

STEWARDSHIP SCIENCE

The SSGF Magazine

2013-2014



PRESSURE PREDICTIONS

How Sandia is refining matter models
by applying first principles

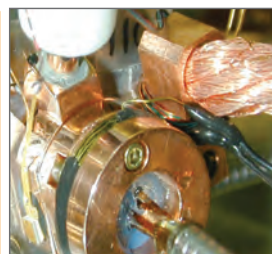
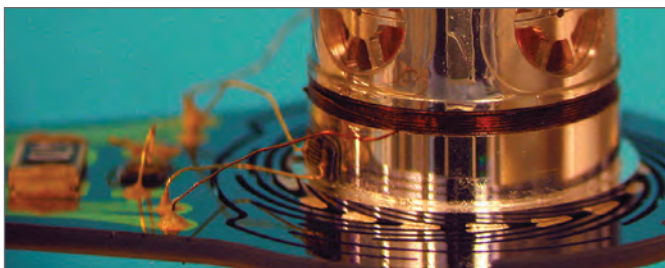
Los Alamos: Neutron
beam record-breaker

Livermore: At the edge
of the periodic table

Plus: Former fellow goes to Washington,
more juice for Z, bringing the big bang
down to size, fission and scission, and
SSGF on the road.

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



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IMAGES

LEFT: A metallic case called a hohlraum holds the fuel capsule for National Ignition Facility experiments at Lawrence Livermore National Laboratory.

MIDDLE: 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.

RIGHT: X-ray laser flashes generated in an undulator, an arrangement of magnets that directs high-energy electrons. Image courtesy of Los Alamos National Laboratory.

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Investing in the Future



Christopher Deeney

MUCH OF the discussion in Washington these days revolves around fiscal restraint, doing more with less and the dreaded “S” word: sequestration. Even in this environment, there is a continuing understanding of the value of science by NNSA leadership and the nation’s elected representatives. This fourth edition of *Stewardship Science: The SSGF Magazine* represents a milestone since the magazine’s publication now spans an entire class of fellows! Our shared commitment to sustaining programs like the Stewardship Science Graduate Fellowship represents the value we place on developing the leaders of tomorrow’s scientific endeavors. The work highlighted in this issue shows the return on those investments.

In missions that range from reducing the risks of nuclear terrorism or the proliferation of nuclear weapons technology to responding to nuclear accidents like the one at Fukushima in Japan, NNSA relies on tools and technology based on a fundamental understanding of nuclear science. The work of fellow Matthew Buckner at Lawrence Livermore National Laboratory (page 4) on Accelerator Mass Spectrometry (AMS) advances the state-of-the-art of a key diagnostic tool. AMS is used in several fields, including detecting signatures of nuclear fuel reprocessing – an important nonproliferation function. Matthew used AutoCAD, along with simulation tools, to build a prototype detector, install it and test it on a Livermore accelerator beamline.

At a more fundamental level, fellow Nicole Fields worked on calibrating a key material during her research practicum at Los Alamos National Laboratory (page 7). Fields examined germanium-76, an isotope researchers hope will find evidence of neutrinoless double-beta decay. This rare interaction is key to understanding neutrinos and can help in advancing our fundamental knowledge of the universe. She used neutron beams from LANSCE, the Los Alamos Neutron Science Center, to simulate cosmic ray exposure so she could calibrate the effects of this radiation for future experiments.

In related work, fellow Joshua Renner conducted his practicum at Livermore (page 7) on the technology for time projection chambers (TPCs). These TPCs also are designed to detect evidence of neutrinoless double-beta decay. Renner worked with physicist Adam Bernstein on the negative ion TPC and used simulation tools to emulate ion drift behavior. These tools provided clues to help maximize the efficiency of Livermore’s detector for these rare interactions.

From fundamental exploration to prototype development, Stewardship Science fellows are advancing the frontiers of nuclear science and helping NNSA build its future.

Christopher Deeney
*Assistant Deputy Administrator
for Stockpile Stewardship
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With assistance from Mark Visosky
*Senior Technical Advisor
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FEATURES

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By Jacob Berkowitz

Sandia's Luke Shulenburg and colleagues are harnessing the power of quantum Monte Carlo methods to boost matter models' accuracy. They're already finding that elements under extreme temperatures and pressures behave in unexpected ways.

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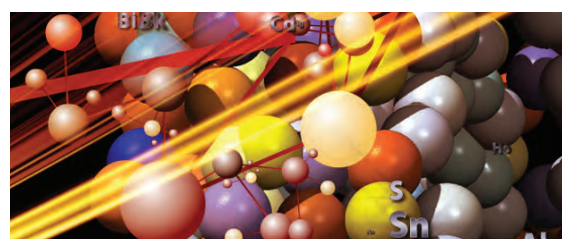
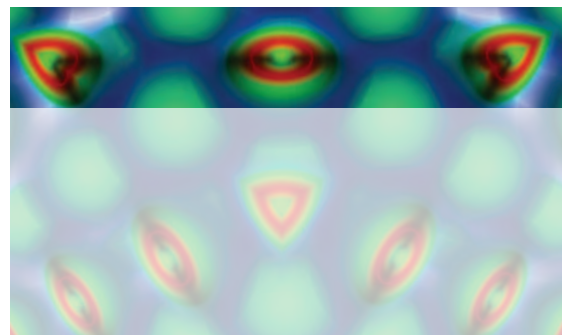
By Karyn Hede

The newest, heaviest elements on the periodic table are difficult to produce and often quickly disappear, making it hard to quantify their properties. Livermore scientists are finding new ways to separate and understand these strange substances.

THE BEAM COUNTERS 19

By Thomas R. O'Donnell

Los Alamos National Laboratory's Trident, a powerful laser that produces fleeting pulses, has racked up a new neutron beam record. The experiment could lead to more precise detectors and to compact neutron sources for science and nuclear forensics.



COVER



FIRST-PRINCIPLE INVESTIGATORS

This visualization by Sandia National Laboratories' Luke Shulenburg shows a charge density map for FeO (iron oxide) calculated with quantum Monte Carlo methods. Iron oxide is of interest to geophysicists, but modeling its electronic structure is challenging. Shulenburg belongs to a corps of young mathematicians – who include Miguel Morales of Lawrence Livermore National Laboratory, an alumnus of the National Nuclear Security Administration Stewardship Science Graduate Fellowship – working out the fundamental properties of this and other materials based on first-principles physics. Read more starting 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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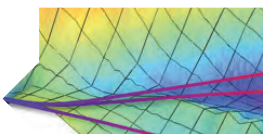
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Deciphering the details of atom splitting.



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Sandia plans to amp up the Z machine in the same space.



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Cover, Luke Shulenburg, Sandia National Laboratories (SNL); page 1, National Nuclear Security Administration; page 4, Walid Younes, Lawrence Livermore National Laboratory (LLNL); page 5, SNL; page 6, ATLAS Experiment/CERN; page 9, Laura Berzak Hopkins; pages 10-12, Shulenburg/SNL; pages 16-17, LLNL; pages 19-20, Markus Roth, Technical University of Darmstadt; page 21, julsdesign (source: Los Alamos National Laboratory [LANL]); pages 22-23, LANL.

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Fission Up Close

Although it releases vast amounts of energy, the process of splitting atomic nuclei is still difficult to understand in detail. Nuclei are infinitesimally small and fission happens incredibly quickly (within 10^{-20} seconds), so it's hard to study in a laboratory.

Undaunted, Lawrence Livermore National Laboratory researchers are looking at fission's microscopic detail with the hope of improving nuclear waste management and recycling and increasing nuclear power production. Describing fission in detail also can help answer basic science questions, such as how heavy elements formed in the universe.

Physicists started delving into fission theoretically 75 years ago by simplifying the problem. Instead of looking at all the protons and neutrons within the nucleus, they considered it as a liquid drop,

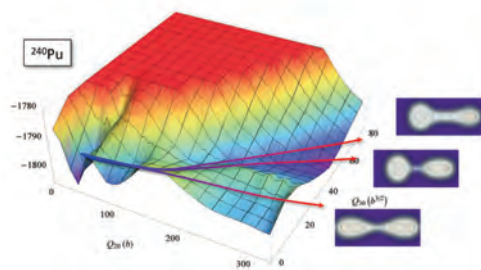
Livermore's Walid Younes says. During fission, the drop would stretch into an oblong peanut shape. At the scission point, the narrow neck in the peanut would break to form two new atomic nuclei and release energy.

Even today, with high-performance computers, the data challenges for

understanding fission remain enormous. If you put all that information into a computer, Younes says, you'd quickly be looking at tens of millions of processor hours as the simulation moves toward scission.

Despite the difficulty, Younes and his colleagues have extended the traditional droplet model. Instead of considering the nucleus as a single stretching blob, their calculation includes protons and neutrons that arrange themselves within the droplet in a way that's energetically favorable. They then stretch the theoretical nucleus until it breaks naturally and probe how that force affects the individual particles. "We don't force it," he says. "We don't take a knife and cut it in two."

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A schematic illustration of microscopic fission calculations for plutonium-240. The arrows represent evolution of the nucleus in the calculation across its energy surface toward its breaking point. On the right are three examples of the nuclear configuration near breaking.

FELLOWS ON LOCATION

Members of DOE National Nuclear Security Administration Stewardship Science Graduate Fellowship's 2013 outgoing class share their national lab research experience.

DETECTOR UPGRADE

Matthew Buckner's practicum at **Lawrence Livermore National Laboratory** was a bit like a high-tech physicists' shop class. His plans for an improved gas ionization chamber detector went from computer modeling to fabrication at a machine shop and testing.



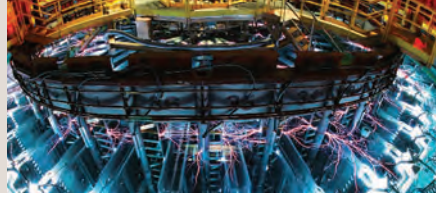
Buckner worked with Scott Tumey at Livermore's Center for Accelerator Mass Spectrometry. Accelerator mass spectrometry, or AMS, speeds ions to high energies, separating isotopes from surrounding material before mass analysis. AMS is used in several fields, including detecting signatures of nuclear fuel reprocessing – an important nonproliferation function.

The device Buckner made uses AMS to measure transition metal activation products. He simulated a previous design on a computer and found that voltages were incorrectly applied for the detector anodes to adequately collect electrons. After some research, he used simulations to tailor the new detector design to transition metal activation products and modified grids, voltages and other aspects.

Using AutoCAD software, Buckner designed a detector enclosure for fabrication at the lab's machine shop, then built the detector and installed it on the accelerator beam line. He and Tumey tested it with relevant materials and Buckner compared its resolving power with that of the original detector. The new detector is more sensitive and bolsters the lab's nuclear forensics capabilities, Tumey says.

The fellow, meanwhile, says the project was a contrast with his doctoral work at the **University of North Carolina at Chapel Hill**. Under Christian Iliadis, Buckner has studied proton capture by rare oxygen isotopes – thermonuclear reactions associated with nucleosynthesis and energy generation in a class of stars and with explosive hydrogen burning during classical novae. During the summer, he reports, "it was really interesting to participate in an application of the nuclear and accelerator physics I'm interested in."

continued on page 7



Z, Supercharged



By far the world's largest, most powerful and most successful pulsed-power accelerator, Sandia National Laboratories' Z machine is poised to become even more powerful.

The Z machine – named for z-pinch, a type of plasma device driven by pulsed-power accelerators – generates an 80-terawatt electrical power pulse. It's 33 meters in diameter and fills the high bay of Building 983 on the lab's Albuquerque, N.M., campus. Thanks to LTD technology, for linear transformer driver, over time Z will become Z 300, a 300-terawatt machine that will fit the same space.

The Z 300 will generate twice the current and four times the power that Z now generates, says William Stygar, manager of the lab's Advanced Accelerator Physics Department, which specializes in pulsed-power accelerator physics. With that capability, Z 300 will be able to perform ultra-precise high energy density physics experiments in support of various Department of Energy missions, including the Stockpile Stewardship Program of the National Nuclear Security Administration.

Stygar is confident that Z 300 will quadruple pressures for conducting material-physics experiments with plutonium, uranium and other critical elements; achieve thermonuclear ignition in an inertially confined deuterium-tritium plasma; quadruple the energy and power radiated by non-thermal X-ray sources for weapon-physics and weapon-effects experiments; and quadruple the energy and power radiated by thermal X-ray sources for laboratory astrophysics, radiation opacity and radiation transport experiments.

John Porter, senior manager of Sandia's Z accelerator sciences group, was the first to propose building a next-generation LTD accelerator that fits inside the same building.

The High Current Electronics Institute (HCEI) at Tomsk, Russia, began work on LTD technology about 10 years ago. Sandia has developed the technology to its present state. Stygar, a Sandia researcher since 1982, says Russia, Israel, France, England, China and other countries already use LTD technology to drive high energy density physics experiments.

LTD technology dates back to 1920s, when Erwin Marx described his self-named generator. Thirty-six Marx generator-driven pulsed-power modules create the 26-megampere, 80-terawatt pulse that powers Z. A Marx generator creates a 1 microsecond-long power pulse. Z experiments, however, require a 100-nanosecond power pulse, so

four stages of pulse compression must reduce the span of the Marx pulse. Pulse-compression hardware introduces electrical impedance mismatches, causing multiple internal reflections of the Z power pulse and reducing Z's efficiency. In addition, Stygar says, pulse compression hardware substantially complicates the design of a machine like Z, increasing maintenance costs and ramping up the difficulty of developing an accurate accelerator circuit model and conducting accelerator simulations.

"An LTD generates a 100-nanosecond power pulse in a single step, which eliminates the need for additional pulse-compression hardware," Stygar says. "As a result, an LTD module is twice as efficient as a Marx-driven module, substantially more compact, less costly to maintain and easier to simulate."

The belly of the LTD beast is a collection of 20 bricks arrayed in a circle like the spokes of a wheel. Each shoebox-sized brick holds a 200-kilovolt switch and two 100-kilovolt capacitors. The bricks are inside an annular enclosed metal cavity that looks like a giant Life Savers candy, Stygar says.

Z 300 will be driven by 90 LTD modules, each consisting of 33 LTD cavities (each cavity is 2 meters in diameter and .22 meters thick) stacked horizontally, like a Life Savers roll. Altogether, Z 300 will have 2,970 cavities, each producing a 100-nanosecond-long, 105-gigawatt power pulse.

"Each cavity converts, in a single step, the energy stored in its capacitors to the 100-nanosecond pulse," Stygar says. "Hence, Z 300 will not need any additional pulse compression hardware."

But it will need some work to upgrade LTD cavities from a 79-gigawatt electrical pulse, the current standard, to the lab's 105-gigawatt pulse goal. To get there, technicians will replace existing switches with new, more advanced ones now under development by researchers from Kinotech Inc. and Sandia. They'll also use upgraded capacitors from technology company General Atomics. Voss Scientific also participates in the project.

Stygar says the plan is to first operate an LTD cavity at 105 gigawatts. Then the team of about 17 technicians and researchers will build an LTD module with 33 cavities that generates a 3.5-terawatt electrical power pulse. "After we demonstrate successful operation of this module, we will be ready to build Z300."

—Tony Fitzpatrick

Little Big Bang

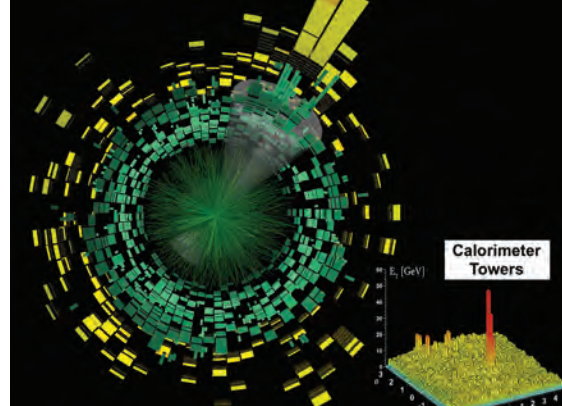
Equipped with particle accelerator-colliders, scientists are glimpsing conditions like those scant microseconds after the Big Bang began our universe 13.8 billion years ago. By bashing together energized heavy gold or lead ions accelerated to near-light speed, they trigger so-called Little Bangs that help reveal states of matter that are even odder than they'd anticipated.

Los Alamos National Laboratory physicist Ivan Vitev is among the theorists attempting to understand these tiny-bang states, known as quark-gluon plasmas, or QGPs. That's because QGPs are "by definition not observable on the time scales at which detectors make experimental measurements," Vitev says.

QGPs themselves refute normal rules of the strong interaction, a fundamental force that keeps matter's core components – quarks and gluons – bound in an unbreakable embrace. Scientists think the Big Bang's stupendous energy burst let quarks and gluons very briefly roam free. But within a few microseconds, they cooled enough to rejoin as the building blocks of protons, neutrons and other contemporary fundamental particles.

Little Bang experiments artificially boost particle energy levels just enough to recreate those last moments when quarks and gluons were still "approximately free," Vitev says. These semi-liberated QGPs were expected to be gaseous. But when the Relativistic Heavy Ion Collider (RHIC) at Brookhaven National Laboratory began producing them in the summer of 2000, puzzled scientists instead found them acting like perfect liquids, flowing with practically no viscosity.

Such discoveries, also observed at CERN accelerators in Europe, "have to be interpreted by theory to extract the information," Vitev says. "We have only a very short time" – about a millionth of a billionth of a second – "when this plasma state lives and develops features we are looking for in experimental data." That's too fleeting for accelerator detector



measurements, so theorists must instead conduct thought experiments. Those reconstruct QGP qualities by using particles formed after the quarks and gluons recombine. "That's what makes the field exciting and at the same time difficult."

Vitev's contributions began with a paper published in 2002, the year he received his doctoral degree from Columbia University. It laid the theoretical foundation for jet tomography, which can be used "once in a blue moon," he says, whenever a comparatively rare heavy ion collision creates especially energetic quarks or gluons. One quark or gluon may collide with another and bounce apart like billiard balls at azimuths roughly 180 degrees apart. After ricocheting, one of the resulting particles continues on at a high speed and energy. The other rapidly loses both in a shower of fragments – the jet – while passing through and interacting with the detector's plasma medium.

Experimentalists can then study the measurable byproducts. For example, if one of the particles is a rare Z boson or a photon, the data can be tagged for comparison with the final byproduct of its counterpart. Researchers know those fragments are spaced by a predictable azimuth and that one has interacted with the plasma medium, whereas the other hasn't. They can reliably use this information to recreate details about the immeasurable QGP itself, such as its density and temperature. Vitev compares this method to positron emission tomography and radiography because both those medical techniques create images by processing signals from particle behavior within a medium.

His theoretical work is "part analytic and part computational," he says, and his codes run on local computer clusters at Los Alamos, where he started in 2004 as a J. Robert Oppenheimer Fellow and now works in the Theoretical Division.

– Monte Basgall

continued from page 4

Although scission – the last part of fission – is incredibly important, it's also the hardest to understand. Physicists would follow the process up to this point of no return but didn't have the tools to examine the nucleus as it fragments. Younes and his team now use their framework to examine scission and have gotten as far as calculating some properties of the resulting nuclear splinters.

Researchers can examine the pairs of nuclei that form as the nucleus comes apart. Most break into a variety of combinations with different energies, so Younes and colleagues are interested in which fragments form and how frequently. Understanding scission is so challenging, in part, because the breakup of a single nucleus into two doubles the complexity: two sets of properties now, plus the nuclei are interacting, introducing still another variable that can affect the system.

This visualizes jet quenching in a lead-lead collision in the Large Hadron Collider's ATLAS detector at a center of mass energy of 2.76 TeV per nucleon-nucleon pair. Green and yellow bars represent particle tracks and energy deposition into the detector subsystems. An energetic jet is clearly visible at 1 o'clock. The gray cone shows there's a jet (a large energy deposition in a narrow cone) in this direction. Its away-side partner at 7 o'clock is completely missing, having dissipated its energy into the plasma.

continued from page 4

ISOTOPE HOPES

It will take some sensitive detectors to answer basic questions about the nature of matter in the universe. Fellow [Nicole Fields'](#) project during her [Los Alamos National Laboratory](#) practicum will help researchers calibrate properties of a key material that could do the job.



Working with Steve Elliott and the Neutron Science and Technology Group's weak interactions team, Fields examined germanium-76, an isotope researchers hope will find evidence of neutrinoless double-beta decay. This rare particle interaction is key to understanding neutrinos – the chargeless, nearly massless byproducts of nuclear reactions – and advance knowledge of the universe.

But germanium-76, when above ground, may interact with naturally occurring cosmic rays, creating radioactive contaminants that could interfere with experiments. The Los Alamos researchers wanted to test other elements that produce similar radioactivity at much higher rates. By counting gamma rays from those other materials, the researchers could estimate how much cosmic ray exposure the germanium received and account for that in their measurements.

Fields exposed foils comprised of the other elements – cadmium, zinc and niobium – to neutron beams at the Los Alamos Neutron Science Center to simulate cosmic ray exposure, but at higher levels. Then she used a detector to count gamma rays and determine which and how many radioactive isotopes resulted. With the neutron flux that hit the foils and the measured cosmic ray neutron flux, Fields could predict which radioactive isotopes would be good indicators of neutron exposure from space.

Fields and her advisor, Juan Collar at the [University of Chicago](#), and Elliott are all collaborators on Majorana, an international experiment that will use germanium-76 to seek signs of neutrinoless double-beta decay.

PARTICLE TRACKER

[Joshua Renner's](#) practicum project at [Livermore](#) was the same as his doctoral research at the [University of California, Berkeley](#), only different.

In both, Renner worked on technology for time projection chambers, or TPCs, designed to detect evidence of neutrinoless double-beta decay. It's key to understanding neutrinos and to advance knowledge of the universe.

TPCs track charged particles released when two larger particles collide or, in some cases, when atoms of fissionable materials split. In essence, the energetic particles scientists seek knock loose electrons from atoms of a gaseous material (the detector medium) in the TPC. The number of freed electrons characterizes the particle's energy.

At UC Berkeley and Lawrence Berkeley National Laboratory, Renner worked under James Siegrist, now associate director of the Department of Energy Office of Science for the High Energy Physics program. The group collaborates with other institutions to develop a prototype detector using xenon as a detector medium – thus the acronym NEXT, for Neutrino Experiment with a Xenon TPC.

At Livermore, Renner worked with physicist Adam Bernstein on the negative ion TPC. It uses negative ion drift, in which freed electrons attach to gas particles, forming negative ions. The ions drift through an electric



Although the LLNL scientists are beginning to get a picture of what scission looks like, questions remain. For example, physicists continue to discuss the role of certain neutrons in the fission process. These scission neutrons, in the neck of that splitting peanut, sometimes are emitted as the nucleus breaks. "We would like to be able to calculate what those neutrons are doing from a microscopic point of view," Younes says. On the atomic scale, this fundamental science also could help researchers understand a variety of scientific problems that come up with multiple

particles. "Scission is such an extreme example of the quantum many-body problem."

Fission is the most computationally challenging problem in nuclear physics, Younes says, partly because it incorporates so many complex dynamic phenomena. "It produces a lot of different kinds of observables and is incredibly rich in the type of phenomena that you can study."

– Sarah Webb

field to a region in which each electron can detach from its ion and create a signal for counting.

Renner learned computer simulation tools to emulate ion drift behavior. The simulations, operating under a set of assumptions about how detachment works, provided clues to maximizing the process in Livermore's detector setup. Learning new computational skills was useful, Renner says, but the experience of working on a new project in a new setting proved unexpectedly valuable.

HIGH-PRESSURE SITUATION

Her practicum at [Livermore](#) set [Kristen John](#) on the road to a high-pressure doctoral thesis. John spent the summer working with Hye-Sook Park and Bruce Remington to learn her way around laser-driven tests of material strength under high pressures and high strains. (See "Laser Days of Summer," *Stewardship Science* 2012-13.)



The practicum became the foundation of her thesis and of a partnership between the Livermore researchers and a group at her university, the [California Institute of Technology](#), that included John's advisor, Guruswami Ravichandran.

At Livermore, John designed experiments using laser-driven compression to study solid-state material properties. She mastered two radiation hydrodynamics computer simulation codes, read papers and talked with colleagues. John also traveled four times to assist with experiments on Omega, the powerful laser at the University of Rochester, and helped analyze the results. The experiments included a study of Rayleigh-Taylor instability in tantalum.

With that knowledge, John helped design experiments investigating iron's properties under the high pressures achievable only at Omega and the National Ignition Facility, known as NIF, Livermore's giant laser complex. The shots, carried out on Omega in summer 2012, indicate iron is stronger than simulations predicted, John says. Nonetheless, her thesis will focus on the tantalum experiments because they're further along.

John also is conducting experiments to recreate the Omega shots on a small scale, using a Caltech gas gun to target ballistic gelatin and tin. The goal is to observe how the materials flow and see if strength

correlates with Rayleigh-Taylor instability growth. John also is learning a Caltech-developed multiscale computer model of strain-induced phase transformations in materials like iron. With Caltech engineering professor Michael Ortiz's group, she's creating simulations and comparing them with the Omega experiments. She'll also use the model to predict results from the gas gun experiments.

IONIC BRAKE-TAPPING

At [Livermore](#), fellow [Alex Zylstra](#) helped set the course for aspects of his supervisor's research and added a branch to his own path. The [Massachusetts Institute of Technology](#) student worked with Gilbert Collins to design experiments probing transport properties in inertial confinement fusion implosions conducted at NIF. Current models are untested because no one has proposed practical experiments in relevant conditions that are able to run on today's facilities.

One set of Zylstra's tests looks at electron-ion equilibration, the rate at which temperatures of the two implosion components even out. Varying temperatures between electrons and ions can substantially affect the implosion's observed behavior, Zylstra says, but experimental data is limited. Zylstra also designed trials to measure ion-stopping power – the way alpha particles lose energy in the implosion hot spot due to complex collision processes. The energy loss rate sets requirements on conditions for an ignition chain reaction, but experiments so far haven't measured ion-stopping power in strongly coupled or degenerate plasmas.

For both investigations, Zylstra simulated the radiation hydrodynamics and made calculations to predict the signal-to-noise ratio and quantify measurement accuracy.

Zylstra's practicum performance was outstanding, Collins says, and his projects helped define a roadmap to benchmark transport properties and provided estimates of uncertainty for these quantities.



The practicum fit well with Zylstra's MIT research under Richard Petrasso, whose group develops diagnostics for NIF and Rochester's Omega laser and explores the physics of fusion and general high energy density plasmas. The project's ion-stopping aspects, Zylstra says, are now part of his doctoral thesis and evolved into a partnership between the Livermore and MIT groups. The researchers carried out the first shots in the ion-stopping experiment earlier this year on Omega, and they're planning for more.

– Thomas R. O'Donnell



CONVERSATION

Laura Berzak Hopkins

*Physicist, Lawrence Livermore
National Laboratory
DOE NNSA SSGF Class of 2010*

As a 2010-11 American Physical Society Congressional Science Fellow, you got an inside look at how science policy develops in Washington. What did you take away from your year in D.C.?

I think the general public has this idea that if you are a scientist you know all kinds of science. I was working in Congress when the Fukushima disaster unfolded. I was asked to write a memo explaining the different features and factors involved in the [Japanese] nuclear power plant and contrasting that to what the media were reporting. I also would get questions because someone thought: "This is science. You give it to the scientist." For example, I did research on poppy growing in Afghanistan and how it affects the opium trade. That's certainly outside my sphere of knowledge. But as scientists, we are trained in research skills. Although we apply them to our specific fields, I learned you also can apply those research skills to a variety of topics. There was a general comfort with getting research questions that you don't know the answer to and figuring out how to answer them.

BRIDGING SCIENCE, POLICY AND THE PUBLIC

Certainly, working in Congress really drove that point home. I learned that there is a critical role for scientists to play in policy. There doesn't have to be this barrier between the policymakers and scientists.

After that year, you could have stayed in Washington and pursued a career in science policy, but you chose to return to a research position at Lawrence Livermore National Laboratory. How did you make that decision?

I am still excited about science and research, so I wasn't certain I was ready to completely step away from research. Livermore provides a lot of opportunities as far as career advancement merging with science policy, so that was definitely a big draw for me.

What are you working on now?

My graduate research was in magnetic fusion. Now I'm part of the research staff at the National Ignition Facility, so I'm working in inertial fusion, which to anyone outside the field is exactly the same. But it's completely different. I'm studying different types of high energy density implosions driven by NIF, which is an enormous laser facility. The goal is to reach ignition, which is a self-sustaining burn of light fuel – deuterium and tritium. I'm in the design physics group, so I work on the type of target the laser hits and on shaping the laser pulse both in power and in time, which is an important part of how the implosion performs.

How did your time as an SSGF Fellow inform your career choices?

During my practicum I worked at Sandia National Laboratories, where I focused on developing advanced materials for plasma-facing components in magnetic fusion reactors. That was an interesting and important introduction

It's important to explain why people's tax dollars should fund what scientists are working on.

to the national lab system and opened my eyes to the career opportunities there. Also, my initial introduction to science policy came through the fellowship. At our annual gatherings there always are opportunities for connections to policymakers in D.C.

You recently co-founded a forum called Why-Sci.com to connect nonscientists with scientists and research. Why should scientists communicate directly with the public?

The reason it's so important to build that bridge is two-fold. In times of fiscal constraint like we are in and will likely continue to be in, it's important to explain why people's tax dollars should fund what scientists are working on. Second, it's important for the public to understand that from their new, quiet refrigerator to their iPod, science goes into all of that. It's important for people to understand that scientific research really does affect them and those investments can improve their lives.

One of the biggest take-home messages I learned in D.C. is that people are excited about science. So many people I met in D.C. who don't know about science were excited to learn more. My office [former Sen. Kent Conrad, D-N.D.] asked me to give a lunchtime mini-lecture on fusion and ongoing plasma physics experiments. It was exciting to see the interest, and I think part of it was the direct interaction with a scientist who was willing to explain what they do. That's the model for Why-Sci.com.



Lab initio

BY JACOB BERKOWITZ

Title image: Snapshot from a simulation of xenon in which liquid atoms (red) are solidifying (green) at a high temperature and pressure.

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

Luke Shulenburg



Scientists at Sandia National Laboratories are out to make first-principles chemical models, hoping to reduce error and illuminate experiments on materials under extreme conditions.

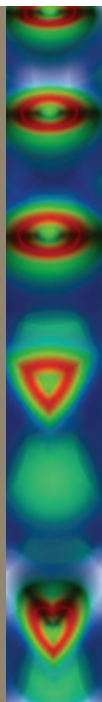
W

hile in high school in Lawrence, Luke Shulenburg would bike or walk up the hill to the University of Kansas, where professors mentored the precocious teen in math, physics, chemistry and computer science.

By his senior year, this extracurricular education had led him to the National Junior Science and Humanities Symposium and his first paper in *Physics Letters A*, co-authored with his mentors and published when he was an undergraduate at the Massachusetts Institute of Technology.

It also led him to a career-defining conundrum. While studying organic chemistry and struggling to memorize reaction rules, he wondered why chemists didn't work like physicists: mathematically, from fundamental first principles.

"Why couldn't you just solve the equations behind everything?" says Shulenburg, now a staff scientist in the high energy density physics theory group at Sandia National Laboratories in New Mexico. "I've been playing around with that ever since."



Today, Shulenburg has found his intellectual home. He's part of a new generation of young Stockpile Stewardship program researchers at National Nuclear Security Administration laboratories who are driven to create models of matter based not primarily on experimental data, but on first-principles physics equations – *ab initio*, literally “from the beginning,” models.

At the heart of this vision is Quantum Monte Carlo (QMC), a computational modeling technique that grew from work at Los Alamos National Laboratory in the early 1950s. Sixty years later, QMC is finding its greatest expression in extreme parallel computing applications on DOE's high-end supercomputers.

As a result, two decades since the last U.S. underground nuclear test, Shulenburg and colleagues are taking stewardship science into a new era. They are harnessing the combination of QMC techniques, dramatic new insights into materials at the extreme and visions of ever more powerful computing to create a new race for accuracy between experimentalists and theorists.

“Experimental results will always be needed to ground our research, but our goal is to provide a more complete picture,” says Shulenburg, who presented his latest QMC work at the American Physical Society meeting in March 2013.

BEYOND APPROXIMATIONS

Shulenburg wasn't the first to dream of theoretically predicting the physical and chemical properties of matter from first principles. The pioneers of quantum theory long shared that vision. The formulation of the Schrödinger equation describing the quantum behavior of electrons held the promise of theoretically solving any chemical interaction. In practice, however, the equation hits a computational Mount Everest. Problems scale exponentially with the number of particles. Thus, even with enormous computing power, exact solutions are obtainable only for molecules with just a few electrons.

To vault this quantum multibody hurdle, computational scientists have developed ways to approximate solutions to the Schrödinger equation. Each approximation –

incorporating a mix of experimental data and what physicists call physics intuition – makes the equation more computationally tractable.

The problem is that every approximation also distorts reality to some extent. Thus, approximations are fertile ground for improvement for the Stockpile Stewardship Program's Predictive Capability Framework, which aims to significantly reduce modeling uncertainties.

“The common thread that links all of my research is the elimination of approximations to develop a more precise ability to simulate materials under extreme conditions,” Shulenburg says.

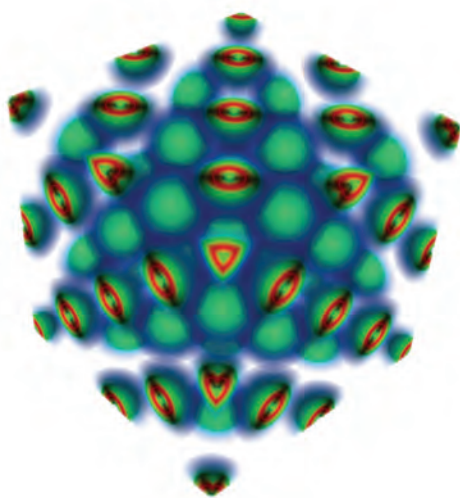
Since joining Sandia in 2010, Shulenburg has taken a two-pronged approach to reduce approximations in models of elements across the periodic table under extreme pressure.

First is adapting and applying QMCPACK, a new QMC code optimized for use on DOE's massively parallel leadership-class computers. (See sidebar, “New Code Tested Against the Elements.”)

The workhorse of quantum computational approximation is density functional theory, or DFT. The technique was developed several decades ago and now has thousands of users and applications agile enough to run on smartphones. But DFT falters in describing how matter behaves under extreme conditions, particularly for heavy atoms.

This is where QMCPACK enters the picture. QMC uses a stochastic, random step-sampling technique to solve wave equations, an approach with a completely different and potentially tinier class of approximations than DFT.

A visualization of a charge density for solid argon, calculated with quantum Monte Carlo methods.



NEW CODE TESTED AGAINST THE ELEMENTS



Miguel Morales

“QMC is an excellent fit with stockpile stewardship because it has the potential to determine materials’ properties with extremely small uncertainties,” Shulenburg says. This is critical to verification and validation – proving models act as intended – and reducing uncertainty. “With QMC you have the opportunity to get the physics right even where your intuition fails you.”

QMC algorithms also are naturally parallelizable on several levels, providing the ideal models for petascale computers that can do quadrillions of scientific calculations a second and exascale machines at least a thousand times more powerful than those. “If you give me a bigger computer to run on – and fortunately the DOE has lots of big computers – I can make the statistical approximation error as small as I want.”

Although QMC provides one avenue for reducing approximations, another approach quantifies how much each of those approximations potentially skews simulations.

Many researchers working to improve QMC’s accuracy have focused on reducing the fixed-node approximation, known to limit *ab initio* calculations of

A pair of young DOE scientists is confident that a new first-principles quantum simulation code will provide unprecedented predictive accuracy in modeling elements across the periodic table under sun-like extremes of temperature and pressure.

Their optimism is based on QMCPACK, for Quantum Monte Carlo Package. Quantum Monte Carlo isn’t a widespread method yet, says Miguel Morales, a staff scientist in the Condensed Matter and Materials Division at Lawrence Livermore National Laboratory. “In terms of stockpile stewardship, the challenge for us is to develop QMCPACK to the point at which there’s trust in its predictive capabilities.”

QMCPACK was created under the leadership of the University of Illinois’ David Ceperley, a pioneer in developing the quantum Monte Carlo family of methods.

Ceperley, also a staff scientist at the university’s National Center for Supercomputing Applications, worked with fellow professor and physicist Richard Martin to mentor a talented group of graduate students. Many of those students now are Department of Energy staff scientists applying QMCPACK to the most challenging stockpile stewardship problems.

Jeongnim Kim, a scientist in the Computational Chemistry and Materials Division at Oak Ridge National Laboratory, leads QMCPACK’s ongoing development.

“QMCPACK is completely designed with extreme parallelism in mind,” Morales says. Test runs on Oak Ridge’s petaflops-capable supercomputer showed the code could be scaled up to the entire machine with little loss in efficiency. In a discipline in which modeling a dozen individual electrons is considered an admirable feat, QMCPACK has demonstrated it’s capable of modeling thousands of particles in a computationally cost-effective way.

Morales and Sandia National Laboratories’ Luke Shulenburg – both of whom, along with Kim, worked with Ceperley on QMCPACK – are testing the code in a benchmarking program to predictively model elements under extreme conditions. “We’re going to touch on elements across the periodic table and identify those areas where we do well and those where we need to work harder,” Morales says. Last

year, with Ceperley and colleagues, he co-wrote a paper on hydrogen and helium under extreme conditions for *Reviews of Modern Physics*.

“Probably for the light elements, we’re there,” says Shulenburg, who recently used QMCPACK to reveal a possible new beryllium solid-solid phase transition under high pressure. “But as you get to the heavier elements, it’s much more difficult from the computational point of view.”

In a 2010 *Proceedings of the National Academy of Sciences* paper, Morales used QMC *ab initio* simulations to confirm and pinpoint a liquid-liquid transition in high-pressure hydrogen of interest to planetary scientists considering giant gas planets like Jupiter.

Morales and Shulenburg are working with Sandia and Livermore colleagues to extend the QMCPACK benchmarking to other elements, including gold, silver and molybdenum. Applying QMCPACK includes porting the code to other supercomputers, including Cielo at Los Alamos and Sequoia, the IBM Blue Gene/Q at Livermore.

The effort also has involved porting QMCPACK to run on graphics processing units, or GPUs. These massively parallel, energy-efficient chips developed for video games are giving a low-cost, high-efficiency boost to high-performance computing. Notes Shulenburg, “With GPUs you almost have to think of your problem in a whole different way – about how to decouple everything into parallel tasks to an extent that’s previously unheard of.” The approach is ideal for QMC, a naturally parallelizable technique.

Titan, a world-leading computer at Oak Ridge, already gets most of its processing power from GPUs. Kenneth Esler of Stone Ridge Technologies, another of Ceperley’s University of Illinois disciples, recently ported QMCPACK to run on them.

Morales says the challenge QMCPACK’s advocates face is to build a series of success stories, convincing others of its accuracy and utility. “To the extent that we can start using correct first-principle predictions of materials at high density, we will start to identify problems in stockpile stewardship models currently being used. There are still many hurdles to cross, but I think it’s just a matter of time.”



Shulenburger's come full circle in his desire to get down to *ab initio* basics.

condensed matter and nuclear reactions. The approximation is a computational compromise that addresses the fermion sign problem, one of the major unsolved problems in modeling the physics of many-particle quantum systems.

In a system with two or more electrons, the wave function has regions with opposite signs: one positive, the other negative. However, for efficiency, QMC typically calculates only in an approximation of the positive space. This fixed-node approximation is the most difficult to eliminate and is a fundamental uncertainty in QMC calculations today.

Shulenburger and colleagues are pursuing a comprehensive solution to the sign problem. He's already made significant progress by showing that, in practice, it might be less important than previously thought in solving important stockpile stewardship problems. "My work has found that it is rarely the determining factor for high-accuracy simulations," Shulenburger says. "The way we partition the problem into tightly bound and chemically active pieces is far more important than this more theoretically fundamental question."

QMC INSIGHTS TO MATTER AT THE EXTREME

Approximations notwithstanding, QMC already has proven its worth in revealing a dramatically new map of matter's terrain at extreme temperatures and pressures.

From first principles, says Lawrence Livermore National Laboratory's Miguel Morales, "we've identified a completely new set of states of matter that appear when you compress materials, and many of these were completely unexpected."

Morales is a Livermore staff scientist and an alumnus of the DOE National Nuclear Security Administration Stewardship Science Graduate Fellowship. He's collaborating with Shulenburger to systematically apply QMCPACK – a code they both helped develop as graduate students at the University of Illinois – to predict the equations of state for elements at high temperatures and pressures.

They've both witnessed the power of *ab initio* models to redefine our understanding of material behaviors at the extreme conditions critical to stockpile stewardship and fields such as planetary geophysics.

For example, previous models assumed that delocalized electrons – ones at high pressure, stripped from their nuclei – form a uniform electron curtain ions interact against. "In practice that's not always what happens," Morales says. Instead, in atoms from such elements as aluminum and sodium under extreme pressure, delocalized electrons congregate in the voids of the ionic lattice, creating stable electroneutral structures. Similarly, Shulenburger says, scientists now are reassessing models of large atoms that ignored inner electrons. "One of the fascinating things about high-pressure

science is you can get to the point where these previously chemically inert inner electrons start to matter, because the energy scales go up and up as you bring the ions closer and closer together, and factoring this in fundamentally changes the properties of materials at these extreme conditions."

Shulenburger was introduced to real-world high-pressure materials problems as a post-doctoral researcher at the Carnegie Institution's Geophysical Laboratory in Washington, D.C. There, researchers study the behavior of minerals squeezed at enormous pressures and temperatures inside the Earth.

In his time at Sandia, Shulenburger's come full circle in his desire to get down to *ab initio* basics. Working closely with Sandia's engineers and experimentalists, his QMC fine-tuning focuses on making this first-principles technique useful in the Stockpile Stewardship Program's applied big picture.

"When I was a grad student at Illinois, if I could tell you about the phenomenon of a solid under pressure, that it metalizes and here's why, you probably wouldn't have cared as much about exactly at what temperature and pressure that happened," he says. But at Sandia, where an engineer may actually incorporate those data into plans for a device, "you care a lot more about the details. So I've gotten a lot more focused in terms of how to produce a high-precision quantitative result rather than just getting a qualitative sense of the physics of a problem." [SS](#)

IN THEIR ELEMENT

BY KARYN HEDE

Lawrence Livermore National Laboratory scientists are probing properties of atoms on the edge of the periodic table. Their rapid separation techniques could have ramifications for nuclear forensics.

For years the periodic table has existed in limbo, its otherwise orderly stacks and rows of elements petering out at the bottom with a series of elements that seemed to signal chemists had exhausted their ideas. Running across the lower right corner, the elements from No. 113 to No. 118 read as a series of U's. One might guess these stood for "unknown."

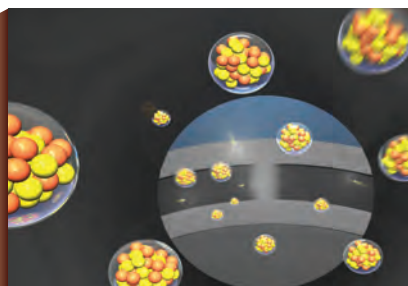
At least some of these orphans finally now have names that acknowledge their discovery. Element 114 is flerovium, after

1 H Hydrogen 1.008	2 He Helium 4.0026																														
3 Li Lithium 6.941	4 Be Beryllium 9.0122	5 B Boron 10.811	6 C Carbon 12.0107	7 N Nitrogen 14.0067	8 O Oxygen 15.9994	9 F Fluorine 18.9984	10 Ne Neon 20.1797																								
11 Na Sodium 22.98977	12 Mg Magnesium 24.304	13 Al Aluminum 26.981538	14 Si Silicon 28.0855	15 P Phosphorus 30.9738	16 S Sulfur 32.065	17 Cl Chlorine 35.453	18 Ar Argon 39.948																								
19 K Potassium 39.0983	20 Ca Calcium 40.078	21 Sc Scandium 44.955912	22 Ti Titanium 47.88	23 V Vanadium 50.9415	24 Cr Chromium 51.9961	25 Mn Manganese 54.938045	26 Fe Iron 55.845	27 Co Cobalt 58.933195	28 Ni Nickel 58.6934	29 Cu Copper 63.546	30 Zn Zinc 65.409	31 Ga Gallium 69.723	32 Ge Germanium 72.64	33 As Arsenic 74.9216	34 Se Selenium 78.96	35 Br Bromine 79.904	36 Kr Krypton 83.798														
37 Rb Rubidium 85.4678	38 Sr Strontium 87.62	39 Y Yttrium 88.90584	40 Zr Zirconium 91.224	41 Nb Niobium 92.90638	42 Mo Molybdenum 95.94	43 Tc Technetium 98	44 Ru Ruthenium 101.07	45 Rh Rhodium 102.9055	46 Pd Palladium 106.42	47 Ag Silver 107.8682	48 Cd Cadmium 112.411	49 In Indium 114.818	50 Sn Tin 118.71	51 Sb Antimony 121.76	52 Te Tellurium 127.6	53 I Iodine 126.9045	54 Xe Xenon 131.293														
55 Cs Cesium 132.90545	56 Ba Barium 137.327	57 La Lanthanum 138.90547	58 Ce Cerium 140.12	59 Pr Praseodymium 140.90765	60 Nd Neodymium 144.242	61 Pm Promethium 145	62 Sm Samarium 150.36	63 Eu Europium 151.964	64 Gd Gadolinium 157.25	65 Tb Terbium 158.92534	66 Dy Dysprosium 162.50018	67 Ho Holmium 164.93032	68 Er Erbium 167.259	69 Tm Thulium 168.9342	70 Yb Ytterbium 173.045	71 Lu Lutetium 174.967	72 Hf Hafnium 178.49	73 Ta Tantalum 180.94788	74 W Tungsten 183.84	75 Re Rhenium 186.207	76 Os Osmium 190.23	77 Ir Iridium 192.222	78 Pt Platinum 195.078	79 Au Gold 196.96657	80 Hg Mercury 200.59	81 Tl Thallium 204.3833	82 Pb Lead 207.2	83 Bi Bismuth 208.9804	84 Po Polonium (209)	85 At Astatine (210)	86 Rn Radon (222)
87 Fr Francium (223)	88 Ra Radium (226)	89 Ac Actinium (227)	90 Th Thorium 232.0377	91 Pa Protactinium 231.03688	92 U Uranium 238.02891	93 Np Neptunium 237	94 Pu Plutonium 244	95 Am Americium 243	96 Cm Curium 247	97 Bk Berkelium 247	98 Cf Californium 251	99 Es Einsteinium 252	100 Fm Fermium 257	101 Md Mendelevium 258	102 No Nobelium 259	103 Lr Lawrencium 262	104 Rf Rutherfordium 261	105 Db Dubnium 262	106 Sg Seaborgium 266	107 Bh Bohrium 264	108 Hs Hassium 277	109 Mt Meitnerium 268	110 Ds Darmstadtium (271)	111 Rg Roentgenium (272)	112 Uub Ununbium (277)	113 Uut Ununtrium —	114 Fl Flerovium (287)	115 Uup Ununpentium —	116 Lv Livermorium (291)	117 Uus Ununseptium —	118 Uuo Ununoctium —

the Flerov Laboratory of Nuclear Reactions in Dubna, Russia, where it was first created. Likewise, No. 116 now is livermorium, after Lawrence Livermore National Laboratory. The labs collaborated on the discoveries and still cooperate on pushing the edge of the periodic table, seeking the outer limit of possible elements.

Perhaps no living scientist is more associated with element discovery than Livermore's Ken Moody, a radiochemist and member of Livermore's super heavy element group. Moody, who was involved in discovering elements 113 to 118, has spent years trying to understand the central issue of how atomic nuclei balance the repulsion between protons with the nuclear glue that binds them. Just how heavy can an element get, he wonders, before clusters of positively charged protons prompt nuclear fission?

This lingering issue motivates nuclear chemists in the super heavy element group. But the tools and technology required to address this fundamental question also have found applications in nuclear forensics, actinide chemistry and other fields.



In this artist's conception, calcium ions travel down an accelerator at a high velocity, about 30,000 kilometers per second, toward a rotating californium target.

Once a new element is discovered, group leader Dawn Shaughnessy says, "the next question is what are (its) chemical properties and how does it relate to its neighboring elements in the periodic table? Doing those experiments is challenging because you are literally doing chemistry on a single atom of something that only lasts a short amount of time."

Their fleeting existence means we have scant or, in some cases, no information about the chemical properties of the heavy elements occupying the last few blocks in period 7, the last row on the periodic table. For example, we know that element 118 existed only by

measuring alpha particles released in its nearly immediate decay to livermorium and then to flerovium. It's the same for nearly all the man-made elements: Scientists only know they've been there by counting radioactive emissions as they decay.

Years ago, Moody described his work to his elementary school-aged daughter. Her incredulous response – "You mean you don't actually know whether you have anything until it goes away?" – encapsulates the difficulties of working with such ephemeral species.

CHEMISTRY BY ANALOGY

Most super heavy elements can be studied only at the few places that have colliders capable of firing ions – calcium, generally – at one of the actinide elements, such as curium or californium, at speeds approaching 30,000 kilometers per second. Experiments using these rarest of elements are both practically and financially

difficult, so the Livermore team wants to probe the chemistry of analogous elements in the same vertical group, whose bonding and chemical behavior should be similar. The idea is to perfect analytical methods using elements that can reliably be made in a standard ion accelerator, then transfer those methods to study the super heavy elements.

Given the challenge of understanding the chemical behavior of an atom with a half-life of less than a minute, the Livermore researchers must develop swift chemical methods and ways to automate often-repetitive experiments. Dubnium, for example, exists in several isotopes that have half-lives from 35 seconds to up to one day. The problem with the more stable form of the element, which is named for the Flerov Laboratory's location, is that generally it's possible to generate only one atom of it per day.

"We need a chemistry where the kinetics are really fast," Shaughnessy says. "It may be that with a standard chemistry on a stable element you can let your experiment sit and equilibrate for a long time. We don't have that luxury."

Livermore uses an automated device that introduces a sample as a gas-borne aerosol to a testing chamber, deposits it on a porous glass frit, adds acids to convert the sample into a liquid and rotates it for subsequent chemical separation and measurement. The device then moves to a cleaning position and rotates back to collect another sample. The device allows the chemists to repeat an experiment about once a minute for days or weeks,



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

Narek Ghariyban, a postdoctoral researcher, works on chemical separations of heavy elements at Lawrence Livermore National Laboratory. The lab is known for its skill at separation methods, which are useful to identify uranium sources.

gathering enough data to understand how heavy elements such as Nos. 104, 105 and 106 adsorb or desorb from a surface.

Following the periodic table would lead scientists to expect that dubnium (element 105) shares properties with tantalum (No. 73, just above dubnium in period 6) and niobium (No. 41, two rows up in period 5), Moody says. “The good news is that it does. But the interesting thing is that you would expect it to be more similar to tantalum than niobium, just because it is closer in atomic weight, but in some systems we have found it is closer to niobium.”

In some ways, the research pits periodic table father Dmitri Mendeleev against Albert Einstein. When a nucleus becomes large enough, its positive charge causes electrons orbiting it to spin so fast that relativistic effects make predicting its behavior difficult.

“If you just put element 114 in the periodic table it should sit under lead,” Shaughnessy says. “But there are nuclear orbital models that say it should not behave

like lead. It should behave like a noble gas, something inert that doesn’t react. And that would be a big deal in terms of how we understand the periodic table.”

The research group’s goal is to understand how element 114, flerovium, behaves. To get there, they are developing very fast chemistry using some of the lighter elements in group 14, such as lead and tin. The researchers are studying ligands, binding agents that can pull lead or tin out of a mixture. They also collaborate with Texas A&M University and the University of Nevada, Las Vegas (UNLV) to study new materials that will separate super heavy elements quickly and efficiently from interfering background products. Several doctoral students have conducted their thesis research on chemical extraction and on analyzing behavior down a specific group in the periodic table.

FINDING AN ATOM IN A HAYSTACK

Livermore scientists mastered isotopic separation methods in an era of open-air nuclear tests before 1962. For example, the lab’s Center for Accelerator Mass Spectrometry can separate and count a handful of uranium-236 atoms from a sample of several grams. Such exacting separations are essential when trying to identify the source of uranium taken from one of dozens of sites where mined ore is processed and enriched for energy production or weapons.

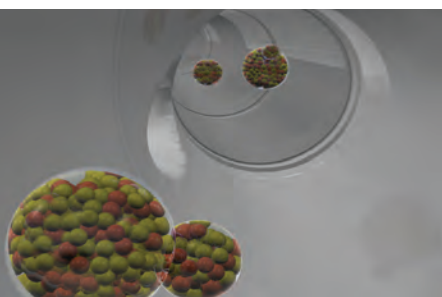
The challenge, Moody says, is taking decades of separations and analytical expertise and applying it to the needs of modern nuclear forensics. In the 1960s, the research team had time to carefully scrutinize a test’s products. Today, the goal is to supply answers that quickly locate the source of, for example, illegally obtained uranium. Perhaps just as important, the researchers want to track the material sources should a terrorist organization succeed in detonating a dirty bomb or other nuclear weapon. In a blast scenario, the nuclear forensics group would analyze debris and reverse-engineer what device was used and how it was built.

“The problems you have doing the heavy element chemistry are often similar to the problems you would have in a (nuclear) forensics type of scenario,” Shaughnessy says. “You are looking for a very small amount of something in a large matrix of background material. You want to separate it quickly because everything is radioactive, and you want to get the answer as soon as possible. We are always looking for new methods of very rapid separation techniques.”

In recent years, Livermore also has cultivated expertise in developing chemical signatures that let the scientists identify where and how a particular sample of uranium was produced. Now they’re working on parsing how it gets to where it’s seized. To that end, Livermore has teamed with UNLV researchers to rapidly identify uranium samples. Graduate students and post-doctoral researchers often split their time between the two locations.

Jonathan Plaue, one such doctoral student, recently discovered that different uranium samples precipitated into unique and reproducible crystalline shapes depending on their origin. This project, which formed an important part of his dissertation, could help to rapidly identify interdicted samples from a specific location or produced through a similar process.

The new element 118 travels through the accelerator to a detector. Quickly separating and observing the new atom is key to understanding its properties.



“If we had a real-world sample, we now believe that simply by looking at the shape or shapes of the particles we may be able to infer the process or processes that were used to produce those particles,” says Ian Hutcheon, a physicist and leader of the chemical & isotopic signatures group in Livermore’s Chemical Sciences Division. Part of Hutcheon’s group specializes in the exacting work of measuring the

abundances of uranium isotopes in surprisingly complex, small samples. (See sidebar, “Rare Earth.”)

Looking ahead, the research team aims to avoid the chemical separation step altogether. Instead, the researchers in Hutcheon’s group are pointing lasers at fallout samples to atomize them. An ionizing laser fired at the cloud would transform only the atoms of interest, usually uranium or plutonium, into an ionized state. Ideally, the uranium or plutonium would absorb the photons, with all other elements invisible, then would be drawn into a mass spectrometer for counting. The method also would be applicable to all the actinide elements, but to make it practical much more information about the atomic energy levels of these elements must be collected. Toward that end, the group collaborates with researchers at the Naval Post Graduate School in Monterey, Calif., to study the atomic energy levels of the heavy elements in the actinide period – the 15 elements between Nos. 89 and 103. That includes uranium to curium, the most interesting ones for nuclear forensics.

“We think that this new technique, called resonance ionization mass spectrometry, gives us the ability to do analyses on the time scale of much less than a day,” Hutcheon says. The required mass spectrometer will be built at Livermore while the basic research project is underway.

Ultimately, Shaughnessy envisions a mobile system that would make nuclear forensics field-deployable.

“We really should be thinking of completely new technology,” she says. “I could think of probably five projects tomorrow that a student could go launch on. That could make a huge difference in nuclear forensics.” **SS**

RARE EARTH

The rare appearance of a meteor streaking over Russia in 2013 shocked local observers but offered scientists another chance to learn more about the origins of the universe. For inside each slice of meteorite debris are some of the earliest building blocks of solid matter – once-molten droplets produced by high-temperature processes at the birth of the solar system.

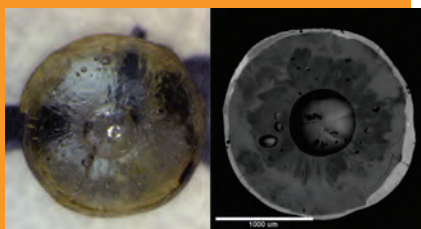
Few opportunities exist to study the remnants of such phenomena here on Earth, but a recent discovery at Lawrence Livermore National Laboratory may have opened up a new possibility.

Ian Hutcheon, a physicist who studies heterogeneous materials in the nanometer to micrometer scales, was examining some of the glassy debris created during outdoor nuclear testing in the 1950s and ‘60s. He realized that microscopic patterns in the glassy spherules created moments after a powerful nuclear blast resemble those in chondrules, the glassy spheres found in primitive meteorites.


“It turns out that these fallout particles, even though they are made of glass, are not homogeneous,” Hutcheon says. “You find large variations in both the elemental composition and, even more intriguing, in the isotopic composition.” Hutcheon’s research team found that within a single marble-like spherule, pockets of uranium-235 (the isotope found in a nuclear device) and uranium-238 (the uranium form found in the environment) exist side-by-side and unmixed, along with various blends of the two.

“What this tells us is that these spherules were made in the aftermath of the detonation by a process or processes that had to mix materials coming from the device with material coming from the environment.”

Hutcheon’s nearly 40 years of experience studying meteorite inclusions may provide clues to the mixing processes that occur in the seconds after a nuclear blast. His research could offer a new avenue for combining nuclear forensics with the physics of early solar system formation.



Cross section of a 2 millimeter-diameter glassy spherule produced during a nuclear test, mounted in epoxy. On the left, an optical micrograph shows a large central cavity surrounded by many smaller bubbles. On the right, a scanning electron microscopic image shows variations in chemical composition that reveal clues to the rate of cooling and solidification. The light band at the perimeter is enriched in calcium and iron.



BY THOMAS R. O'DONNELL

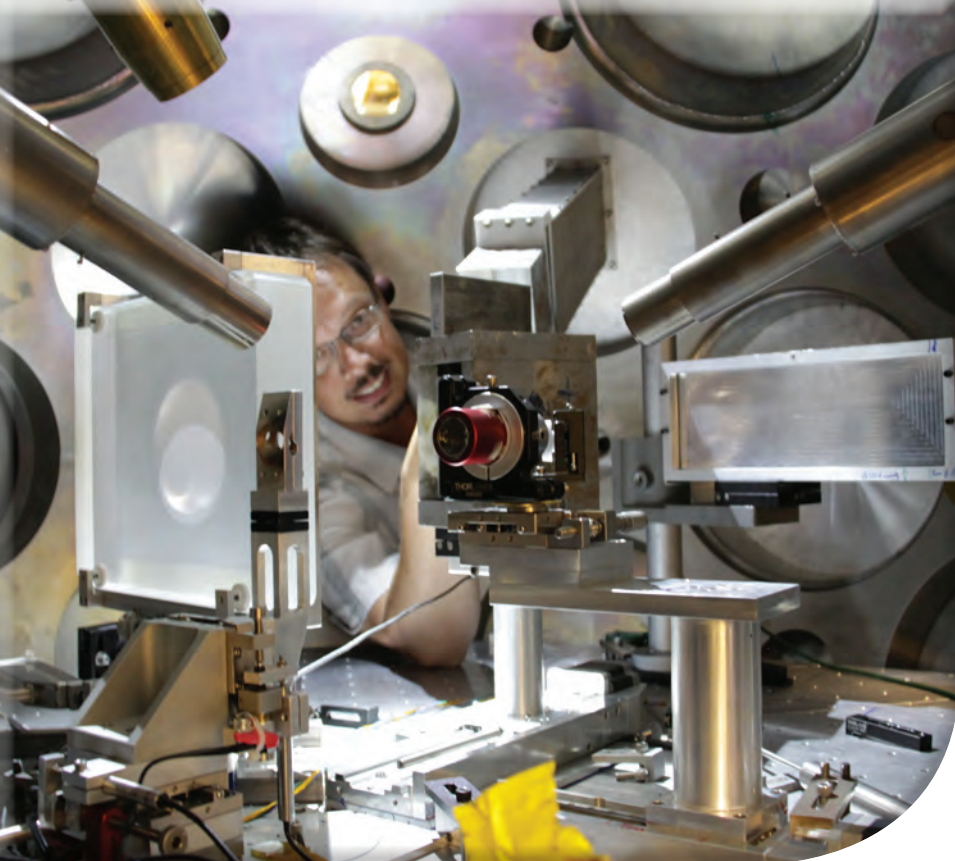
The BEAM COUNTERS

RESEARCHERS USING LOS ALAMOS NATIONAL LABORATORY'S TRIDENT LASER HAVE GENERATED POTENT NEUTRON PULSES, OPENING NEW AVENUES FOR SCIENCE.

A Trident laser shot, delivering as much as 200 quintillion watts of energy per square centimeter to a deuterium-carbon target.

THE INTERCOM ECHOES THROUGH THE TRIDENT LASER

FACILITY AT LOS ALAMOS NATIONAL LABORATORY. A technician speaks. *We are preparing for a system shot to the north target area. She warns staff to avoid high-voltage hardware and the laser bay. Do not break any interlocks.*



Researcher Markus Roth at work in the target chamber at Los Alamos National Laboratory's Trident laser, where scientists often join lab technicians in preparing shots.

The sheer number of energetic neutrons, delivered in incredibly short bursts, makes the Trident beams suitable for multiple uses, from deciphering the fundamentals of radiation damage to identifying illicit nuclear materials. The technology also may advance neutron research as institutions without the space and money for linear accelerators embrace compact neutron-generating lasers.

"That's probably the most exciting aspect," says Frank Merrill, a neutron scientist and team leader for the advanced imaging group in Los Alamos' Physics Division. "It's this novel way of generating neutrons that may open applications nobody has thought about because (neutron beams) were so expensive to generate and build."

Trident's unusual properties – and some physics wizardry – make it possible.

LASER JOCKS

The voice on the intercom indicates the power level of capacitors that soon will discharge in Trident's high-intensity beam. *Twenty-five percent charge.*

Fernández and Roth, Merrill says, are "laser jocks: physicists who know how to use short-pulse lasers to do all kinds of fascinating things." Although the two collaborators are unsure about the nickname – "No self-respecting laser scientist would call us laser jocks," Fernández jokes – they agree lasers are key to their research. "Juan and I are more the users," Roth says. "We really are the experimental side."

Scientists Juan Fernández and Markus Roth listen from a nearby office. Fernández leads Los Alamos' experimental plasma physics group. Roth is a laser plasma physicist from Germany's Technical University of Darmstadt. Shots are "always a little bit like a rocket launch," Roth says. But instead of sending off satellites, Trident is firing oodles of high-energy neutrons.

It's February, and Roth is taking a break between shot setups on his second Trident visit in under a year. In spring and summer 2012, he was a Rosen Scholar, serving a research fellowship at LANSCE, the Los Alamos Neutron Science Center. LANSCE includes the Lujan Center, where a kilometer-long accelerator generates neutron beams for investigating materials, protein structures, nanomaterials and other subjects.

Some of what the Lujan Center does in a kilometer, Trident now does in a few millimeters, thanks to a collaboration involving Roth, Fernández and other researchers from Germany and from Los Alamos and Sandia National Laboratories. The 2012 experiments produced the largest neutron beams a short-pulse laser has ever made: An object placed a centimeter from the source would get a burst of neutrons at a density of $4 \text{ quintillion} - 10^{18}$ – per square centimeter per second. Those neutrons also move fast, with energies as high as 150 megaelectron volts (MeV, or a million electron volts). Conventional accelerator technology like that at the Lujan Center delivers many more neutrons but over a long period. That makes the two techniques complementary, Fernández says.

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.

Merrill's specialty is detectors to count neutrons and measure their energies. He and his colleagues develop sensitive diagnostics for the National Ignition Facility, or NIF, the giant laser built at Lawrence Livermore National Laboratory to implode tiny hydrogen-filled capsules and, if successful, trigger nuclear fusion.

NIF is in demand and shots are difficult and expensive, so routinely using the laser to test diagnostics isn't feasible. Merrill and his collaborators need a NIF stand-in: someplace that readily generates copious neutrons in a short pulse.

Trident, a neodymium glass laser, can deliver 200 trillion watts of energy in pulses as short as half a picosecond, a trillionth of a second. Roth says its reputation as one of the world's best short-pulse laser systems drew him to Los Alamos. Although he's a plasma physicist, "I had neutrons always on my mind" and worked on previous attempts to produce them with lasers. Older systems, however, weren't powerful enough to yield significant numbers or energies.

Merrill, of course, also had neutrons on his mind. Roth, after arriving at the lab last year, gave a seminar on his plans. Merrill caught him later in a hallway. The Los Alamos detector researcher needed a source for bright neutron pulses. The German visitor wanted to show lasers could provide them. A team assembled to find a solution.

Experiments at the Trident laser hit a thin, carbon-deuterium foil with an intense laser pulse, driving deuterium nuclei into a beryllium rod. The nuclei displace beryllium neutrons and also break apart, generating an intense neutron beam.

ON TARGET

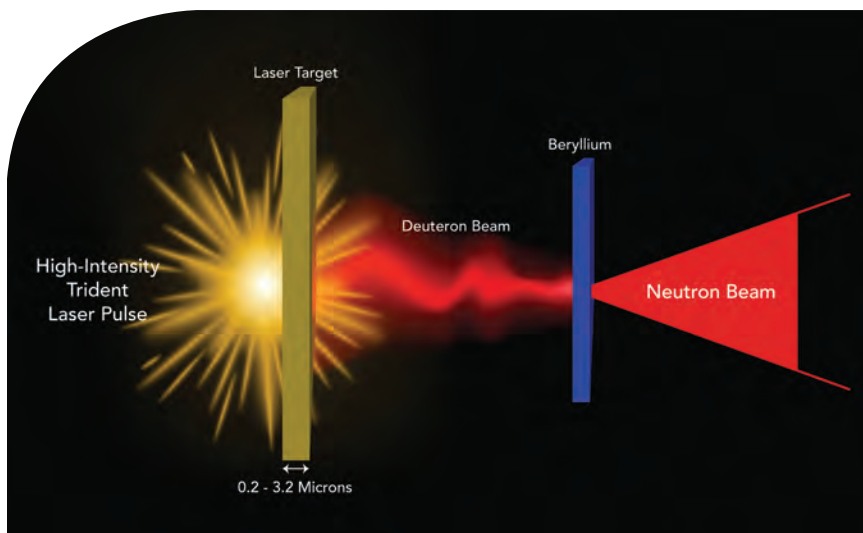
Fifty percent charge.

Compared to larger laser facilities, like NIF and the University of Rochester's Omega, research at Trident is more hands-on, Fernández and Roth say. Los Alamos technicians are involved, but the scientists themselves often work together to set up targets and instruments, "getting their hands dirty," Fernández says. Graduate students work alongside them to make as many shots as possible in a day. Roth adds, "To sum it up, we are having a party here." He laughs. "It's really a great team, but of course we are working hard."

For the neutron beam experiment, Trident targets a super-thin plastic foil. Few big lasers can use such foils because of prepulse – a weak but significant burst of light that heats or destroys the target before the main pulse can hit it. Trident is known for its high contrast, meaning the prepulse is negligible. "You can shoot targets that are very thin," Fernández says, so "you can move the whole foil at once, as opposed to a fraction." That helps to accelerate the resulting plasma ions to unprecedented energies.

The foil's other key property is its composition: carbon and deuterium, a hydrogen isotope that pairs a neutron with each atom's lone proton. The researchers focus Trident's beam tightly and fire it in just trillionths of a second, hitting the foil with 200 quintillion watts of energy per square centimeter, equivalent to focusing all the sun's light into a spot the size of a pencil's tip. The target is reduced to a plasma of electrons and deuterons – deuterium nuclei, comprised of one neutron and one proton.

The physics legerdemain that occurs next is vital to creating a powerful neutron beam without a giant linear accelerator. Most plasmas are opaque to lasers; they reflect the beam like a mirror. But under Trident's high intensity, plasma generated from the foil becomes "relativistically transparent," Roth and Fernández say. It



*Like a cue ball hitting a clump of billiard balls,
the deuterons send beryllium neutrons flying.*

starts when electromagnetic waves from the laser light push electrons into the target. The number of electrons available steadily decreases as they're pushed to the back of the foil.

At the same time, the laser intensity ramps up, Roth says. "The electrons have to oscillate in that electromagnetic wave. Because the intensity is so high, the electrons are accelerated to the speed of light, stop, accelerated to the speed of light, stop, at every cycle of the laser pulse." That means most of the time electrons are accelerated to near light speed.

Here's where Einstein steps in. Under relativity, electrons become heavy as they accelerate. With laser intensity increasing, they're no longer able to follow the beam "because to stop a very heavy electron takes a longer time than to stop a light electron," Roth says. In quadrillionths of a second, the electrons can no longer follow the electromagnetic waves, the foil becomes transparent and the beam passes. "Suddenly, the laser breaks through that foil and catches up with the electrons that are already pulling on the ions on the other side." The laser couples efficiently to all electrons in the volume, not just those on the plasma surface.

The researchers call this effect "breakout afterburner" – the laser breaks through the foil and transfers energy through the electrons to the deuterons, accelerating them in a burst. The linked proton and neutron slam into a shielded beryllium rod placed just 5 millimeters beyond the foil.

Beryllium atoms have a large cross section, meaning their neutrons have a high probability of interacting with incoming protons and neutrons. Like a cue ball hitting a clump of billiard balls, the deuterons send beryllium neutrons flying. Meanwhile, some deuterons break apart, generating additional neutrons, Merrill says. "You get some added oomph. What we found is you get higher-energy neutrons from that piece of the process."

The neutron beam could be even bigger, Fernández says, if the foils were pure or nearly pure frozen deuterium – an idea Roth plans to try later this year.

For Merrill and his detector-developing colleagues, the tough part was finding the neutrons amid the noise – X-ray and electromagnetic radiation byproducts. They sifted them with a time-gated system, essentially a high-speed shutter that opens after X-rays pass but before neutrons arrive. "We could find the sweet spot," admitting the neutrons of interest while "in essence, everything else was quiet."

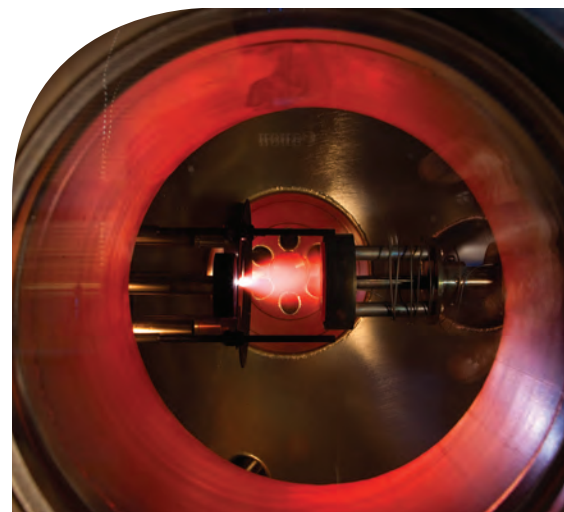
If anything, the laser researchers did their jobs too well, Merrill says, producing neutrons at energies greater than he and his colleagues need for NIF neutron detectors. (See sidebar, "Capturing Neutrons.")

ON THE PHYSICS EDGE

Seventy-five percent charge.

Before these experiments, Trident had never accelerated deuterium ions. "This whole relativistic regime is really the edge of the known physics," Roth says. But the researchers had some guidance: Theorists at Los Alamos' Computational Physics Division, including Brian Albright, Chengkun Huang, Lin Yin and Huichun Wu, predicted optimum target thicknesses for a given laser intensity. That helped the experimentalists generate neutrons on the first shot, not counting two others done to check alignment. "I knew Trident

A Trident shot as seen through a target chamber port. The laser is known for its high contrast, meaning it has little or no prepulse – a short, weak burst of light before the main laser pulse.



was a great laser, but I never would have dreamed that we'd get results on the third shot on the first day," Roth says.

Although far smaller than a linear accelerator, Trident still isn't portable because it's a multipurpose research facility. A system designed specifically to generate neutrons could fit on a truck, making the technology available for a range of research and practical uses, including stockpile stewardship experiments.

One use is flash radiography to assemble detailed movies of mass evolution over tiny time increments. With a neutron source firing 60-nanosecond pulses, Merrill says, researchers could string together freeze-frames of fast, dynamic events like how metal deforms under an explosive force. Because materials absorb neutrons at different energies, beams also could peer inside materials in ways X-rays can't. Neutron radiography tells researchers not only how much of a material is present – the mass – but also what kind of material it is – perhaps aluminum in one part and steel in another.

In a similar way, the high-intensity, high-energy beams Trident produces are suited for "active interrogation" – scanning containers to spot hidden nuclear materials, perhaps at ports and border crossings. Detectors could track particles and radiation emitted when a neutron beam passes through a container, providing investigators signatures of materials inside, says research team member Andrea Favalli, a scientist in Los Alamos' Nuclear Engineering and Nonproliferation Division. He's studying the Trident beam for active interrogation applications. Other such systems have been tested, says Favalli, a native Italian, including one he helped develop at the Joint Research Centre of the European

CAPTURING NEUTRONS

There already are neutron detectors at NIF, the National Ignition Facility, Frank Merrill says, but researchers need better ones.



In a sense, the instruments are like digital cameras. A camera with more pixels captures a finer image. A detector with better resolution provides a more accurate picture of neutron generation and distribution in NIF shots.

"NIF implosions are little tiny things," involving capsules of about 100 microns in diameter, says Merrill, team leader for the Advanced Imaging Group in Los Alamos National Laboratory's Physics Division. "You don't want to just see there's a neutron source 100 microns in diameter. You want to see some of the details inside." Top resolution now is about 10 microns and researchers are constantly investigating ways to improve it. "It would be wonderful if we got to 1 micron, but that's a fairly significant technical challenge," he adds.

With bright neutron sources like the one Merrill and other researchers developed at Los Alamos' Trident laser, detector scientists will have greater access to testing. But in some ways, Trident is too good. NIF typically produces neutrons with energies of around 14 megaelectron volts (MeV). The laser-driven neutrons at Los Alamos are up to 150 MeV. "It's nice to have the higher energies," Merrill says, but "we were interested in the sweet spot, kind of zero to 30 MeV."

Never fear: The scientists use a high-tech gating system – essentially a precise shutter – to filter out the speediest neutrons. Since they move faster, they arrive at the detectors first. Neutrons the scientists seek come a hair later – only after the "shutter" opens. "That gated system is how we were able to only look at the energy range we were interested in," Merrill adds.

Commission. Those, however, often relied on multiple measurements or measurements over long periods. The laser-driven beam could generate neutron signatures with a single rapid burst. "There are many, many possible applications and more are coming," Favalli says.

The current round of shots, in fact, is studying active interrogation. The team found that passing the beam through a depleted uranium sample clearly delayed many of the neutrons. Delayed neutrons is a signature of fission, indicating the presence of a nuclear material.

One hundred percent.

Shot 23-73 is complete. All areas are clear.

With that and many other shots, research on the Trident neutron beam continues. Many are part of Favalli's active interrogation project, but scientists also will study optimizing the pulse to produce neutrons with a specific range of peak energies, Merrill says. The researchers also will address fluctuations in the number of neutrons each pulse generates. [SS](#)

Bottling the Sun

BY EVAN DAVIS



Evan Davis

A metallic feminine voice rings out through the control room: ... *Three. Two. One. Zero. Entering pulse.* Dozens of scientists and engineers hold their breath and fix their eyes on the large computer display at the front of the room. A warm, guttural hum fills the air, the ground softly vibrates, and a flash of light appears on monitors throughout the room.

In fractions of a second, millions of watts of power heat dilute gas to 200 million degrees Fahrenheit, 10 times the temperature of the sun's core. At this temperature, the gas atoms are stripped of their electrons and their positively charged nuclei whiz by at 1 million miles per hour. Some of these nuclei smash into each other with just the right orientation and speed to fuse, forming an altogether different nucleus and releasing an enormous amount of energy.

The pulse ends almost as soon as it began. The gas cools, the glow fades from the monitors, and scientists scramble to analyze the data. *Ten minutes until next shot,* the voice states, reminding the researchers they must work quickly so they're ready to coax every last bit of performance out of their machine in the next experiment.

It's a typical day of operation at the Massachusetts Institute of Technology's Alcator C-Mod reactor, located down a humble side street in urban Cambridge, Mass. C-Mod is a compact nuclear fusion reactor designed to study the scientific and engineering challenges that must be overcome to make this technology a viable energy source.

Fusion is the energy of the sun and stars. Many scientists and engineers, including my MIT colleagues and me, want to bottle the sun for power generation on Earth. When fully developed, fusion will provide continuous power from abundant, virtually inexhaustible fuels, such as deuterium, a hydrogen isotope harvested from seawater. Fusion power plants will not directly produce any greenhouse gases. They also would produce no long-lived nuclear waste, and there is no risk of a meltdown or nuclear materials spreading for use in weapons.

Tokamaks like C-Mod are the leading candidates for successful fusion reactor designs. These doughnut-shaped vacuum vessels use powerful magnetic fields (2 to 3 Tesla, about the strength used in typical magnetic resonance imaging (MRI) medical devices) to suspend a plasma in space, preventing the hot core from touching any material walls. To prevent

melting the walls, the plasma temperature must drop from hundreds of millions of degrees in the core to a few thousand at the reactor wall, creating one of the largest thermal gradients in the universe.

Unfortunately, small-scale turbulence allows the plasma to leak through the tokamak's magnetic fields. Indeed, Nobel laureate Richard Feynman once described confining plasma within a tokamak as trying to hold Jell-O with rubber bands: it's possible, but it's taxing and you'll probably lose at least part of the Jell-O. A dozen or so scientists work on C-Mod with the express purpose of understanding and controlling this turbulence.

Researchers at C-Mod and several other tokamaks over the past two decades have identified several desirable operating modes that suppress these detrimental turbulent fluctuations. In particular, we've discovered that the potential fusion gain in tokamaks is strongly controlled by parameters in the last inch or so of the plasma's edge.

My colleagues and I are working to develop and test a first-principles computer model of this edge turbulence so that we can predict and optimize a device's performance before it's even built. Developing such a model requires a strong coupling between experiment, computation, and theory. That means you'll find me scrambling to set-up C-Mod's phase contrast interferometer before the day's experiments begin and fervently analyzing the measured turbulent density fluctuations between shots. In the evenings, I run edge turbulence simulations on the world's most powerful supercomputers, aiming to validate the code by comparing it with my experimental measurements. It's a long, arduous process, but this crucial element of physics must be understood if we're to advance to a viable reactor.

Fusion science has progressed exponentially since its inception, and we now stand poised to make a viable reactor for the first time. An international collaboration is constructing ITER, the first device expected to reach and exceed fusion breakeven – the point at which energy put into the reaction equals the energy it produces.

C-Mod is the only tokamak that operates at the same densities and heat fluxes as those expected in ITER, so it's thrilling to be here – and extremely important that our research continue.

The author is a third-year fellow at the Massachusetts Institute of Technology and this his winning entry in the 2013 SSGF Essay Slam.

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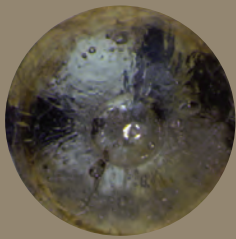
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SSGF PROGRAM

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TAW INSPIRING

The game of marbles reached its zenith in the 1950s and '60s, giving birth to the term "taw," for a glass sphere of exceptional quality. This taw – 2 millimeters across, much smaller than a standard marble – was made in the same era but is the hardest of all to come by: It's the byproduct of outdoor nuclear weapons testing. Lawrence Livermore National Laboratory scientists discovered that spherules like this one make good earthly stand-ins for primitive meteorites, which yield information about the chemical makeup of the early solar system. They also provide clues to the mixing processes right after a nuclear blast, offering a potentially powerful new tool in nuclear forensics. Further details appear on page 18.



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