STEWARDSHIP SCIENCE

The SSGF Magazine 2011-2012

THE BIG MIX-UP

Los Alamos group teases out the physics of turbulence

Sandia: An in-depth look at suns

Livermore: Bill Goldstein's path to stewardship science

Plus: Gas blasts, strange water, SSGF fellows on location and a talk with the leader of a new approach to countering nuclear threats

STEWARDSHIP SCIENCE GRADUATE FELLOWSHIP

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SSGF

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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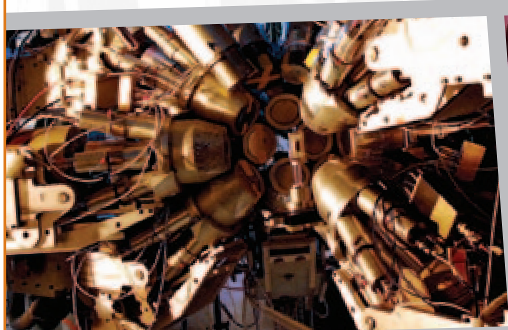
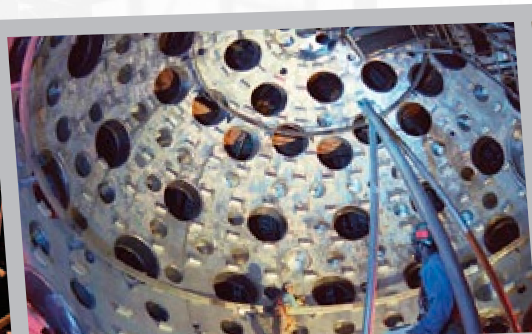
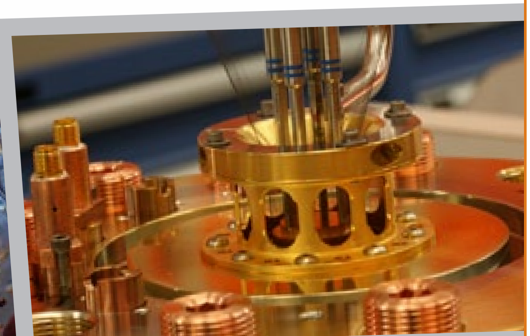


Germanium Array for Neutron-Induced Excitations at Los Alamos Neutron Science Center - courtesy of Los Alamos National Laboratory



The 10-meter-diameter target chamber of the National Ignition Facility (NIF) was assembled from 10-centimeter-thick aluminum panels. Holes in the chamber provide access for the laser beams and viewing ports for NIF diagnostics - courtesy of Lawrence Livermore National Laboratory



A z-pinch wire array is prepared for shooting on the Z inertial confinement fusion facility at Sandia National Laboratories in New Mexico - courtesy of Sandia National Laboratories

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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.


Deeney

Diversity, Passion, Talent

DIVERSITY IS A MUCH-USED WORD IN MANAGEMENT THESE DAYS. This is a powerful concept valued at NNSA. Anyone reading the articles in this magazine must be struck by what great examples of diversity our community, our technical challenges and our science experiments represent. Indeed, one of the great attractions of NNSA's science, technology and engineering program is its multidisciplinary nature. The research highlighted here is truly inspiring and exemplifies "multidisciplinary."

Multidisciplinary is a must when solving the diverse and complex challenges we face. From understanding the explosion of a star, to impacting the power balance of the Cold War through the Strategic Defense Initiative, to the call to protect national security and to assist at Fukushima Daiichi, the disabled Japanese nuclear power plant, the diverse science, technology and engineering of our labs frequently is found on the leading edge.

The magnitude of the challenges we face requires the best people from a range of backgrounds and with many skills to solve them, hence the motivation for the SSGF to train the best. Moreover, Deputy Administrator Donald Cook notes that the ability to "re-invent" yourself is beneficial when the challenges change. The diversity and networking integrated into the SSGF experience helps foster the breadth our fellows need to prepare for change.

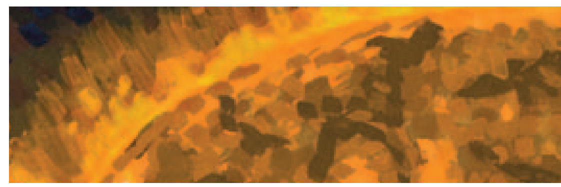
So even embedded in an already technically diverse community, you will find plasma scientists working on material science, experimentalists transforming into computationalists and even scientists and engineers becoming managers! The exciting opportunities for an SSGF fellow and others who may end up at laboratories are endless; certainly, boredom is not a likely prospect. Enjoy the great stories in this magazine, and respect and seek out the diversity of talents and views around you. Not surprisingly, there can be occasional friction among passionate and talented individuals. When it surfaces, gather up the team, and over a cup of coffee or a suitable dark beer conduct one of Rob Gore's mix experiments (page 10), then talk and listen. Great things will happen!

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

STEWARDSHIP SCIENCE

The SSGF Magazine 2011-2012

FEATURES



COVER

PERTURBING THE UNIVERSE

To understand what happens at the heart of exploding stars and inside fusion reactors (among other phenomena), Robert Gore and his colleagues at Los Alamos National Laboratory (LANL) study the turbulent boundary between two mixing fluids. Forces accelerate the fluid flows and density differences lead to instabilities at their interface; these perturbations grow and create secondary disturbances, leading to turbulence. If acceleration is constant, the flow is called a Rayleigh-Taylor instability, named for the scientists who described the phenomenon. The cover visualization represents the largest instability simulation ever performed, showing asymmetry in the density field of a Rayleigh-Taylor mixing layer. For those taking notes, Daniel Livescu and Mark Petersen performed the simulation with a novel parallel, hardware-accelerated analytical ray-casting algorithm. Steve Martin and Patrick McCormick developed the visualization. All of them work in LANL's Computer, Computational and Statistical Sciences Division.

Stewardship Science: The SSGF Magazine showcases researchers and graduate students at U.S. Department of Energy National Nuclear Security Administration (NNSA) national laboratories. Stewardship Science is published annually by the Krell Institute for the NNSA Office of Defense Science's Stewardship Science Graduate Fellowship 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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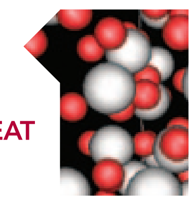
DEPARTMENTS

FRONT LINES



SAMPLINGS

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Fellows' portraits and title illustration for "A Place in the Sun" by Tom Dunne. Unless otherwise noted, images provided by national laboratories and the individuals featured in the accompanying articles.

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Gassing Up the Big Gun

After two years, JASPER is shooting again. The Joint Actinide Shock Physics Experimental Research (JASPER) Facility at the Department of Energy's Nevada Test Site hosts one of the world's most powerful gas guns. The shocks created when projectiles meet their half-dollar-sized targets at velocities of up to 18,000 miles per hour tell scientists about the properties of plutonium and other materials under extreme pressure and temperature.

JASPER resumed operation with a test on March 9, firing an aluminum projectile at a target of the same material. The gas gun and measurement instruments all performed as expected. Neil Holmes, the experiment's chief scientist and a senior scientist at Lawrence Livermore National Laboratory, is analyzing the data.

Holmes and his colleagues have waited as JASPER was brought into compliance with new DOE safety regulations. Originally classified as a radiological installation, the department now has designated JASPER a Nuclear Hazard Category 3 Facility because it tests plutonium. "It's like the difference between running something like a regular lab and running a nuclear reactor," Holmes says, with "extreme control of every aspect of operation."

Since its first experiments in 2003, the gas gun has produced plutonium data of unprecedented quality. "The thing that really distinguishes JASPER is the precision at which it's able to make these measurements" – with an average uncertainty of less than 0.5 percent, says Holmes. The goal is to understand the materials' properties well enough to reduce the uncertainty in weapons simulations.

Plutonium shots are expected to resume by September, pending more tests on tantalum targets.

It's about time, Holmes says. "There are goals we have to meet for the country that are important. These are not just measurements. We have a chance to make discoveries."

~ Thomas R. O'Donnell

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 2011 outgoing class.

MINERAL SQUEEZE PLAY

KRYSTLE CATALLI
Massachusetts Institute of Technology
Practicum: Lawrence Livermore National Laboratory

There was a lot of pressure during Krystle Catalli's practicum, but most of it was on materials she studied.

Catalli's experiments use a diamond-anvil cell to squeeze small amounts of minerals between two diamonds. Working under advisors William J. Evans and Hyunchae Cynn at Lawrence Livermore National Laboratory, she and her colleagues used bright X-ray beams to probe how pressure affects the spin state of ferric iron – the ion Fe^{3+} – in magnesium-silicate perovskite and how that influences the mineral's elastic properties.

Perovskite is Earth's most abundant silicate mineral, but its structure is stable only under pressures found at depths of 660 to 2,700 kilometers. Spin state pertains to electron energy levels. In low-spin states, electrons fill low-energy orbitals first. In a high-spin state, electrons fill a higher-energy orbital before matching lower-energy electrons.

The researchers made magnesium-silicate perovskite containing all ferric iron and subjected it to pressures of more than 100 gigapascals (GPa) while using X-ray instruments at Argonne National Laboratory's Advanced Photon Source to observe its behavior.

The researchers noted that when subjected to pressures above 50 GPa (found in the Earth's mid-lower mantle), ferric iron atoms appear to enter into dodecahedral and octahedral crystal sites about equally. Below 50 GPa high-spin ferric iron is present in both crystal sites, but low-spin is found only in the octahedral form.

The group's data showed that ferric iron in the octahedral site undergoes a gradual spin transition to mid-lower mantle pressures – between

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TIME PROJECTION CHAMBER MAKING TRACKS

Radioactive particles have begun swarming through a unique detector positioned in a neutron beam at Los Alamos National Laboratory (LANL). Color-coded by their energy levels in detector data, these tracks mark the passage of alpha particles and fragments of radioactive nuclei riding along an electric field.

For five months ending in December 2010, scientists tested 192 of 6,000 separate electronic channels in the small yet complex device known as a time projection chamber (TPC). The run culminated nearly seven years of development on the instrument, which is designed to help researchers analyze nuclear fission processes in unprecedented detail.

As a preview to the delivery of the first production model in fall 2011, this trial allowed researchers from Los Alamos, Lawrence Livermore National Laboratory (LLNL) and Idaho National Laboratory (INL) and several collaborating universities to test a working prototype. Testing on 512 more channels, this time using a radioactive source at LLNL instead of a beam, continues into the fall.

"Things went surprisingly smoothly," says Fredrik Tovesson, a nuclear scientist who leads LANL's participation in the project. "Everything worked out the way we had anticipated. Within a few days we started to get signals. Almost immediately, we could see particle tracks."

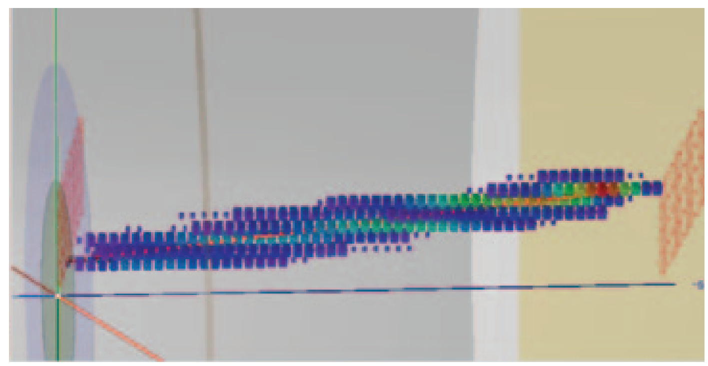
First envisioned by LLNL and now co-directed along with INL and the two other labs, the project aims to improve scientific knowledge of "nuclear cross sections," which define reactions most likely to occur in a particular nuclear fission event.

Whereas full-scale TPCs are the size of basketball courts and track electrically charged fragments in huge subatomic particle colliders, this new TPC design incorporates a reaction chamber and is tiny – no larger than a coffee can with two surrounding hexagonal plates, each about 20 inches in diameter. The device captures the byproducts of nuclear fission events diorama-like, tracing them in three dimensions.

In those plates, which resemble the solar panels on a Star Wars TIE fighter, is enough microelectronic circuitry to handle half a trillion bytes of data per second. That processing power is needed to follow what happens when diagnostic neutron beams passing through the chamber strike minuscule samples of radioactive materials like uranium-235 and plutonium-239.

Resulting fission events send subatomic fragments zipping through the chamber's electric field, liberating charged electrons. Meanwhile, the passing neutrons also collide with protons in the chamber's hydrogen atmosphere, producing more charged fragments.

All this charged flotsam sets ionization trails drifting toward those thousands of electronic-channel readout pads on the inner edges of the hex plates. Farther out, those plates are covered with hundreds of pairs of circuit boards that boost and shape signals from the pads, then convert the data from analog to digital for computation.



In a particle track image, each dot corresponds to a pixel in a detector. The colors differ according to the amount of charge deposited by a particle (seen here, an alpha particle). The particle loses energy as it traverses the detector's gas volume.

The goal is to create 3D-movie-like images that will let researchers observe and interpret particles emerging from fission events. This cross-section view is important for designing nuclear reactors, predicting the composition of nuclear wastes and preserving the reliability of nuclear weapons without underground testing.

Although the neutron-beam tests are in their early stages, the computer displays from this new-generation TPC already are groundbreaking.

Says Tovesson, "I think it's safe to say that these are the first three-dimensional images of fission particles or fission tracks."

– Monte Basgall

This is a followup to an article in the last issue of Stewardship Science.

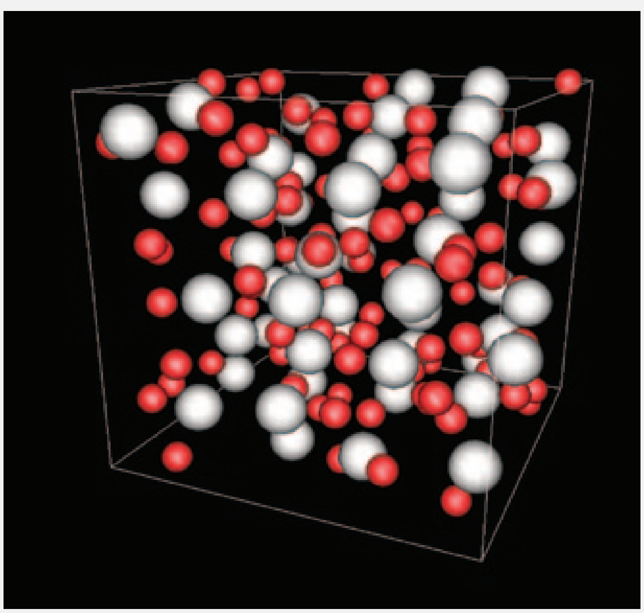
Otherworldly Water

Imagine finding yourself at a party where the ice cube in your drink flowed like a liquid while maintaining its shape. It might be possible if the party were on Neptune.

A new computational model suggests that under the extreme conditions on Neptune and Uranus, water takes on a so-called superionic state in which it simultaneously behaves as solid and liquid. The model extends what's known about the electrical conductivity of water under extreme temperature and pressure and agrees closely with a multilayer model that explains the magnetic fields of these so-called ice giants . "The structural model is intriguingly similar to the layered planet necessary to generate the anomalous magnetic fields of the two planets" that the Voyager spacecraft measured, says Thomas Mattsson, a computational physicist at Sandia National Laboratories in Albuquerque, N.M. "When you compare the two models, there is a striking similarity."

What's more, the result amazed scientists because the project began not to model planets but to predict how a thimbleful of water would behave under extreme pressure. Mattsson and colleagues at Sandia needed the data to model the Z machine, a pulsed-power accelerator designed to explore the high energy density physics of materials. This research certifies safety and reliability of the U.S. nuclear weapons stockpile. The Z machine sends 20-megaampere electrical pulses through water switches that concentrate the pulse and, once a certain threshold is reached, release the energy all at once. Early simulations of warm, dense water defied predictions. It became imperative to pinpoint how water would act at these extreme conditions.

The structure of superionic water at 4,000 degrees Kelvin and a density of 3.3 grams per cubic centimeter. Oxygen atoms are white, hydrogen atoms red. The oxygen atoms are arranged in a lattice.



Mattsson and his colleagues stepped in, with funding from the National Nuclear Security Administration, and extended an existing program that models the behavior of subatomic particles using quantum mechanical principles by adding in routines to measure electrical and ionic behavior.

The result was a new phase diagram – basically a chart that predicts the state (solid, liquid or gas) in which water exists at a given temperature and pressure. We all know water boils at 100 degrees Celsius. But heated water under high pressure behaves literally otherworldly, rearranging into viscous plasma and, at 4,000 times atmospheric pressure, into the predicted superionic solid-liquid hybrid. In this state, the larger oxygen ions arrange themselves into a solid ice-like lattice, leaving the hydrogen ions swimming among them in a liquid-like soup.

Working with collaborators Ronald Redmer, Nadine Nettelmann and Martin French, all of the University of Rostock, Germany, Mattsson applied his model on a planetary scale, requiring the combined supercomputing muscle of Sandia's Red Storm and a system in Rostock.

The model that emerged improves our knowledge of our outer planets and perhaps beyond, Mattsson says.

"There are exoplanets outside our solar system that are heavier and that go to much higher density and much higher pressure. So you could have metallic superionic water there."

– Karyn Hede

continued from page 4

about 50 and 60 GPa – where all ferric iron in the octahedral site becomes low-spin. Meanwhile, ferric iron in the dodecahedral site remained solely high spin up to at least 136 GPa. The data suggest that perovskite is more compressible during the spin transition but less compressible when complete.

Catalli, who is working with Sang-Heon Shim at MIT, incorporated the results into her doctoral thesis.

CRACKING THE NUCLEAR SHELL

ANGELO SIGNORACCI
Michigan State University
Practicum: Lawrence Livermore National Laboratory

Angelo Signoracci played shell games during his practicum – as in the nuclear shell model of atomic nuclei's low-energy properties.

The model describes the nucleus in terms of energy levels. Calculating those levels, however, is a complex problem, with each particle interacting with all of the others where the fundamental forces involved are not well understood.

Working under advisor W. Erich Ormand, Signoracci parallelized the shell-model code NuShellX to run more efficiently, improving calculation times by an order of magnitude. He also used the energy density functional (EDF) method to compute the binding energy and single particle energies of the isotope nickel-68. Using data from those calculations, Signoracci used the configuration interaction (CI) method to determine energies for the isotopes nickel-67, -68 and -69, cobalt-67 and copper-69 for comparison to experiments and other calculations.

Signoracci's work could have lasting impact at the lab. The scale of the calculations was unprecedented, Ormand says, and NuShellX is now available on LLNL's supercomputers for his group to use in its research.

The work complemented Signoracci's doctoral research under Alex Brown, which aimed to combine CI and EDF. CI is accurate but limited in its application and demands high computing power as atomic mass increases. EDF is broader in application and demands fewer computer resources, but has limited accuracy and can calculate only certain nuclear states. Signoracci's hybrid approach has led to accurate calculations of the properties of many nuclei for comparison with experiments and to predictions of unknown nuclei.

A DANCE WITH ARSENIC

PAUL ELLISON
University of California, Berkeley
Practicum: Los Alamos National Laboratory

Most commonly known as a poison, arsenic also is a bellwether for reactions that drive nuclear weapons and form heavy elements in exploding stars. But to fully understand what it's telling them, scientists first must know how arsenic-75, the element's only stable isotope, reacts when neutrons hit it.

Paul Ellison, working with David Vieira, helped illuminate those reactions during his practicum. He analyzed data from arsenic-75 experiments conducted at the Detector for Advanced Neutron Capture Experiments (DANCE) at the Los Alamos Neutron Science Center. DANCE zapped the arsenic with neutrons, then recorded gamma ray emissions. Gamma rays are a byproduct when an arsenic-75 nucleus captures a neutron and transforms into a new isotope.

Ellison began by calibrating the gamma ray energy and timing of DANCE's detectors. He also determined background gamma-ray rates to calculate the best net counts in the arsenic-75 data. Ellison analyzed neutron energy resonance peaks to determine the detector's efficiency, then combined the data to calculate the cross section as a function of neutron energy. The results, Vieira wrote in an evaluation, will help improve simulations used to certify the safety and reliability of the nation's nuclear stockpile.

The practicum gave Ellison, who is studying with Heino Nitsche at UC-Berkeley, the opportunity to get feedback from lab personnel on his thesis investigations into americium-240 production.

NEUTRON-STAR BABY PICTURES

LUKE ROBERTS
University of California, Santa Cruz
Practicum: Los Alamos National Laboratory

The computer model Luke Roberts developed during his practicum can help scientists virtually witness the birth of supernovae residues called neutron stars.

A neutron star forms when a massive star's core collapses in a type II supernova – like the famed Supernova 1987A – forcing protons and electrons together into neutrons clumped so densely a teaspoonful of the resulting matter would weigh billions of tons on Earth. As the neutron star cools, it emits a huge number of neutrinos – almost massless, neutral, weakly interacting fundamental particles. Neutrino behavior may provide a direct window into neutron star formation and the properties of matter at super-nuclear densities.

Working with Sanjay Reddy and Vincenzo Cirigliano at Los Alamos, Roberts developed a computer code to simulate how neutron stars cool by neutrino emission in the first hundred seconds of their existence. The neutrino transport/stellar structure code uses advanced microphysics for the nuclear equation of state (EOS), which describes the relationship between pressure and density at densities greater than those found in nuclei on earth. Microphysics in the code portrays the processes of neutrino interactions with nuclear matter. The code also calculates energy transport by convection to characterize the effects of hydrodynamic instabilities in the young neutron star's interior.

The results could help explain how hydrodynamic instabilities, variations in neutrino interaction rates and the nuclear EOS affect the rate at which neutrinos are emitted and the energy of those neutrinos. This information can then be used to predict how such events would look in Earth-bound neutrino detectors.

Roberts, whose doctoral advisor is Stan Woosley, and his collaborators have determined how to disentangle the effects of hydrodynamic instabilities on the neutrino signal from the effects of microphysics variations. Comparing these models with neutrino data collected from 1987A or future nearby supernovae can help constrain the properties of weak interactions in dense matter and the properties of nuclear matter.

SEEING THE LIGHT AT Z

MATTHEW GOMEZ
University of Michigan
Practicum: Sandia National Laboratories, New Mexico

Sandia scientists are getting additional insights into the fine reactions generated by their formidable Z machine, thanks to former fellow Matthew Gomez.

The machine fires powerful, intensely short pulses of electric current through hundreds of minuscule tungsten wires arranged in a small cylinder. The pulse ablates the wires, and the strong magnetic force the current generates rapidly compresses material, which implodes on axis and generates X-rays. The X-rays are used to compress and heat a target capsule that often contains hydrogen isotopes. Z generates data for use in stockpile stewardship simulations and for experiments on a possible approach to nuclear fusion energy.

The Z machine's fiber optic system had been removed during an upgrade. Working with Mike Cuneo, Gomez tested, installed and recalibrated the system and later operated it during several experiments. Gomez also designed hardware to measure aspects of the post-hole convolute, a device that combines the current from multiple transmission lines and transfers it to the target in the Z machine and similar pulsed-power devices. That work played into his doctoral research, which focused on current losses in the convolute. Working with advisor Ronald Gilgenbach on the Michigan Accelerator for Inductive Z-pinch Experiments, Gomez studied how plasma formation in the gap between the convolute's cathode (or hole) and anode (or post) relates to current loss.

Gomez received his doctoral degree in early 2011 and now works at Sandia.

– Thomas R. O'Donnell

CONVERSATION

AVERTING THE THREAT

Kim Budil

N Program Manager
Lawrence Livermore National Laboratory

Steering Committee Member
Stewardship Science Graduate Fellowship

Former Senior Advisor
to the Under Secretary for Science
Department of Energy

You recently were named manager for LLNL's new N Program, which coordinates research and development activities designed to counter the threat of nuclear terrorism, including nuclear detection, forensics, threat assessment and support for nuclear incident response. How did the program come about?

The Obama Administration's nuclear posture review put countering the threat of nuclear proliferation and nuclear terrorism as a first priority. It has embraced the notion that the nuclear security mission is more than just our stockpile. It's a very interesting time, and NNSA owns the expertise across that full mission space. Most people who focus on NNSA see the defense programs mission and the U.S. stockpile, but there are very large programs in nonproliferation and nuclear counterterrorism. Most of the activity on securing nuclear materials worldwide comes through NNSA. NNSA supports the development of science and technology to understand this complex threat space and to diminish the threat worldwide. At LLNL, we decided to bring together the pieces of work in the broader nuclear threat space into a single program to give it the kind of visibility of our core stockpile program.

What are some of the emerging scientific challenges within that mission?

Nuclear forensics is one area – understanding signatures of nuclear materials. If we find material it can be analyzed to determine the processes it has been through and the likely source. If a device were detonated somewhere in the world, we would use forensic analysis to reconstruct what kind of device was used and provide that information to support attribution. It's an incredibly hard scientific problem to reverse-engineer one of these very complex devices.

Another major challenge is developing methods for high-confidence detection of nuclear materials or devices at a distance. Standard radiation detection techniques work best when you are close, backgrounds are very low and the material is unshielded – not really a realistic scenario. So methods that allow you to see through shielding or to detect materials from greater distances would be very powerful ways to identify potential threats.

How as a nation do we attract our best and brightest scientists to the national security mission?

First, people should understand that we do a lot of basic science research that gets published, and people have exciting scientific careers while also contributing to these national security missions. So the notion that if you decide to go into a security arena your whole life goes under the cover of darkness is not true. Students who come into the national laboratories and see the work that we do, the facilities and tools at our disposal – that creates a lure. If people experience that environment, it will change the way they think about working in these mission areas. You get to do world-class science and make a difference on very important challenges facing the nation.

You've been a strong advocate for women scientists and engineers. What can the national labs offer this group?

Women earn between 15 and 18 percent of doctoral degrees in physics, so we start off very underrepresented. Therefore, the size of the institution makes a big difference. Because there are more scientists and engineers, there are more women scientists and engineers. I have a network of women colleagues all across the laboratory and, as my career has progressed, that network has become even more important, providing support and helping me develop confidence. I have advocated for a long time that the national labs have a responsibility to be a model for how scientific and technical organizations should operate since the government provides the vast majority of our funding. Like at any big organization, there are issues, but I think that labs really do strive to live up to that ideal.

COVER STORY

MIXING

BY THOMAS R. O'DONNELL

A LOS ALAMOS NATIONAL LABORATORY TEAM PROBES THE PHENOMENA BEHIND TURBULENT MIXING, FROM INERTIAL CONFINEMENT FUSION TO SUPERNOVAE.

Density field data is visualized in homogeneous multi-fluid mixing, with red indicating low density, blue higher density, and white mixed fluid.

ROBERT GORE NEVER DRINKS HIS COFFEE BLACK. Withholding the cream would deny him his daily experiment. "I take that dark, hot coffee and pour in thick, cold cream and watch the swirls develop and form, and then it slowly turns into a murky brown," says Gore, a project leader in Science Campaigns at Los Alamos National Laboratory (LANL). "That's the easily understood application of everything I'm doing."

Gore and his colleagues decipher the complicated mechanism of turbulent mixing at the boundary between two fluids. They pay particular attention to variable density (VD) flows in which one fluid is denser than the other, like cream and coffee. Forces accelerate the fluid flows and the density differences lead to instabilities at their interface. These perturbations grow and interact to create secondary disturbances, leading to turbulence.

If acceleration is constant, as gravity is, the flow is a Rayleigh-Taylor instability (RTI). If a shock accelerates the interface between the fluids, it's a Richtmyer-Meshkov instability (RMI). Both were named for scientists who were instrumental in describing the phenomena.

VD flows comprise everyday processes like ocean and atmospheric circulation and more exotic phenomena like supernovae and inertial confinement fusion (ICF). In ICF – a goal of the National Ignition Facility at Lawrence Livermore National Laboratory (LLNL) – hydrogen isotopes inside a tiny capsule are compressed and heated so greatly and quickly that they fuse, producing energy. "We have to understand these processes because the capsules are designed to minimize mixing between the shell that holds the fusing gas and the fusing gas itself," Gore says.

Gore and his colleagues also apply their findings to computer simulations that help maintain the nation's nuclear weapon stockpile. Since it stopped nuclear weapons testing in 1992, the United States has depended on modeling to ensure its arsenal is reliable, even as it ages.

LANL researchers are collaborating to characterize the complex processes that drive VD flows and turbulence. Numerical modelers like Daniel Livescu, Fluid Dynamics Team leader in LANL's Computer and Computational Sciences Division, develop direct numerical simulations (DNS) to solve equations that describe fluid flow. DNS designers can target specific processes or try to match experiments. Simulation often is the only way to understand phenomena that are impossible to recreate experimentally, like supernovae.

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. *He wrote the cover story for last year's* Stewardship Science *magazine.*

Experimentalists like Kathy Prestridge, Extreme Fluids Team leader in LANL's Physics Division, use the latest laser instruments to gather data that's more detailed than ever, measuring what's happening at tiny scales in shocked fluid interfaces.

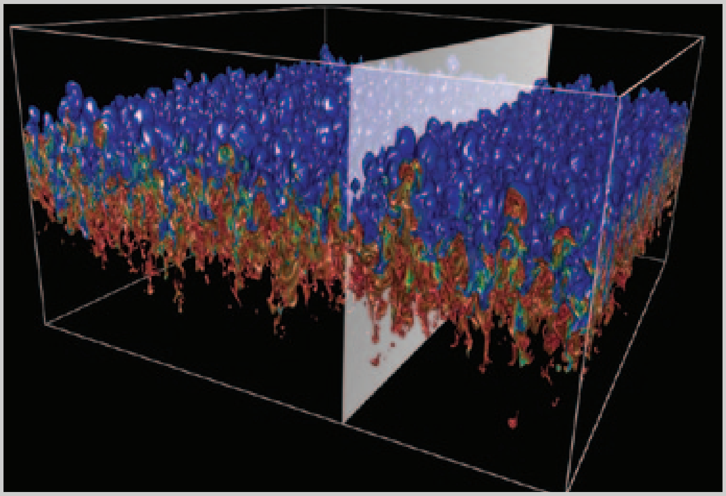
"It starts out big," Prestridge says. "There's a big shock wave and there are these big structures in the flow, but then it starts to mix and go to smaller and smaller scales." Because computers aren't powerful enough to calculate the small-scale effects as part of a large-scale DNS, researchers incorporate them in model parameters. The information Prestridge and colleagues provide helps others set simulation parameters and physics at realistic levels.

Another group of researchers focuses on theory and modeling – developing equations that go into simulations to describe instabilities and turbulent flows. Gore, meanwhile, works on validation: comparing model results with experiments, then seeking better theories or new and different experiments, depending on the results.

TURBULENT COLLABORATION

"We're all working together," Gore says, "so the experimentalists talk to the modelers, and the modelers talk to the experimentalists, and the DNS researchers try to benchmark their simulations against the experiments."

Characterizing turbulent instabilities is tough. Shock models must cope with the sudden pressure jumps that shocks create. The shocks change pressure among only a few molecules at a time but profoundly affect the bulk flow. Both qualities create a span in scales that's demanding for equations and computer resources.



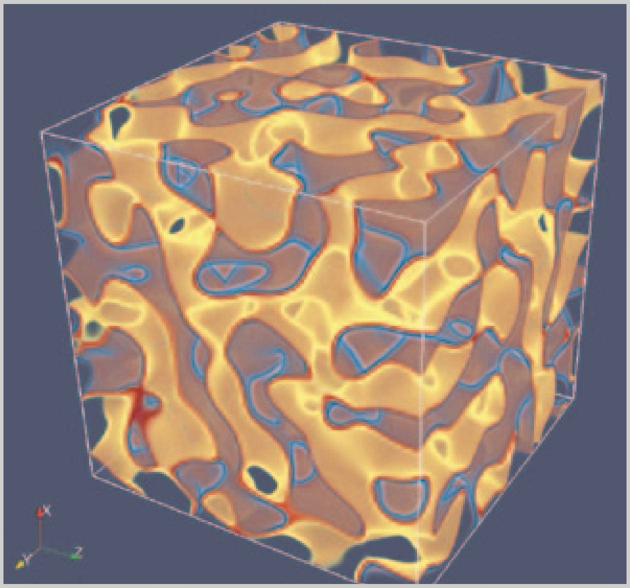
This three-dimensional visualization, representing the largest instability simulation ever performed, shows asymmetry in the density field of a Rayleigh-Taylor mixing layer at an Atwood number of 0.75. Bubbles form on the heavy fluid side (at top) and spikes on the light fluid side.

RTI problems may include interfaces between a gas and solid, a liquid and gas, two gases or other combinations. "Just think of how that interface evolves differently, depending on those cases," Gore says. "How much information do we have on what exactly is going on and how do we come up with models that can span that different type of behavior?"

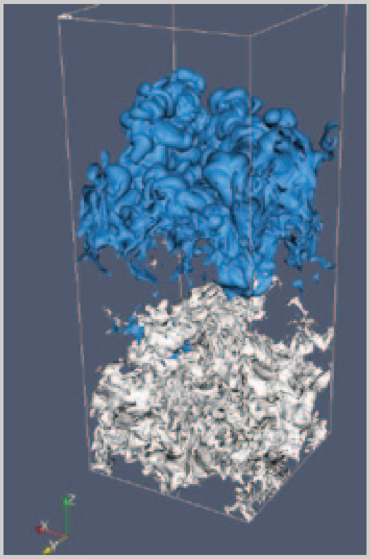
Computational difficulty increases with the size of the domain being simulated – with a supernova at the enormous end – and with turbulence, as measured by the Reynolds number. The Reynolds number is the ratio of inertial forces to viscous forces, quantifying the impact of viscosity on a fluid's ability to flow. Thick fluids, like cream, have a low Reynolds number and low likelihood of turbulence. Thin fluids, like smoke or air, have a high Reynolds number and a high propensity for turbulence.

In a computational context, the Reynolds number also indicates the range of spatial scales a simulation portrays. A higher number captures a greater span, Livescu says. "These flows are strongly nonlinear," and like the proverbial "butterfly effect," small-scale actions can affect large-scale behavior. "Everything is interconnected, and to do an accurate simulation we need to accurately solve all the scales of motion."

Representing even low Reynolds number experiments is beyond most computer capabilities, Gore says, but that's changing. The latest supercomputers are nearly capable of running models matching turbulence seen in experiments. "It's an exciting time. We're starting to get the really high Reynolds number in these flows."



The flame surface in reacting turbulence with microphysics similar to those found in type Ia supernovae.



Mixing layer edges in high Reynolds number Rayleigh-Taylor turbulence.

ASYMMETRICAL CONCLUSION

One example is a January 2009 *Journal of Turbulence* paper by Livescu, Ray Ristorcelli, Sumner Dean and Gore from LANL and LLNL's William Cabot and Andrew Cook. They were the first to describe mixing symmetry in an RTI layer.

Using LLNL's Dawn, an IBM Blue Gene/P, the researchers ran a variable density RTI simulation that Cabot and Cook devised. It calculated the physics at each of almost 29 billion data points spread through three dimensions and achieved a turbulent Reynolds number of 4,600.

Another key parameter is Atwood number, which characterizes the density differences between two mixing fluids. An Atwood number near 0 indicates a small difference; a number near 1 means the fluids differ greatly in density. The Atwood number was 0.5 in the simulation described in the *Journal of Turbulence*.

As the simulation progressed, the "bubble and spike" mixing pattern characteristic of RTI developed symmetrically along the inner region of the mixing layer but became asymmetric at the edges. Greater mixing also occurred on the light-fluid side of the layer than on the heavy-fluid side.

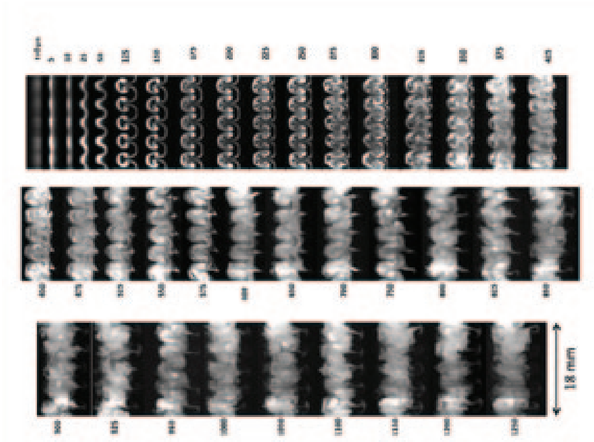
That's surprising, Gore says, and indicates that dynamic turbulence – a mostly mechanical process – drives mixing along with the chemical process of molecular diffusion. "That wasn't obvious beforehand. The chemical process of molecular diffusion is always there, but the key here is that this also has an effect on a mechanical level."

Another revelation, Livescu says, was that small-scale turbulent structures that develop are anisotropic – buoyancy forces drive their development more in one direction than in others. Researchers had assumed that small-scale structures were isotropic, growing on average at the same rate in all directions. "People thought that buoyancy acts only at large scales" and could be disregarded at small scales. "What we showed was that was not true. Buoyancy has a sizable influence at small scales, too."

To be reliable, equations that comprise mixing models must account for these physics. Asymmetrical instability could affect models of weapons, ICF, chemical reactions and pollutant dispersion. Modelers may need to incorporate small-scale anisotropy into large-scale turbulent modeling techniques, like large eddy simulation, which implicitly account for small-scale activity to make problems simpler to compute.

INSTRUMENTAL IMPROVEMENTS

Just as more powerful computers have led to leaps in modeling and simulation, new instruments developed the past 12 to 15 years have garnered new data from turbulent mixing experiments. High-speed digital cameras freeze images of reactions in microsecond increments with high resolution. Lasers fire ever faster pulses and computers coordinate everything with ever greater precision.



A series of planar laser-induced fluorescence (PLIF) images shows the evolution of turbulent structures in a gas curtain over time after it was hit by a shock wave traveling at 1.5 times the speed of sound. Times are in microseconds, starting from top left.

"You can imagine that you have these mixing materials and how much harder it is to get at and measure things inside that versus, say, air blowing over an airplane wing," Gore says. "That level of difficulty is just being overcome within the last 10 years. We're now getting statistics on these classes of flows for the very first time."

For years, turbulence researchers studied images of dye-tinted flows for clues to density, velocity and other properties. The new diagnostics remove much of the subjectivity. "It makes it quantitative," Prestridge says. "It makes it easy to say whether you're matching with simulation or not because you're not just looking at pictures. Your feet are really held to the fire, in terms of the simulations, because you can't fake it. If your average velocity is wrong, for example, it just doesn't match." Researchers must look to the simulation or the experiment to root out the disparity's source.

Experimentalists have two powerful instruments in their arsenal: Planar laser-induced fluorescence (PLIF) lets researchers gather data about velocity, species concentration, pressure and other flow properties; particle-image velocimetry (PIV) tracks the velocity of reflective particles that spread through flows.

"This is the key: doing PIV and PLIF together," Prestridge says. That allows researchers to measure both density and velocity at the same time and point in space and draw correlations. These cross-correlation measurements provide key turbulence quantities for comparison to simulations.

Prestridge applies these high-speed diagnostics to experiments in a 17-foot-long, 3-inch-square shock tube. Air or another gas is pressurized in a driver cylinder. A mechanism punctures a membrane in the driver cylinder, sending a shock at speeds faster than sound down the tube. The shock hits a column or curtain of a heavier gas, such as sulfur hexafluoride, that's usually mixed with a substance like acetone that reflects laser light. It takes just milliseconds, but the PIV and PLIF cameras give researchers precise pictures of the air-gas interface.

In a June 2009 *Physics of Fluids* paper, University of New Mexico graduate student Greg Orlicz, LANL scientists B.J. Balakumar and Chris Tomkins, and Prestridge compared PLIF images of thin streams of shocked sulfur hexafluoride gas that resembled vertical blinds, or what they called "curtains." The researchers hit the gas with shocks of Mach 1.2 and 1.5 (1.2 and 1.5 times the speed of sound). When the shocks hit, the gas streams quickly formed large-scale, mushroom-shaped instabilities that curled into turbulent vortices under the caps. The researchers measured the integral width – the distance between the farthest upstream and downstream locations where the gas was present. Integral width is a simple metric for mixing.

Integral width ended up greater in the higher-shock experiment. But when the researchers normalized the time scales for the two experiments and made an adjustment for differences in the experiment's initial conditions, the rate at which the integral width grew was nearly identical. That indicates that the growth rate, independent of size, is disconnected from Mach number – at least in the range of shocks the researchers studied.

The growth rate curves also nearly matched a numerical simulation, suggesting it employs the right physics to portray large-scale mixing trends. But integral mixing doesn't include mixing that happens at tiny scales. The team also computed the total mixing rate from diffusion – the tiny intermingling driven by natural molecular movements – and found it was nearly twice as high over time for the Mach 1.5 shock as for the weaker shock. That means integral width alone insufficiently describes the physics driving fluid flow and mixing.

Quantifying turbulence in shocked flows to this degree is relatively new, and modelers are clamoring to put the data in their simulations.

Says Prestridge, "You're not talking turbulence until you measure these quantities experimentally and you're not really testing your code until you see how (it compares with results)."

A PLACE IN THE SUN

BY SARAH WEBB

MONITORING THE U.S. NUCLEAR STOCKPILE IN AN ERA THAT BANS WEAPONS TESTING REQUIRES DEEP UNDERSTANDING OF HIGH ENERGY DENSITY PHYSICS. EXPERIMENTS AT SANDIA NATIONAL LABORATORIES’ Z MACHINE OFFER A GLIMPSE INSIDE THE SUN – AND A HANDLE ON PHENOMENA THAT STELLAR INTERIORS SHARE WITH NUCLEAR WEAPONS.

FOR ALL THAT OUR SUN DOES FOR THE EARTH – not the least, warming our planet to just the right temperature to sustain life – scientists still have a surprising number of questions about the high energy density physics that fuels it and other stars throughout the universe.

What we know about the physics going on inside the sun, 150 million kilometers away, is based on a variety of models astrophysicists have built. These specialized tools replicate the extreme conditions of the sun – temperatures of millions of degrees and pressures millions of times those of the Earth's atmosphere – here on our planet.

The Z machine at Sandia National Laboratories in Albuquerque, N.M., gives scientists access to some of the conditions inside the sun on a much smaller scale and under controlled conditions that enable accurate measurements. This instrument concentrates electrical energy into a powerful pulse of up to 80 trillion watts, says Keith Matzen, director of pulsed power sciences at Sandia. That pulse is released in billionths of seconds to produce X-rays and gamma rays.

Fundamental science questions take up roughly 5 to 10 percent of the available experimental time on the Z machine, Matzen says. These tests offer Sandia scientists an opportunity to tap into a broader community. "Those scientists will have good ideas for doing new physics and stimulate improved understanding on many topics," among them studying nuclear phenomena for monitoring the safety of the U.S. nuclear weapons stockpile.

It's exciting, says Jim Bailey, a distinguished member of the technical staff at Sandia, to produce in the lab matter the mass of a few grains of sand that shares characteristics with the sun. "It's an amazing opportunity to re-create a little chunk of the sun in our lab to study."

JOURNEY TO THE CENTER OF THE SUN

The sun produces energy through fusion reactions. Under the extreme temperatures and pressures found at its core, the single protons in the nuclei of hydrogen atoms smash together to form heavier helium nuclei. The energy that's produced radiates from the core in packets known as photons. But those energy packets don't have an unobstructed path on the hundreds of thousands of kilometers they travel to the sun's surface. Stellar interiors are incredibly hot and extremely dense, filled with plasma, a super-hot mixture of more than 20 elements. Most of the stellar plasma is hydrogen and helium, but the other constituent elements sometimes play a key role in stellar structure and evolution.

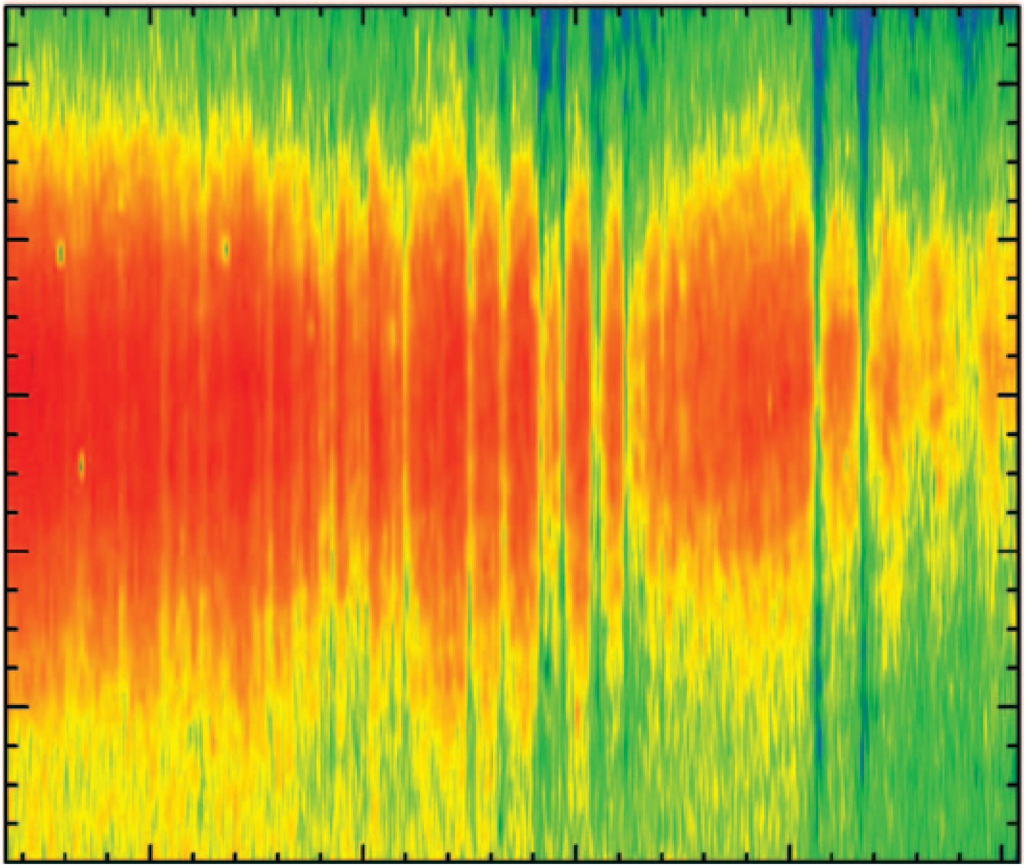
Sarah Webb is a New York-based freelancer. She has covered chemistry and materials science for Science News *and has worked at* Discover *and* Popular Science*. She holds a Ph.D. in chemistry and studied organic chemistry in Germany on a Fulbright fellowship.*

The photons, in the form of X-rays and gamma rays, constantly collide with this dense plasma soup, which impedes their movement from the core. Because of the extreme density and pressure of this intrastellar plasma, it can take tens of millions of years for that energy to reach the star surface.

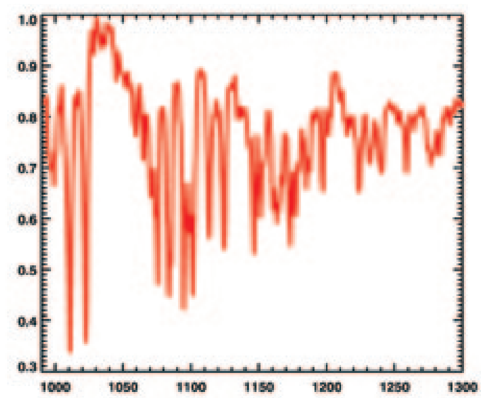
How effectively this energy moves outward depends on how the materials inside obstruct the energy passing through them, a property known as opacity. In this way, the hot plasma acts much like tinted windows on a car, Bailey says, filtering the energy that shines through. Opacity controls how quickly the radiation flows through this soup.

Opacity depends on a number of factors. At the higher temperatures closer to the core of the star, stellar matter is more likely to be ionized, which lowers the opacity. This portion of the star's center, where energy moves primarily as radiation, is called the radiative core. In the sun, this portion extends across 70 percent of the distance from the core. "When radiation is the dominant energy transport mechanism, opacity is the main material property that controls how quickly or effectively energy moves out of the sun," Bailey says.

Closer to the star's surface the temperature cools. Electrons are more likely to be bound to atoms within the plasma, and opacity increases further. At that critical point nearly three-quarters' distance from the sun's center, the opacity increases to the extent that radiation becomes relatively inefficient at transporting energy. At



Left: An X-ray spectrum image for iron absorption helped Sandia researchers determine the sun's opacity. The horizontal axis corresponds to photon energy, the vertical transmission. The bright red regions indicate high transmission, or low opacity; the thin green or blue vertical stripes correspond to absorption, or high opacity. Transitions between different atomic energy levels make the vertical stripes; those same transitions account for absorption in the solar interior. **Below:** An experimental transmission spectrum. The bumps and wiggles encode physical information about radiation transport near the sun's convection-radiation zone boundary; the peaks and dips correspond to lower and higher opacity, respectively.



this boundary, convection takes over. In this zone closer to the sun's surface, energy burbles toward the surface through the plasma, much like bubbles in a pot of boiling water.

This radiation-convection zone boundary, where opacity has its greatest impact, is the target for study. The scientific team includes Bailey and other Sandia scientists, researchers from Lawrence Livermore National Laboratory, Los Alamos National Laboratory, the CEA laboratory in France, Ohio State University and the University of Nevada in Reno.

A SOLAR PUZZLE

About 10 years ago, scientists revised estimates of the sun's chemical composition. For example, they estimated that the sun contained only half the oxygen previously thought. Because the sun's physics relies on the mixture of elements inside, those changes meant that scientists needed to recalculate mathematical models of our star. With these new calculations, the astrophysical models now don't match observations based on helioseismology, studies of earthquake-like vibrations.

Bailey and his colleagues realized they might be able to help sort out these problems. Opacity also varies depending on the element, and the Z machine was powerful enough to create conditions to measure this property for individual elements.

Maybe the chemical composition estimates were incorrect, maybe the opacities were wrong or maybe the solar models needed refinement, Bailey says. But the Z machine could help scientists figure out whether the opacity values of the individual elements were accurate.

The team's opacity measurement was closer than any other at achieving conditions inside the sun.

"The sun is our very best opportunity to understand any star. If we don't understand the sun, it hinders us from understanding all the other stars."

THE COMPLEXITY OF IRON

Even with the strongest pulsed-power accelerator in the world available to them, scientists at Sandia faced a daunting task when it came to measuring the opacity of individual elements. Ideally, the team would like to measure the opacity for each. But measuring just a single element is challenging and a long-term investment.

Because opacity is a fundamental material property, the researchers needed to choose single elements to tease out each one's contribution to the overall opacity. Iron contributes 20 percent of the sun's opacity. It's also complicated, which led Bailey and his colleagues to select iron as a starting point. "Because it's more complicated, we're more suspicious of it."

The team has been working on iron for more than five years, and they're not finished yet.

The complexity that lurks within the opacity of iron arises from the atom's 26 electrons, the most of any of the sun's major elements. With a larger number of electrons, an element also has a larger number of energy states. A larger number of energy states also exponentially increases the number of possible paths between those states. Those paths between energy states, known as bound-bound transitions, make a large contribution to the opacity value.

A large number of bound states also implies a large number of possible bound-free transitions, corresponding to liberation of bound electrons. This is another major opacity source.

MEASURING OPACITY

To measure opacity with the Z machine, experimenters blast an iron sample with energy to produce conditions approaching those at the convection-radiation zone boundary. This small approximation of one solar component is backlit with an intense X-ray light source, and on the sample's opposite side, a spectrometer measures the energy that penetrates the hot iron plasma.

The X-rays moving through the iron have re-created temperatures up to 80 percent (1.7 million degrees Kelvin) of that at the sun's radiation-convection zone boundary and a density a factor of 10 smaller than that of the boundary zone. When Bailey and his team reported this result in *Physical Review Letters* in 2007 it was as close as any opacity measurement had come to achieving the conditions inside the sun. The spectral details contain an enormous amount of physical information in their bumps and wiggles. "Part of the challenge is to be able to use that information and decode the spectrum in such a way that you can test the physics ingredients of the opacity model," Bailey says. Detailed models for iron fit these experimental measurements very well, he says – better than many scientists expected.

That doesn't necessarily mean, Bailey cautions, that opacity models are adequate for stellar-interior understanding. Generating a theoretical opacity model for a single element like iron at a single point of temperature and density is difficult. But generating accurate opacity information for a multi-element stellar mixture over the entire range of temperatures that exist inside a star is even more challenging. Bailey and his team are now performing comparisons with the opacity calculations that are regularly used for stellar physics. The team also is continuing to work on measuring opacity data for iron at conditions that more closely mimic the sun's, within 5 percent of the temperature and density at the radiation-convection boundary.

The complexity of the sun and stars requires that Bailey and his colleagues figure out which components of the opacity models are essential for defining iron's contribution to a star's opacity. "We have to test the physical underpinnings of the models, not just verify that they match experiments performed at one specific set of conditions." They also will need to add opacity data from other complex atoms in the sun, such as neon and oxygen. Bailey and his team hope to work on those atoms next. SS

SCIENTIST TO THE STOCKPILE

BY JACOB BERKOWITZ

The Stockpile Stewardship Program substituted science for detonations to ensure the safety and reliability of the U.S. nuclear weapon arsenal. One of the Department of Energy scientists assigned to this ambitious task: Lawrence Livermore National Laboratory's Bill Goldstein.

Nuclear weapons get very hot and produce plasmas and X-rays.

In 1983, as a newly minted theoretical physicist from Columbia University, Bill Goldstein was alive with the hope that one day he would discover something. Maybe some little detail about the underlying nature of fundamental particles, maybe a broader theoretical insight.

But two years later, when he drove from San Francisco over the Dublin Grade to the Department of Energy's (DOE) Lawrence Livermore National Laboratory (LLNL) to report for his first day of work, the young physicist also intersected the last gasp of the Cold War. His doctoral dissertation two years earlier dealt with an esoteric realm of theoretical particle physics (with the *Alice in Wonderland*-ish title "Spontaneous CP-Violation in Extended Technicolor Models"). But he'd landed a very practical job as part of President Ronald Reagan's so-called Star Wars initiative, an effort to create a futuristic ballistic missile defense shield.

Within a decade, however, world politics changed dramatically and with it Goldstein's scientific future. When the Cold War ended in 1991, American nuclear weapons policy took a U-turn, leading to the creation of a previously unthinkable scientific project. Through the Stockpile Stewardship Program (SSP), the United States would ensure the safety and reliability of its nuclear arsenal without tests; the nation would replace nuclear blasts with science. It was an audacious policy on par with the legendary Manhattan Project – a massive, collaborative venture at the intersection of international politics and frontier science. And one of the Department of Energy scientists assigned to this historic task? Bill Goldstein.

LASERS, PLASMA AND STAR WARS

Today, now in his mid-50s and associate director of physical and life sciences at LLNL, Goldstein recalls his arrival in Livermore as ancient history. Told that his dissertation is available online, he laughs that it reminds him of a recent news story about people outliving themselves through their virtual, online presence.

Previous page: Bill Goldstein in his Livermore office, circa 1990. **Above:** As he appears today.

It's an apt analogy for Goldstein's professional trajectory, literally bridging two worlds – and helping bring the second into existence.

One of the potential cornerstones of the Strategic Defense Initiative (SDI), the official name for what was nicknamed the Star Wars anti-missile program, was a system of nuclear X-ray laser weapons, destructive X-ray laser pulses powered by nuclear explosions. Goldstein was originally hired to interpret data from some of the earliest X-ray laser experiments. But he didn't yet have Q clearance – DOE's top-secret designation for those working with nuclear weapons information. Nor did an Israeli group working at LLNL to develop atomic modeling tools for laser-induced plasmas.

Together, Goldstein and the group from Hebrew University developed a landmark computer code and programming techniques for using X-ray spectroscopy to analyze plasmas. Insights from HULLAC (the Hebrew University Lawrence Livermore Atomic Codes) have since been applied in fields from X-ray lasers to fusion, astrophysics and stockpile stewardship.

For Goldstein, this first collaboration provided a necessary education in computation.

"I was a pencil-and-paper theorist," he says. "I hadn't done any computer work or programming in the course of my Ph.D. So it was a new tool to learn, and the Israeli group was very experienced. It was a lot of fun."

The linchpin in the work was developing new ways to analyze and predict the behavior of plasmas. Called the fourth state of matter – with gases, liquids and solids – a plasma is superheated matter, such as inside a star or atomic weapon, in which electrons are ripped from atoms creating a complex soup of charged particles.

"From a physics-modeling perspective plasmas are just a mess. Modeling a plasma was almost an intractable problem on the computers that existed when I arrived here. There were just too many possible states for each atom to be in. You couldn't keep track of them."

Jacob Berkowitz is a science writer and author. His latest book, The Stardust Revolution: The New Science of Our Origin in the Stars, *is due in 2012 from Prometheus Books.*

However, with his Israeli collaborators, Goldstein developed an ingenious way of modeling plasma behavior and testing the accuracy of their simulations by examining the plasma's X-ray fingerprint. This fingerprinting method exploits the fact that when electrons in an ionized atom change energy level, they emit or absorb energy at the X-ray wavelength. The X-rays given off by a plasma are a telltale marker of the plasma's contents and the interactions of the myriad particles.

"Once we could model plasma systems using approximations, then we could predict the kinds of X-rays that would come out," explains Goldstein, who in 1989 was appointed group leader for computational physics in LLNL's nuclear test program. "And then you measure this in an experiment and see whether you've accurately determined what was going on in the plasma."

Although the work was applied to the classified Star Wars nuclear X-ray laser program, it also proved critical to the stars in other ways. In the 1980s, astrophysicists were poring over data from NASA's first space-based X-ray observatory, the Einstein Observatory, also known as HEAO-2.

"The X-ray spectra that were being measured by these instruments weren't understood. They presented a number of mysteries, and there's nothing like a scientific mystery to get people interested. We were able to take some of the insights gained from looking at the X-ray spectra of plasmas in the laboratory and apply that in astrophysics, particularly in understanding photo-ionized plasmas."

The work resulted in ongoing collaborations with astrophysicists and led Goldstein to pioneer the use of lasers in high-energy astrophysics experiments at LLNL.

Goldstein's groundbreaking work in plasma modeling and diagnostics was cited in 2009 during his election as a Fellow of the American Association for the Advancement of Science. The award also noted his leadership in support of DOE national security programs.

By the early 1990s, Goldstein's role in these programs was about to change profoundly.

A look inside the target chamber at the Jupiter Laser Facility. Bill Goldstein set up Jupiter a decade ago at Livermore to conduct high energy density physics experiments for the Stockpile Stewardship Program.

FROM TESTS TO STEWARDSHIP

The Soviet Union's collapse in August 1991 set events in motion that transformed the U.S. nuclear weapons program. The next year saw the last U.S. nuclear test. And in September 1996, President Bill Clinton signed the Comprehensive Test Ban Treaty formally pledging an end to nuclear testing (though Congress hasn't yet ratified the CTBT).

"At some point between the last test in 1992 and the signing of the CTBT it became clear that, as a matter of policy, the U.S. was not going to be testing again," recalls Goldstein, who by 1994 had risen to the role of deputy division leader for high-temperature atomic physics in the lab's Physics and Space Technology Directorate. "The weapons program had to undergo a paradigm shift. The paradigm at the time of testing was you design a system and you take it out and see if it works. That finished, and it had to be replaced with the science-based Stockpile Stewardship Program."

It was a dramatic, controversial and deeply challenging transformation of almost 50 years of the status quo with U.S. nuclear weapons design. The nuclear arsenal would become like a well-protected garage full of classic cars, with the all-important caveat that they must be in *perfect* working condition but can never be started to test that fact.

SSP, the Stockpile Stewardship Program, is based on three science pillars: the analysis of previous nuclear test data; advanced computational modeling; and sub-critical experimentation – experiments that test not a full nuclear weapon but rather some critical part of it. Under the auspices of the National Nuclear Security Administration (NNSA), SSP science happens primarily at the three DOE weapons

A LEADERSHIP AWAKENING

Bill Goldstein didn't dream of being a top science administrator. He woke up to it.

"It's not always clear when it's happening, and then when you realize that it's happened, that's a bit of a wake-up call. Then you've changed what you do," he says with a laugh from his Livermore office.

In 2010, Goldstein marked his 25th year at the lab, where in the mid-1980s, fresh from a post-doctoral position, he started his first job doing plasma X-ray research. Today, as associate director of physical and life sciences, he helps lead one of the nation's core national security programs, the Stockpile Stewardship Program.

"For me, the tradeoff to actually doing the science myself is that my job is to create an environment that allows scientists to flourish as scientists and to have an impact on national security problems."

It's a delicate scientific work balance, he says. The national security mission is essential. Yet achieving this at the highest level requires a broader vision of "pursuing science at the frontiers. That's not always where the immediate impact is on the security programs. So balancing peoples' work between programmatic research and basic research and creating an environment where these two aspects feed each other to the maximum benefit of both, that's where the rubber hits the road. As a manager, that's the thing that needs constant attention."

As for the psychological challenge of managing a large scientific team responsible for a key piece of the national security agenda, Goldstein says his peace of mind comes from the quality of the Livermore and DOE team of which he's a part.

"My way of dealing with the programmatic challenges is to hire the best possible scientists to work on them. If we're bringing in the best people, then I feel that we will answer the call."

labs: Sandia National Laboratory, Los Alamos National Laboratory and LLNL.

In 1997, Goldstein was appointed to lead a significant part of the underlying science of this effort, as program leader for physical data research in the Livermore SSP.

Before 1992, Goldstein says, the critical question for weapons designers was primarily whether the weapon exploded and delivered the expected yield. Between Trinity, the first U.S. bomb test in the New Mexico desert in 1945, and 1992 the U.S. tested 1,035 nuclear weapons. However, with the advent of the SSP, the question became "not just whether the bomb went off, but *why* it went off, or why it hadn't if it hadn't."

Goldstein's group developed new models, designed and performed basic science experiments and combed through the existing nuclear test data to elucidate the fundamental physics, particularly the equations of state (the relationships between temperature, pressure and density as they relate to the materials) in an exploding weapon.

This SSP physics work drew heavily on Goldstein's plasma research, in particular how radiation transports through hot plasmas.

"Nuclear weapons get very hot and produce plasmas and X-rays. So understanding how nuclear weapons operate means understanding accurately just how the X-rays interact with the matter."

This physical data in turn provided the cornerstone information for the enormous SSP computational codes developed to simulate nuclear blasts as part of the DOE's Accelerated Strategic Computing Initiative, or ASCI (now ASC, for Advanced Simulation and Computing).

"One of the big successes of the SSP has been to develop the ability to do fully three-dimensional models of exploding nuclear weapons."

A NEW SSP GENERATION

The year 2012 marks the 20th anniversary of the last U.S. nuclear test, a major moment for taking stock of the SSP. The U.S. nuclear strategy released in April 2010, called the Nuclear Posture Review, concluded that the SSP clearly provides for the safety and assures the reliability of the nuclear stockpile, with no need for future testing to maintain this confidence. It's a position supported by the three nuclear weapons labs' directors.

For SSP scientists, the Review was another endorsement of their approach. They've not only developed the scientific underpinning of the SSP – they've also nurtured a new generation of SSP scientists, Goldstein notes.

"The imperative to develop a group of scientists who without experience of nuclear tests could still be called upon to certify that the stockpile is secure and reliable has been a huge challenge, and a major deliverable of the SSP."

Yet, he says, the SSP still presents grand challenges, in particular fine-tuning the approximations in models with more exact data and, critically, understanding how plutonium changes over time.

"Plutonium is the heart of a weapon. Since it's radioactive, it's changing even if we don't change anything. So the most critical question that we've had to answer and need to continue to understand is how does plutonium age?"

He says the new National Ignition Facility (NIF) at LLNL will help provide answers. Under construction for more than a decade, the billion-dollar NIF, which boasts the world's most powerful laser, is a critical piece of the SSP. NIF is being used to produce the enormously energetic plasmas involved in nuclear fusion.

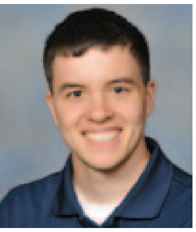
"For the first time, NIF will enable us to experiment with the fusion ignition that happens in nuclear bombs. NIF will allow us to do integral, full-scale fusion ignition experiments that we'll be able to compare with codes. That's a last piece that goes into the puzzle of assuring that our simulation capability is accurate."

NIF symbolizes Goldstein's journey to date at LLNL: the union of fundamental plasma research and national security. During his plasma work in the late 1990s, Goldstein developed the initial experimental concepts for NIF, and it is central to the SSP. What's clear is that a quarter century after arriving, the lab is a professional home that this scientist has shaped and where he feels deeply comfortable.

There's warmth and passion in Goldstein's voice when he talks about what the lab and the SSP program have to offer a new generation of scientists.

"At the laboratory you get the chance to work on some of the most advanced scientific tools that exist in the world today. The laboratory offers access to the most powerful computers, the biggest, most powerful laser that exists and on top of that a group of people, equipment and experimental capabilities that is unmatched any place else. People tell me this all the time, that they don't really understand it until they come to the lab. We have such a large scientific organization that it doesn't matter where your scientific interests take you, you'll find people here who'll help you go there."

For this issue, we asked Stewardship Science Graduate Fellows what drew them to science and to stewardship science in particular. Here are two answers.



Aware of Our Surroundings

BY JOSH RENNER

Third-year fellow

Physics includes things we can see and things we can't. The mountains, lakes, and forests we see are made up of well-known particles: protons, neutrons and electrons. In large numbers these particles construct our familiar world, but individually they are minuscule and can move about, invisible to the eye. They are joined by other less familiar particles, too short-lived or elusive to appear in our daily observations but still surrounding us, some passing right through us.

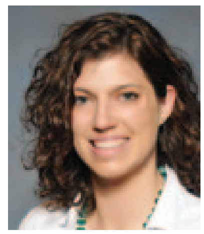
There's often a tendency to ignore things we can't see, but it's important to stop and think about what's really going on around us.

My research involves improving ways to detect and study particles in forms that are infrequently encountered but are important to technological advances and to understanding physics. I develop technology to search for a nuclear reaction, yet to be observed, called neutrinoless double-beta decay. In short, I work on particle detectors.

Particles invisible to the eye can be detected in other ways because they have energy. Just as a stone thrown into a pond creates a splash, a particle deposits a small pocket of energy when it interacts with a particle detector. Atoms in the detector material receive this energy. Small energy exchanges may simply bump an atom like colliding billiard balls, but larger amounts of energy may knock electrons out of an atom. These electrons are one component of the energy splash that can be measured to confirm a particle's presence.

Highly energetic, fast-moving particles are classified as radiation. Radiation can originate from radioactive matter on Earth or from high-energy particles that are expelled from the sun and other entities in space. We have learned to redirect energy from radiation sources on Earth into nuclear power and have used radiation to develop cancer treatments. Our manipulation of nuclear material also has generated nuclear waste – radioactive material that must be kept isolated until it is no longer dangerous. Without proper attention, these materials could present a hazard or fall into hands that seek to transform them into threatening weapons. We must ensure we can efficiently identify nuclear materials, monitor them carefully and make educated decisions about their use.

Stewardship science aims to understand radiation and know its whereabouts. Greater knowledge ensures more responsible development and use of nuclear materials, and future security for our planet. We must remain diligent or radioactive materials could slip by unnoticed. I study stewardship science because I'd like to know what is going on around me, whether I can see it or not.



A Science Nerd Spreads the Word

BY STEPHANIE LYONS

Second-year fellow

I've always been a science nerd. When my second grade teacher asked, "And what do you want to be when you grow up?" I answered, "I want to be an entomologist!" Not knowing what an entomologist was, she replied, "Oh. Umm, well, that's nice." As my fear of spiders and other creepy-crawlies grew, my interest in being an entomologist waned and my aspirations shifted toward forensic expert, geneticist and finally to physicist.

A turning point came in my senior year of high school, when I reluctantly took an introductory physics course. As the semester began, I noticed correlations between it and my calculus class. Simple equations that could model a baseball's flight through the air or a particle's motion in a cyclotron fascinated me. In college I started a double major in physics and biology, then dropped biology. After working in the University of Notre Dame's nuclear structure lab one summer, I was hooked.

During my first year of graduate studies, I saw that family members and nontechnical friends held misconceptions about what scientists do and what science can provide. Without science, many wonderful devices and technologies – from cell phones and transportation to life-saving medical equipment – would be impossible. Yet when it comes to energy resources, public fears hinder technology's advancement.

Being able to communicate possible advances and breakthroughs is what drew me to stewardship science, and I have since become active in science outreach events at and around Notre Dame. People must better understand scientific advances to make informed decisions in their day-to-day lives. In this sense, all science can be steered toward stewardship. To lead the way, scientists should give back to the community through communication and outreach.

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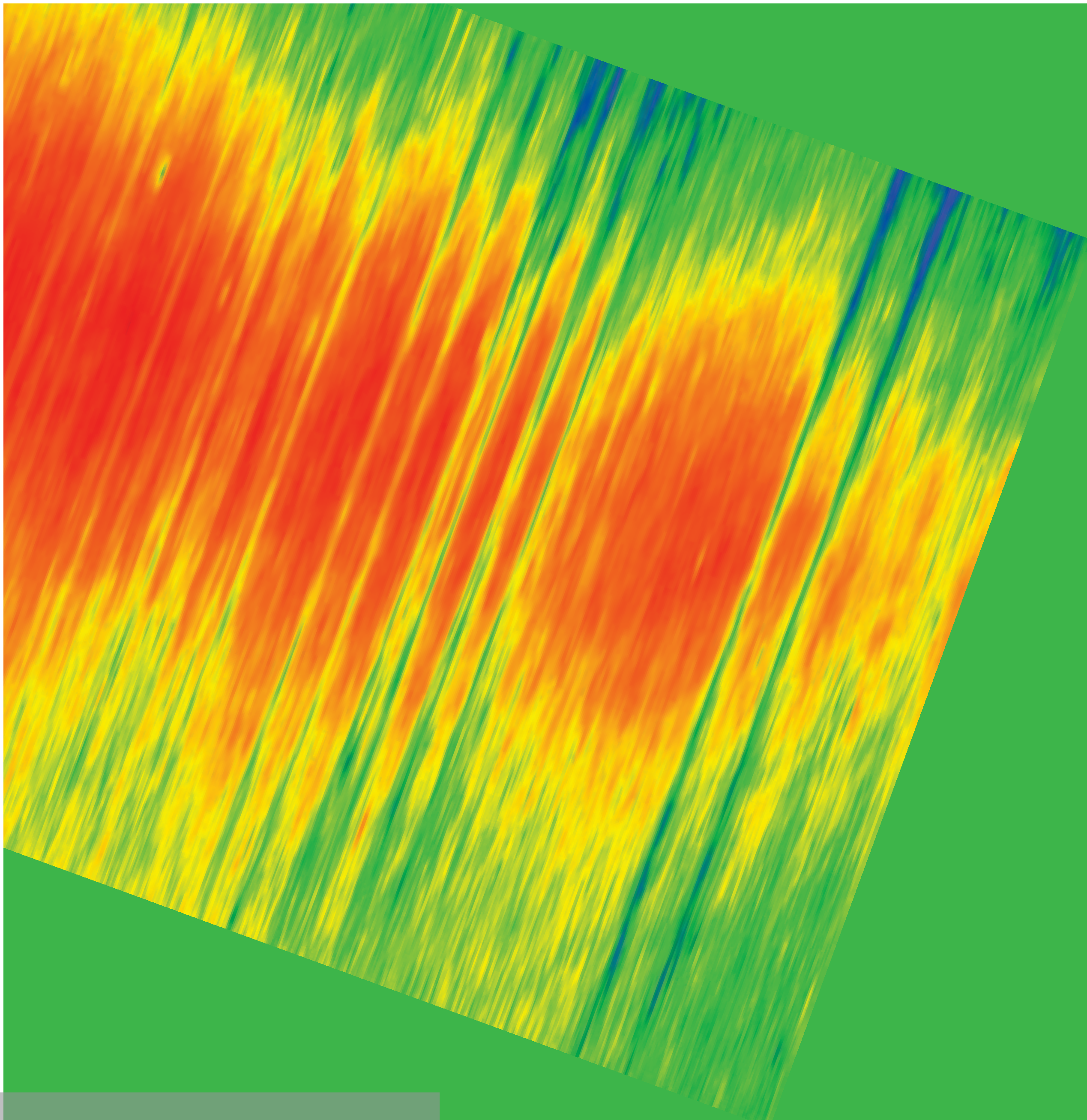

STELLAR VIEW

Sandia National Laboratories' Jim Bailey is "often asked how we can determine the behavior of atoms in exotic matter" – such as iron at the sun's convection-radiation boundary, represented here in an X-ray spectrum. "This picture is one way to answer that – a way to see quantum mechanics in action, real data exhibiting the real behavior of iron atoms." For more on this image and the bigger picture surrounding it, see "A Place in the Sun," which begins on p. 15.

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