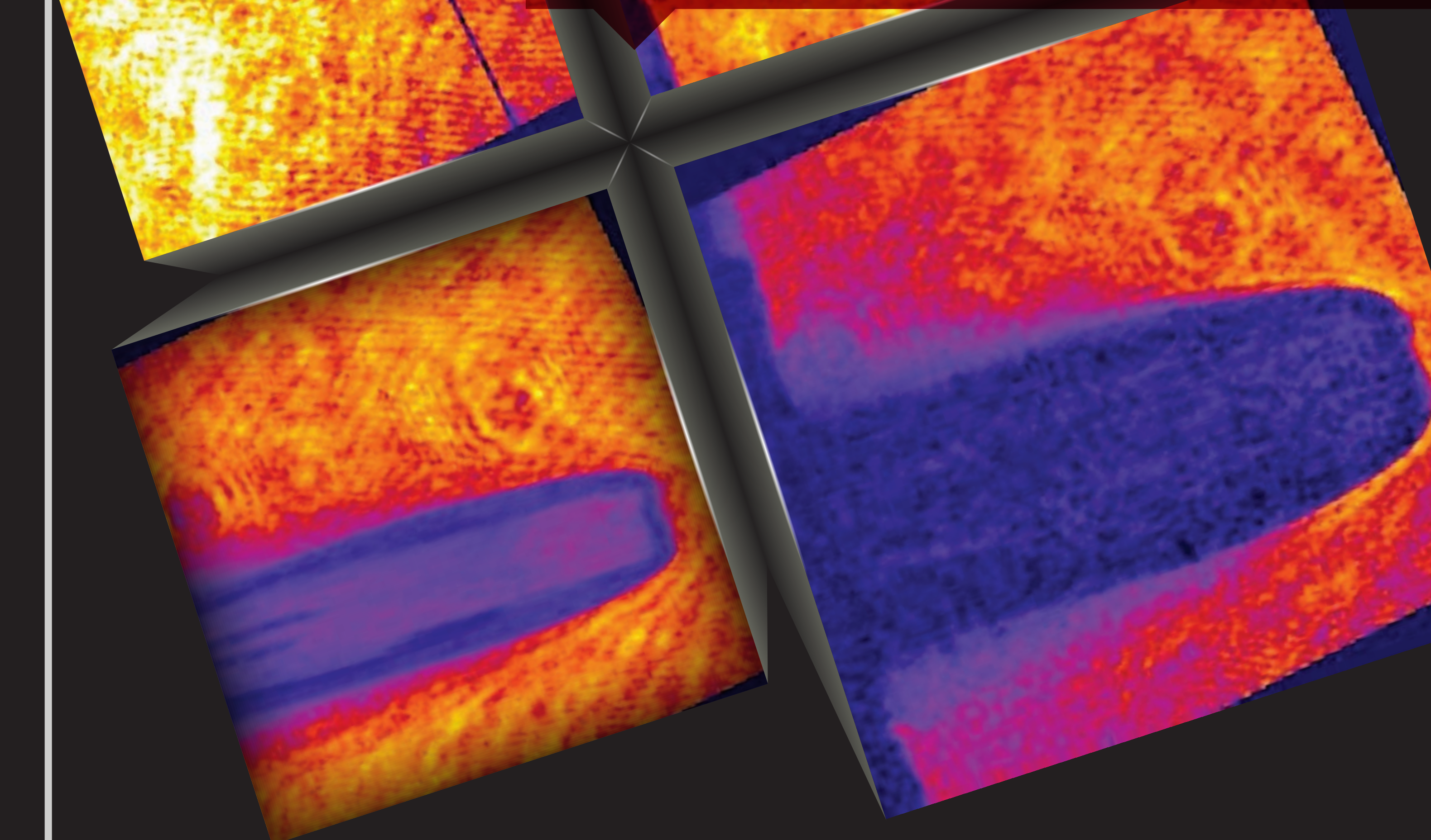
2018-2019

The SSGF Magazine

STEWARDSHIP SCIENCE



SEEING BETWEEN THE FRAMES

Sandia scientists' ultrafast cameras capture fusion's fleeting moments

Livermore: Machine learning informs experiments

Los Alamos: Printed metals make the grade

Plus: Many fellows, lots of locations; lab briefs: a Big Bang head-scratcher, Z's visionary lens, a building and its contents under extreme pressure; and NNSA's top scientist talks about research with a purpose

LETTER FROM THE EDITORS

A BIG Year

DURING ITS DOZEN YEARS IN EXISTENCE, the Department of Energy National Nuclear Security Administration Stewardship Science Graduate Fellowship (DOE NNSA SSGF) has never celebrated more outgoing fellows in a single year than 2018: 10. The graduating classes are usually about half that number, closely tracking the handful of new fellows admitted to the SSGF program each year. But sometimes a fellow, for various reasons, needs more time or less time in the program on the way to a doctorate and the research career that follows – often at a DOE NNSA national lab. The balances of final-year fellows can shrink (two last year) or swell accordingly. You can read accounts of this year's diverse record-setting class starting on page 4.

Elsewhere in this issue, we sample DOE NNSA lab stewardship science on the leading edge, from the mystery of elements cooked in the primordial soup ("Big Bang, Big Questions," page 5) to tough metals manufactured in surprising new ways ("Shattering the Metal Ceiling," page 20) and from our premier pulsed-power machine's beefed-up optic ("Z's New X-Ray Vision," page 5) to imaging much, much faster than the blink of an, um, just about anything ("The Fast Picture Show," page 10).

Not least, we allow the last word to Dimitri Kusnezov, NNSA chief scientist, who notes ("Conversation," page 24) that the NNSA labs "do science that makes a difference. … We can define how it will impact the world and the country. It's not for everybody, but if you want to make a difference, it could be for you."

– The Editors, *Stewardship Science: The SSGF Magazine*

2018 2019

STEWARDSHIP SCIENCE

DEPARTMENTS

COVER

FAST FACTS

Two ultrafast X-ray imaging cameras captured these frames, snapped at 2-nanosecond intervals, of a blast wave evolving in a laser-heated gas. Sandia National Laboratories researchers used the instruments to study the early stages of an experimental fusion technique. More on their work to accelerate imaging and document the previously unobservable begins on page 10.

SSGF

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 Program's Stewardship Science Graduate Fellowship (SSGF) program, which Krell manages for NNSA under cooperative agreement DE-NA0002135. Krell is a nonprofit organization serving the science, technology and education communities.

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FEATURES

IMAGE CREDITS

Pages 4-8 (portraits), Krell Institute; page 5, Alex Zylstra, Los Alamos National Laboratory (LANL); page 6, Philipp Mösta, TAPIR/California Institute of Technology; page 7 (olivine), Cameron Meyers; page 7 (lens), Sandia National Laboratories (SNL); page 8 (implosion), Alison Saunders; page 8 (target chamber), Collin Stillman; page 9, Lawrence Livermore National Laboratory (LLNL); pages 10, 11, SNL; page 12, National Ignition Facility; page 13 (device inset), SNL; page 13 (portrait and instrument), Randy Montoya; page 14, SNL; page 15, University of Texas at Austin; page 17, LLNL; pages 18, 19 LLNL; pages 22, 23, LANL; page 24, Krell Institute.

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This year's 10 outgoing DOE National Nuclear Security Administration Stewardship Science Graduate Fellowship recipients share their research experiences. For longer versions of their stories, see https://www.krellinst.org/ssgf/fellows/fellow-reflections.

Charles Epstein

ELECTRONS ON THE REBOUND

Charles Epstein focuses on the physics of electrons and other subatomic particles at the **Massachusetts Institute of Technology**. Working with advisor Richard Milner, he directs an experiment designed to better understand Møller scattering, when electrons collide and ricochet, generating radiation. It's important in experiments that track nuclei-electron beam interactions, especially in new high-precision, low-energy facilities where electron mass – often ignored in high-energy physics – becomes significant.

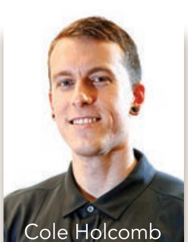
Epstein built software that simulates electron-electron and positron-electron scattering while accounting for electron mass, generating predictions of what detectors will record from the dispersed particles.

To check the code's results, he and his colleagues are developing an experiment at MIT's High Voltage Research Laboratory that will send electrons into a carbon target. Complex spectrometers will measure the energies and angles of electrons the collisions knock loose, helping pin down the effects of electron mass at low energies.

The project's demands have led Epstein to program his own software for data analysis and other purposes. He's even written code to help estimate gas flow and pumping power required for the near-vacuums the experiment requires. The team eventually will run the experiment on a low-energy device at Virginia's Thomas Jefferson National Accelerator Facility.

STORMING GALACTIC WINDS

Princeton University's Cole Holcomb's quest for fundamental understanding led him to study cosmic rays with James Stone and Anatoly Spitkovsky. His computer models track how these subatomic charged particles contribute energy to a galaxy's magnetic field, producing a particle wind that pushes out gas and inhibits star formation and structural evolution.



Cole Holcomb

His models inject simulated rays into a magnetic field running through the interstellar background plasma. The relatively sparse rays rarely collide with the plasma's gas particles but influence it via the field, pumping in energy and exciting waves.

If the fluctuations reach large amplitudes, the rays become trapped, inhibiting their ability to transport energy and momentum to the galaxy's outer regions. On the other hand, Holcomb says, "if this instability saturates at a low amplitude, cosmic rays escape the galaxy without affecting the interstellar plasma at all."

Holcomb's simulations suggest a third scenario, a sweet spot in which the excited waves resonate with the background plasma, losing energy as heat and limiting their amplitude so they efficiently drive galactic winds.

Holcomb will apply his approach to real-world astrophysical phenomena. It also may be useful for stewardship science applications.

RESPECTING LOCALITY

At the **University of California, Berkeley, Fabio Iunes Sanches** studies how gravity relates to locality, which arises from Albert Einstein's Theory of Special Relativity: Nothing moves faster than light, limiting communication between two points.

At the same time, however, quantum physics says an electron can be in superposition, simultaneously occupying two points. Quantum field theory unites these concepts and explains all particle interactions – except for gravity. Sanches studies this force as a holographic theory – three-dimensional at its foundation but organized to appear as if there's a fourth dimension.

Fabio Iunes Sanches

A cylinder, for example, has two dimensions, circumference and length, but the interior gives it a third dimension. Gravity in all those dimensions is "described by a theory that we say lives on the boundary, which is the circle and the long side, the time direction," Sanches says. "If there's gravity, then inside the cylinder I can imagine objects" such as black holes, stars or particles. "But if those things are inside, how are they secretly only encoded as a hologram on the boundary, which is one dimension lower?"

His research with Yasunori Nomura hopes to understand how it's possible for objects to respect locality if they're encoded in a lower-dimensional boundary.

Big Bang, Big Questions

The OMEGA target chamber, where Los Alamos National Laboratory's Alex Zylstra tests ideas about the birth of elements in the early universe.

The universe began nearly 14 billion years ago with an explosion: the Big Bang. It started out tiny and unimaginably hot, a burst of light and a swirling primordial soup of subatomic particles – neutrons and neutrinos, protons and photons, and electrons. As the universe expanded, during a small window called the Big Bang nucleosynthesis, or BBNS, hydrogen nuclei fused into heavier elements without immediately coming apart. Deuterium, helium and lithium were all produced a few minutes after the Big Bang; heavier elements came later, forged inside stars.

Today, researchers are investigating whether BBNS theory matches observations of these early materials. Although two isotopes of hydrogen and two isotopes of helium fit its predictions, lithium isotopes present a conundrum.

Lithium – a soft, silvery metal that forms two stable isotopes, lithium-6 and, as it's found most often, lithium-7 – is commonly used in cellphone and electric vehicle batteries. It can be used as nuclear fuel – and lies at the heart of the big BBNS puzzle.

"Our observations for lithium-6 don't seem to match the models of the Big Bang nucleosynthesis," says Alex Zylstra, a Los Alamos National Laboratory plasma physicist and alumnus of the Department of Energy National Nuclear Security Administration Stewardship Science Graduate Fellowship, or DOE NNSA SSGF.

Zylstra and colleagues have been using the Laboratory for Laser Energetics' OMEGA laser in Rochester, New York, to study this quandary, which has plagued nuclear astrophysicists for years.

At OMEGA, a stewardship science workhorse, lasers deliver large amounts of energy – about 30 kilojoules – in nanosecond bursts. That energy is absorbed in capsules just 860 micrometers in diameter – about the size of a pinhead – that contain fuel for fusion reactions. The laser energy crushes the fuel at high pressure for about 100 trillionths of a second, generating plasmas that can reach hundreds of millions of degrees Kelvin – conditions relevant in astrophysics. The fusion reactions ultimately produce gamma rays that can be analyzed to ascertain fusion-reaction rates.

Starting in 2013, Zylstra and his colleagues attempted to verify whether one instance of fusion that's thought to produce lithium-6 could explain the primordial soup mystery – specifically, whether hydrogen-3, also known as tritium, could react enough with helium-3 to produce lithium-6.

Using OMEGA, the researchers found that this reaction rate in compressed tritium-helium-3, derived from the gamma rays they detected, was far too low to explain the astrophysical observations of lithium-6 abundance in the universe.

"It turned out that we couldn't solve the mystery," Zylstra says. "But even being able to rule out one explanation is very valuable because it means the other ones are more likely to be true."

The differences in lithium-6 abundances continue to perplex Zylstra. "The nuclear physics behind it is pretty solid, but it can't explain these discrepancies."

One possible explanation may lie in how lithium is measured. Typically, astronomers analyze spectra from stars, hoping to catch the chemical signature for lithium-6. But it turns out that gauging lithium is tricky – turbulence in stellar atmospheres can throw off calculations.

Now Zylstra and his colleagues are looking at other reactions that could generate lithium-6, such as the fusion between two helium-3 nuclei, a reaction that generates half the energy in the sun. His team is following up initial research at OMEGA with experiments at the National Ignition Facility (NIF), at Lawrence Livermore National Laboratory.

The results from these astrophysics studies feed back into the main stockpile stewardship program at Los Alamos. Understanding gamma rays – produced by many nuclear reactions besides the fusion of hydrogen-3 and helium-3 – improves diagnostics and capabilities. "Obtaining better fusion performance is critical for our stewardship mission, and measuring gamma rays is a key way we gain insight into what happens on our current experiments," Zylstra says. "In fact, an instrument originally motivated by our astrophysics work is now being used for programmatic measurements on NIF."

– Wudan Yan

NUCLEAR PUMMELING ▶

Leo Kirsch, another fellow based at the **University of California, Berkeley**, collaborated on GRETINA, a detector for nuclear physics experiments that a Lawrence Berkeley National Laboratory team is developing. It uses germanium crystals and other equipment to precisely track the trajectories and energies of gamma rays emitted in nuclear reactions.

"That pathway tells you a lot about the emission properties of gamma rays" and the nuclei that produce them, Kirsch says.

He and advisor Lee Bernstein analyzed GRETINA data captured when protons struck targets of iron-56 (^{56}Fe) at Argonne National Laboratory. They found a surprising result with roots in the Doppler effect: When struck by a proton, an ^{56}Fe nucleus recoiled, altering the frequency of the emitted gamma rays. Kirsch and Bernstein found that as the recoiling nuclei stuck other nearby nuclei, they slowed and changed direction.


Leo Kirsch

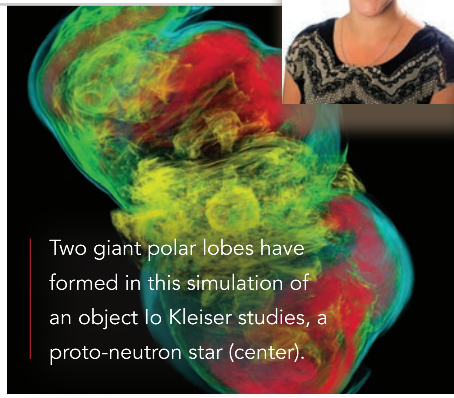
That information combined with proton data and the slowing-down theory of charged nuclei gives researchers a new tool to study nuclei, Kirsch says, helping them better understand how much energy it takes to knock a gamma ray, neutron or proton from a nucleus – vital to know when modeling nuclear reactions and possibly useful for stewardship science.

EXPLOSIVE FAST FADE ▶

The **California Institute of Technology's Io Kleiser** was drawn to supernovae because of their variety and urgency in a field that measures time in billions of years. An exploding star discovery gets immediate attention, and theorists like her try to develop models that explain data gathered from it.

She also explores supernovae as labs for high-energy and exotic physics. With advisors Sterl Phinney at Caltech and Dan Kasen at the University of California, Berkeley, Kleiser simulates stars that have lost all their outer hydrogen to see if some lead to unusual supernovae that fade within weeks.

She uses two codes: MESA, which evolves the stars up to the ends of their lives, and SEDONA, which calculates radiation transport through matter flying off the supernova and predicts what astronomers should see from the explosions. She wrote a hydrodynamics code that makes stars modeled with MESA explode and connects it to SEDONA.


Two giant polar lobes have formed in this simulation of an object Io Kleiser studies, a proto-neutron star (center).

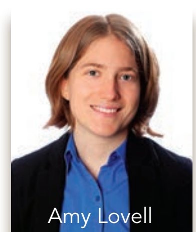
With multiple model runs, she and her colleagues have predicted how luminous and long-lasting a supernova should be under a particular set of circumstances. The results could help observers, theorists and modelers connect examples of this new supernova class to physical conditions that may have produced them.

UNCERTAINTY FINE-TUNED ▶

After a brief undergraduate foray into architecture, **Michigan State University's Amy Lovell** now studies theoretical low-energy reactions, particularly probing uncertainty quantification, or UQ: calculations of how much physicists can trust their reaction models. Without that knowledge, it will be difficult for them to interpret experiments designed to understand nuclear reactions involving heavier nuclei and less-stable isotopes.

Lovell and advisor Filomena Nunes found that much of uncertainty arises from data used to determine model parameters, perhaps because many phenomenological nuclear potentials are based on observations rather than fundamental evaluations of proton-neutron interaction.

Using Bayesian inference and Monte Carlo mathematical methods, they calculated differential cross sections for a range of heavy isotopes, including calcium-48 and zirconium-90, struck by deuterons at various energies and compared their results with data from experiments and a simpler UQ model.

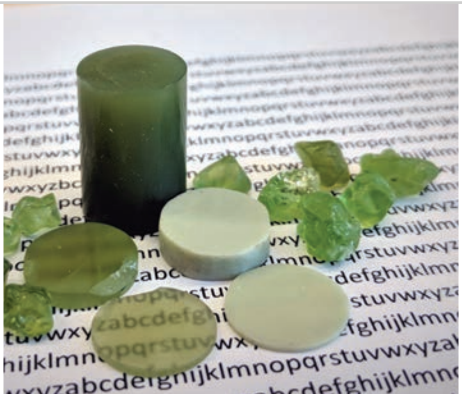

Amy Lovell

Previously researchers had assumed parameterizing interactions led to uncertainties of 10 to 30 percent. Lovell and her colleagues found it could be between 20 and 120 percent. They also found that reducing experimental error by half reduced uncertainty by only 30 percent.

Lovell says the results suggest that researchers should use different kinds of data when fitting models.

FAKE-ROCK STAR ▶

An insight the **University of Minnesota's Cameron Meyers** gained during his 2016 practicum at Lawrence Livermore National Laboratory led him to improve samples for the rock and mineral physics experiments he conducts with David Kohlstedt.



Olivine gems surround synthetic olivine samples. The transparent coin-shaped samples and the column at center were made with Cameron Meyers' evacuated hot-press process.

Meyers saw Livermore researchers use 3-D printing to produce transparent ceramic laser-gain media, material that boosts a laser's power. That made him wonder why the synthetic olivine he uses in small-scale experiments that emulate processes that occur deep underground is opaque rather than transparent like the gems they come from.

To make the samples, researchers pulverize olivine to a micron-scale powder then squeeze it under high pressures and temperatures. The resulting opaque samples meant something was scattering light that should have passed through. Tests found the samples contained tiny voids that can retard crystal grain growth.

With Kohlstedt and research associate Mark Zimmerman, Meyers developed evacuated hot pressing, which squeezes and heats the crystals while under a vacuum so contaminants and pore spaces are vented. The result: dense, transparent synthetic rocks that resemble the gem-quality starting material.

Meyers is using samples made with this new technique in his rock deformation research, trying to understand how their characteristics might change experimental outcomes.

TO FOIL THE FOIL ▶

At the **University of California, Berkeley, Alison Saunders** has worked with Roger Falcone and Lawrence Livermore National Laboratory's Tilo Doeppner to perfect X-ray Thomson scattering (XRTS) experiments.

In XRTS, X-rays are fired into warm dense matter, where they interact with electrons and scatter. Spectrometers measure how the emerging X-rays' frequencies changed, providing information about energy they deposited into the sample. That, in turn, offers details about the plasma's initial state.

XRTS has advantages over other diagnostics, but it's a difficult measurement to make. The probability of a photon scattering off an electron at a given angle is low, so it's often difficult to collect enough signal data. In addition, laser

Z's New X-Ray Vision

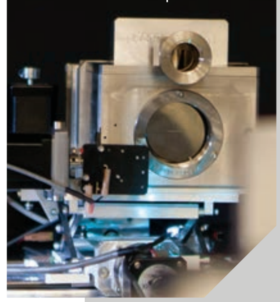
Sandia National Laboratories' Z machine uses massive electrical pulses to subject materials to conditions like those in a nuclear detonation, helping validate physics models for the nation's Stockpile Stewardship Program.

Z also happens to be the brightest X-ray source on Earth, notes Sandia's Jeff Fein, part of a large team from his lab and other research groups fitting the facility with a new X-ray lens.

"We can use the X-rays to study both the fundamental physics that generate them and to drive other experiments to study the effects of radiation on materials," explains Fein, a postdoctoral researcher in the Albuquerque lab's Pulsed Power Program.

To produce two-dimensional X-ray images of a target the size of an eraser, researchers have developed a Wolter optic – a hollow cylinder a couple of inches in diameter and half again as long.

The Wolter optic will shed more light on Sandia National Laboratories' Z machine experiments.



The optic is comprised of two barrel-like mirror surfaces – one elliptical section curved like an egg, the other shaped like a half hourglass – that focus Z-emitted X-rays to a point on a detector several meters away.

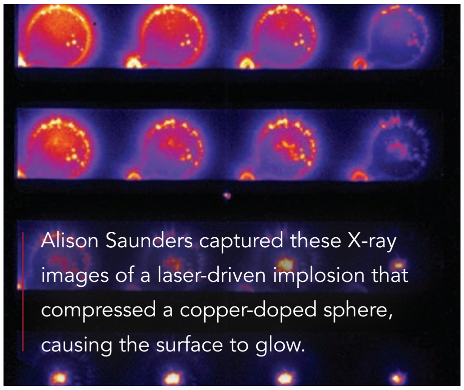
Z's previous optic captured X-rays passing through a tiny opening. The Wolter optic collects them over a wider range of angles and should gather several times more X-rays.

A Lawrence Livermore National Laboratory (LLNL) team is designing and calibrating the optic. Key collaborators include NASA's Marshall Space Flight Center (MSFC) and the Harvard Smithsonian Center for Astrophysics (CfA). MSFC is fabricating a mandrel, a metal substrate with a precision-machined surface that determines the X-ray mirror's shape and, ultimately, the image's quality. The mirror is coated with alternating, few-nanometers-thick tungsten and silicon layers deposited on the mandrel's surface. CfA is depositing and replicating the multilayer coatings from the mandrel.

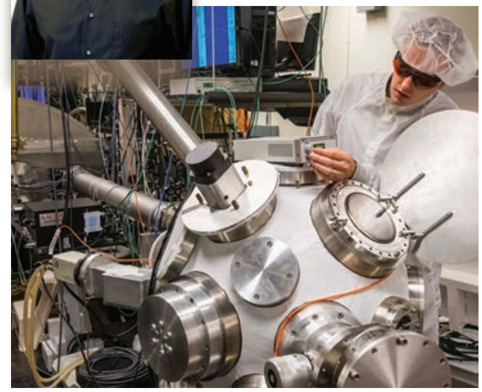
The mirror "lets us pick out a fairly narrow region of the spectrum of X-rays that an object" may emit, Fein says. "Knowing that the X-rays in our image came from a specific part of the spectrum helps us hone in on the specific physical processes that would generate" them.

Boosting the image resolution will help researchers "optimize the sources to ultimately make them even brighter."

– Tony Fitzpatrick



Alison Saunders captured these X-ray images of a laser-driven implosion that compressed a copper-doped sphere, causing the surface to glow.



Collin Stillman configures the target chamber for a plasma experiment at the University of Rochester's Laboratory for Laser Energetics.

facilities where experiments are conducted don't have powerful X-ray sources, so researchers must shine lasers on metal foils to produce bright X-rays.

"The problem is, plasma from that foil starts squirting everywhere," Saunders says, so experimenters must add shielding to block the instrument's direct view of the foil.

She's worked with multiple researchers to field experiments at the University of Rochester's Omega Laser Facility. What they learn can help benchmark computational models that attempt to predict properties of matter under extreme conditions.

PLASMA: THE MOVIE ▶

The **University of Rochester's Collin Stillman** taps powerful lasers at Rochester's Laboratory for Laser Energetics (LLE) to create miniature versions of the dense, hot plasma found inside stars and in other high energy density physics systems, letting him study their radiative and material properties. The data also help improve model predictions of these otherworldly phenomena.

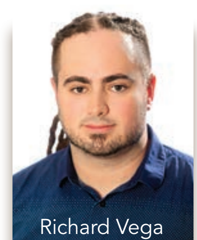
Stillman targets opacity, the degree to which these plasmas absorb radiation. It's difficult to calculate theoretically and experiments have struggled to provide high-quality benchmark data to compare with models.

In Stillman's experiments with advisor Dustin Froula, ultrafast bursts from LLE's lasers zap plastic foils sandwiching a slim metal layer. The foil heats before it can react, producing a dense, hot (as much as 3 million degrees Kelvin) near-uniform plasma. Ultrafast instruments record X-ray radiation emerging from the target, providing a brief one-dimensional plasma "movie." The data on how atoms and ions behave help researchers understand how radiation flows through dense plasma environments.

Besides conducting experiments, Stillman also has helped develop high-tech tools to record these fast radiation bursts and to track changing conditions over trillionths of a second. Interpreting the resulting data is challenging, especially determining which signatures correspond to physical processes in the plasma.

COMPUTATIONAL TIME-SLICER ▶

Once a high-school dropout, **Texas A&M University** fellow **Richard Vega** now is an intern at Sandia National Laboratories in New Mexico, where, with advisor Marvin Adams, he researches ways to solve the Boltzmann transport equation, a key to calculating nuclear reaction rates and other factors governing nuclear power and weaponry.



Richard Vega

In simulations, algorithms discretize the physical space being modeled into a mesh of cells for processing on a parallel computer. Vega focuses on the slice balance approach (SBA), which extends one-dimensional discretization to a three-dimensional configuration and combines it with linear discontinuous finite element discretization. The problem: As the algorithm sweeps through the domain, the resulting data exceed storage capacity, so every property must be recalculated with each of thousands of sweeps, wasting time.

Vega implemented the SBA on graphics processing units, reducing time spent on recalculation from 90 percent to around 5 percent. To overcome SBA's difficulties with discontinuities – domain irregularities that generate large changes in conditions and require added computation – he created sub-slices that allow them to propagate into downstream cells, improving the simulation's accuracy.

The extended SBA, as Vega named his technique, could be used to calculate particle transport in nuclear reactors, plasma physics and more.

Fire Within

The Stockpile Stewardship Program monitors aging weapons in the country's nuclear arsenal – and must ensure their safety and reliability without actually detonating any of them. Lawrence Livermore National Laboratory's Contained Firing Facility (CFF) is a key tool.

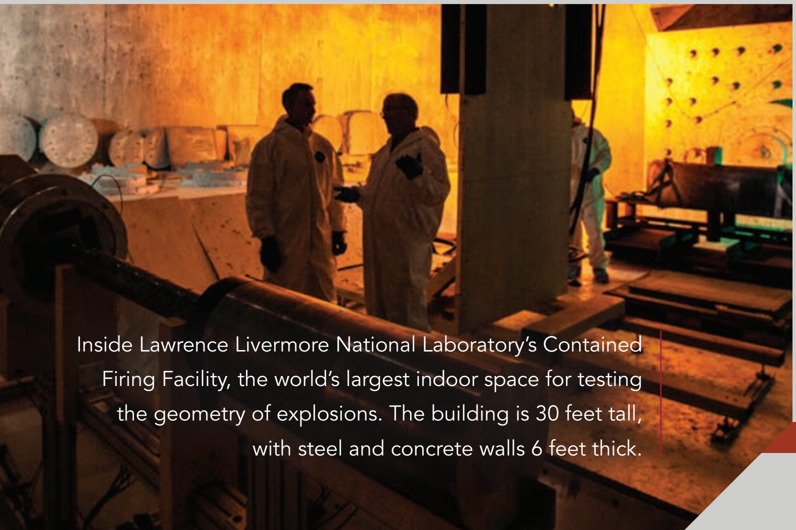
"Our job is not blowing up things, but collecting data," CFF manager Karen Folks says. "The data are all collected as the experiment goes boom."

The CFF is located about 50 miles east of San Francisco at the lab's Experimental Test Site, which began operations in 1955. By 1982, the facility had added a flash X-ray radiography (FXR) linear induction accelerator, which takes snapshots of explosion dynamics at an ultrafast, 55-nanosecond shutter speed. In 2000, LLNL scientists and engineers built the CFF around that device.

With a 50-by-50-feet base and at 30 feet tall, the CFF is the world's largest indoor firing chamber. Its nearly 6-feet-thick steel-lined concrete walls can contain the forces from as much as 132 pounds of high explosives without damaging the building or contaminating the surrounding environment. In many cases, those explosions come from weapon-geometry tests that include all components except the nuclear material.

CFF scientists use a variety of diagnostic and analytical tools to capture an explosion's nuances. The FXR captures wide-angle X-rays while half a dozen or more cameras operate at up to 2.5 million frames per second.

Digitizers collect the data and feed it to supercomputers for analysis. "It takes many small components to simulate a nuclear explosion," says Juliana Hsu, deputy director of LLNL's Weapon Physics and Design Program. "This requires information on material properties and many areas of expertise." Researchers then integrate information about material properties and other features into the models.



Inside Lawrence Livermore National Laboratory's Contained Firing Facility, the world's largest indoor space for testing the geometry of explosions. The building is 30 feet tall, with steel and concrete walls 6 feet thick.

The CFF also protects the surrounding environment. Although it produces some solid waste, "we have a pretty much zero-emissions facility," Folks says. CFF encloses all the gases, particulates and other potential contaminants created in a test. Air from a test is released only after passing through HEPA-grade filters and an acid-gas scrubber. "The emitted air is cleaner than the air that comes in."

Cleaning up after an experiment also uses 3,000 to 9,000 gallons of water. The facility filters the used water to remove all particulates larger than 2 microns, then stores it for reuse after future experiments.

Filters and other solid materials are considered low-level radioactive waste and can be disposed of in a designated landfill. Workers encapsulate test-explosion residue from chamber walls, enlisting techniques borrowed from the asbestos-abatement industry. Once the facility is cleaned and tested for lingering pollutants, other personnel in protective gear can enter.

How the experiment unfolds and how the system captures the data are crucial. "It doesn't do scientists any good to have a beautiful X-ray shot 20 milliseconds after they wanted it," Folks says.

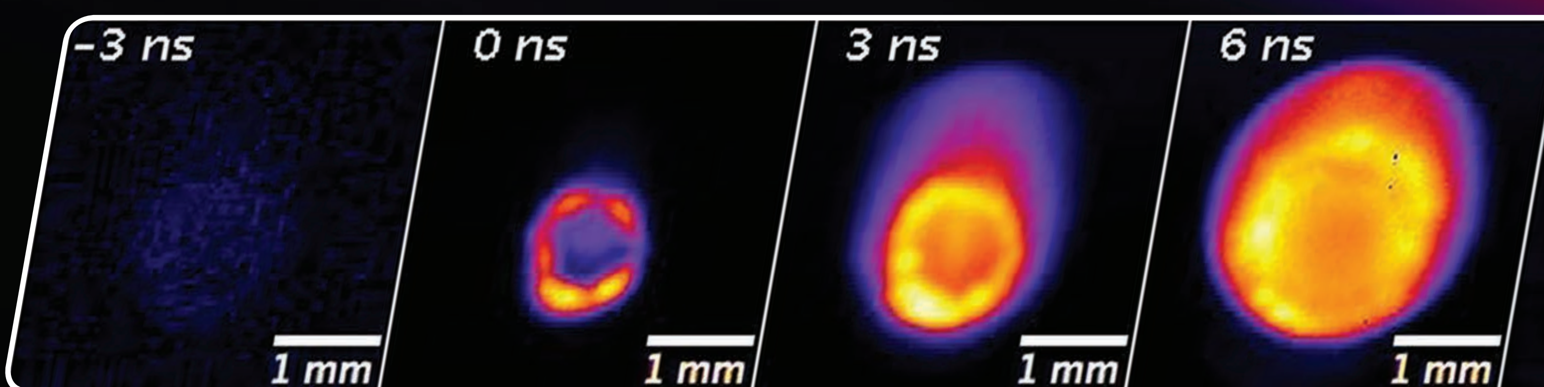
Just as CFF has improved on the FXR accelerator, the site continues to evolve experimental planning and execution approaches and add capabilities to keep pace with national security challenges.

For example, CFF formerly focused on one-off firing configurations, but the team now tries to set up simultaneous shots. "We have done up to four at once," Folks says, "and we can have a subset of experiments in each shot." In this way, the CFF team can gather more data in less time and at a lower cost.

To produce even more information, scientists are exploring ways to improve throughput from CFF instruments. For example, the current FXR produces single pulses, but the LLNL team is working on ways to do multiple pulses, which will provide multiple images in a test. Says Hsu, "Today we can get even better data on some aspects of warheads than we could before the nuclear-testing ban."

– Mike May

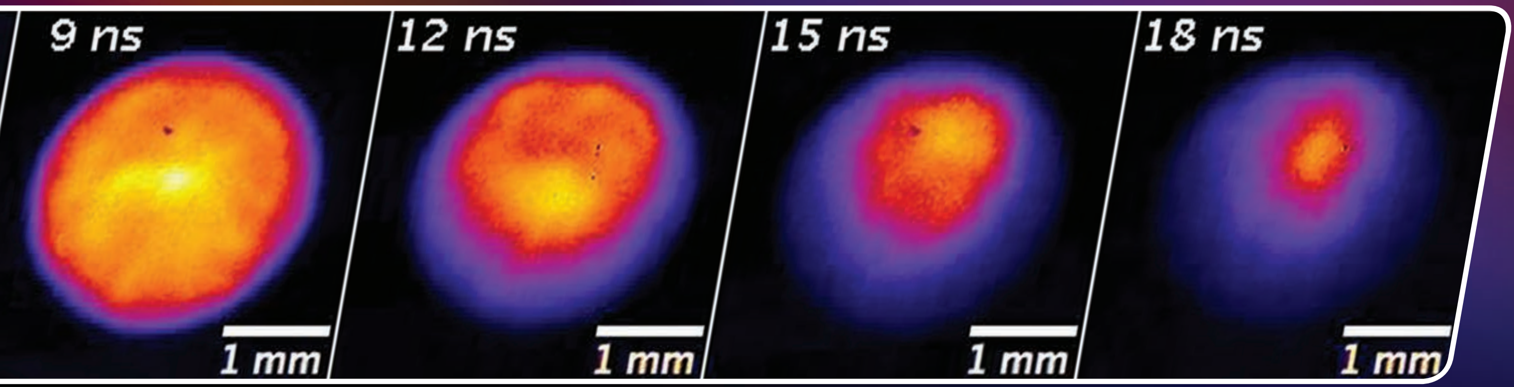
BY THOMAS R. O'DONNELL



A sequence of axial X-ray emission images, captured by an ultrafast X-ray imager (UXI), of a magnetized liner inertial fusion (MagLIF) experiment viewed from one end while Sandia's Z-Beamlet laser heats the cylindrical target. MagLIF is a promising technology researchers are pursuing to achieve ignition, the point at which the fusion reaction becomes self-sustaining.

THE FAST PICTURE SHOW

Sandia's hybrid imaging sensor could put moviemaking capacity in the hands of fusion researchers.



OUTSIDE HIS JOB as a technical manager at Sandia National Laboratories' New Mexico facility, John Porter occasionally served as videographer for his son's soccer teams. "He and his friends loved to replay the few moments of highlights," Porter says.

Similarly, Sandia scientists want to review critical moments of experiments – "to slow down and replay some fleeting event," Porter says. Soccer goal-shots can happen with lightning speed, but they may as well take centuries when compared to the tests, measured in billionths or trillionths of a second, conducted at Sandia and other Department of Energy National Nuclear Security Administration facilities.

Understanding what's happening in these evanescent events has always been difficult. The tiny and violent experiments explore the physics of fusing atomic nuclei or squeezing materials to pressures and temperatures found inside massive planets. But detectors haven't been fast enough to gather every detail. It's been like trying to analyze an imploded building's collapse with a camera that takes just one photo every 10 seconds: A lot goes on between frames.

"No matter what picture you take (you wonder) what happened either next or in between or before," Porter says. The missing information could help clarify the steps toward ignition – when a fusion reaction becomes self-sustaining – and why experiments don't perform as computer models predict.

After a 10-year quest, Porter and his colleagues have devised an elegant solution: a high-tech digital camera capable of snapping multiple frames in a span of nanoseconds (billionths of a second), each with an exposure as fast as 1.5 nanoseconds. The award-winning ultrafast X-ray imager (UXI) now is a key component in three generations of high-speed diagnostics for inertial confinement fusion, or ICF, experiments at the National Ignition Facility (NIF) at Lawrence Livermore National Laboratory.

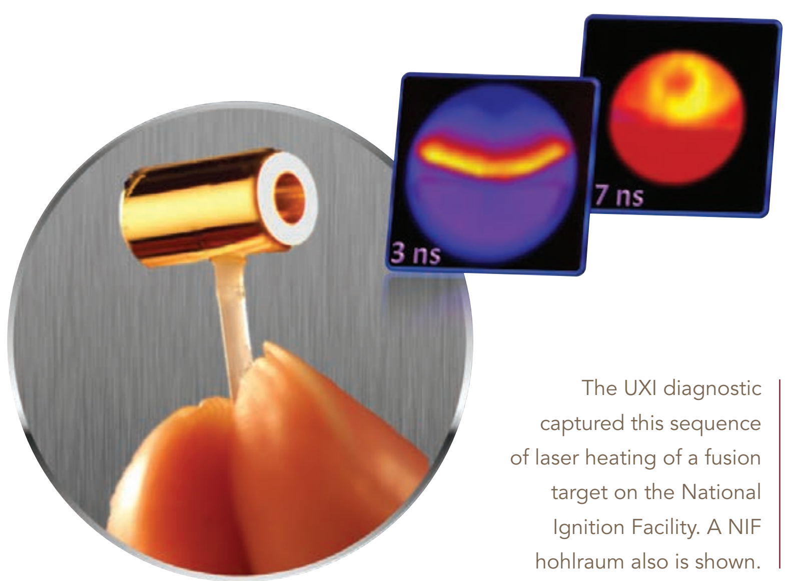
At NIF, 192 powerful lasers enter holes in the ends of a hohlraum, a gold tube about the size of a pencil eraser, heating it and bathing a peppercorn-sized, hydrogen-filled capsule in X-rays. If the radiation compresses the capsule quickly and symmetrically, the hydrogen nuclei fuse, releasing tremendous energy.

Sandia's Z Pulsed Power Facility, or Z machine, takes a different approach to ICF. It's named for the z pinch that squeezes plasma using magnetic fields from parallel currents flowing in the direction labeled as the z axis in three-dimensional plots. Capacitor banks deliver a thousand times the charge of a lightning bolt but in a time span 20,000 times shorter. In nanoseconds, the surge produces a potent, focused magnetic field that crushes tiny cylinders and compresses hydrogen isotopes.

X-rays are best to image these experiments, Porter says. They work like a dental radiograph: Rays pass through a sample, with some blocked by dense regions in the material to reveal hidden structure. At Sandia, the X-rays come from the Z-Beamlet Laser Facility, which Porter oversees.

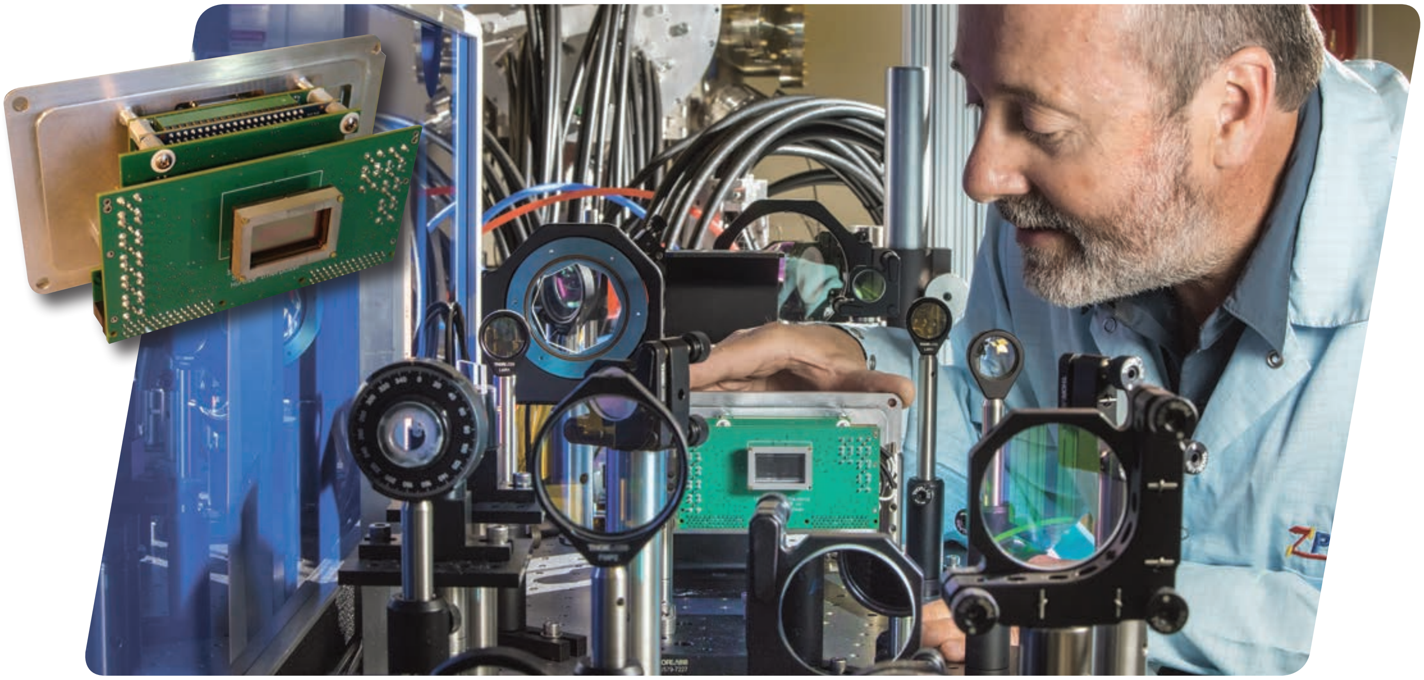
The z pinch itself produces radiation the laser X-rays must outshine. Detectors also must withstand a barrage of radiation, subatomic particles and explosive power. And because the most critical phase, when the plasma is contained before everything explodes, lasts 10 to 20 nanoseconds, "you'd like nanosecond resolution," Porter says.

The Z-Beamlet radiography diagnostic can capture just one or two time-separated images of pulsed-power experiments. Researchers want as many as 10 – enough, perhaps, to make short movies – but "there was no practical way using existing detector technology to do that," Porter says. Without a fast sensor, more images also would be blurred like a speeding car in a photograph.



The UXI diagnostic captured this sequence of laser heating of a fusion target on the National Ignition Facility. A NIF hohlraum also is shown.

Thomas R. O'Donnell is senior science editor for the Krell Institute. He has written extensively about research at the DOE national laboratories.



Sandia's John Porter sets in place a multiframe UXI in the lab's Z-Beamlet Laser Facility. Inset: The UXI with shielding and electronics. The rectangular object on the nearest circuit board is the UXI sensor.

Scientists had one promising approach: solid-state detectors called silicon photodiodes. When visible light or an X-ray hit the device – smaller than a square millimeter – it sent an electric current to a transient digitizer, a high-tech oscilloscope that recorded the time history of the generated voltage.

"They were beautiful detectors," with great sensitivity and time response, Porter says, and inexpensive. The digitizers, though, cost tens of thousands of dollars. "You ended up only fielding a handful of photodiodes on an experiment."

Porter and his colleagues suggested that if specialized integrated circuits – in essence, microchips – replaced the bulky digitizers, researchers could create a sensor with a million photodiodes, similar to a megapixel in a digital camera. In the early 2000s Sandia opened MESA, the Microsystems and Engineering Sciences Application facility. The microchip-making installation investigates electronics for refurbished nuclear weapons, but its manager at the time, Donald Cook, also sought projects to meet other missions.

Porter proposed the photodiode-integrated circuit merger. Building on technology developed to capture particle collision data at Europe's Large Hadron Collider, MESA microelectronics engineers, led by Marcos Sanchez and Liam Claus, began 10 years of research. "We knew it would work at a one-pixel level," Porter says, but "would a million pixels work in the Z environment?"

The UXI is a hybrid: Nearly half a million photosensors, each 25 microns (millionths of a meter) square, are directly connected to individual readout electronics in the radiation-hardened integrated circuit. Altogether, the sensor array is 25 millimeters by 11 millimeters – about an inch by a half-inch. In essence, each sensor-circuit pair is a pixel in a 448-pixel by 1,024-pixel digital camera. The UXI's electronics can be tuned to convert a range of radiation – visible light, X-rays, electrons, ions or neutrons – into electrical current. The individual pixel circuits capture and store the current for later readout.

Scientists can program how long the signal is recorded, letting them adjust the exposure time and time between frames in a range from billionths to thousandths of a second. Early UXI sensors stored two frames, but a recent iteration called Icarus 2 can operate each half of the sensor as two independent cameras, capturing up to eight frames in a 16-nanosecond experiment. With improved fabrication technology, Porter says, the exposure and time between frames could be reduced to less than a nanosecond.

The UXI's performance and low cost earned it recognition from R&D Magazine as one of the top applied technology advances of 2016. The sensor also earned the magazine's Market Disruptor Product Special Recognition Award.

NIF researchers incorporated the UXI into the gated laser entry hole (G-LEH) imager to capture the hohlraum interior during fusion experiments. Previous instruments "could take only one image that was over the entire temporal history of an experiment, from beginning to end, all overlapped," says Nathan Palmer, a NIF target diagnostics engineer. Those static images suggested that, as simulations predicted, the plasma's shape changed significantly during the implosion but provided little information on how. "We couldn't see the dynamic change."

The G-LEH, in contrast, takes two images per experiment with 2-nanosecond exposures. "The snapshots still aren't quite as fast as we would like," but even so, Palmer says, "we can start to see the difference in the plasma shape from the beginning of the experiment to the middle to the end." Scientists are comparing the data against simulations to better understand plasma evolution and improve modeling.

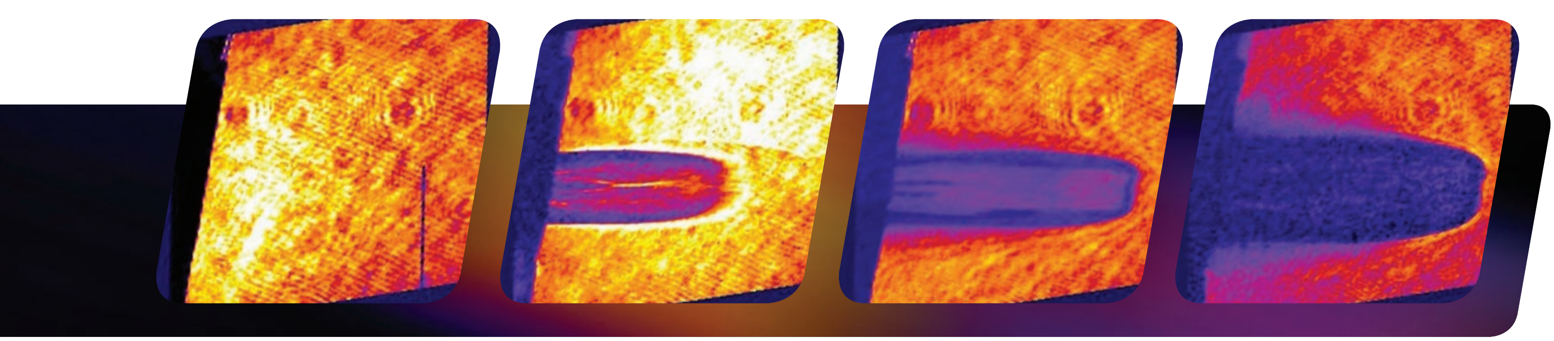
The UXI in G-LEH, called Furi, had been slated for a quick upgrade, but it's still in use as work on other instruments has taken precedence. "Our little instrument that was supposed to be a prototype running for six months or so has now been running" for nearly three years and hundreds of experiments, Palmer says, chuckling. "It's really become a workhorse diagnostic." Its replacement Icarus sensor, in testing, will capture four more closely-spaced frames per experiment with a slightly faster shutter speed and higher X-ray sensitivity.

That's good enough to capture plasma evolution but still too slow to image other critical aspects of NIF implosions. As in z-pinch shots, the final stages of these reactions are vital but a thousand times faster.

"The whole burn width of an implosion at NIF is about 100 picoseconds," says Terance Hilsabeck, a science manager for contractor General Atomics. Held in place by the inertia of the imploding capsule, the fuel stagnates – squeezed to a tiny volume, with pressures and temperatures similar to a star's interior, producing a hot spot of fusing nuclei. "Once you have this hot plasma in the middle, you need to keep it there for a while so it will burn" and produce energy before rapidly rebounding in an explosion. If the compression isn't symmetric, confinement time will be limited, reducing burn and energy yield.

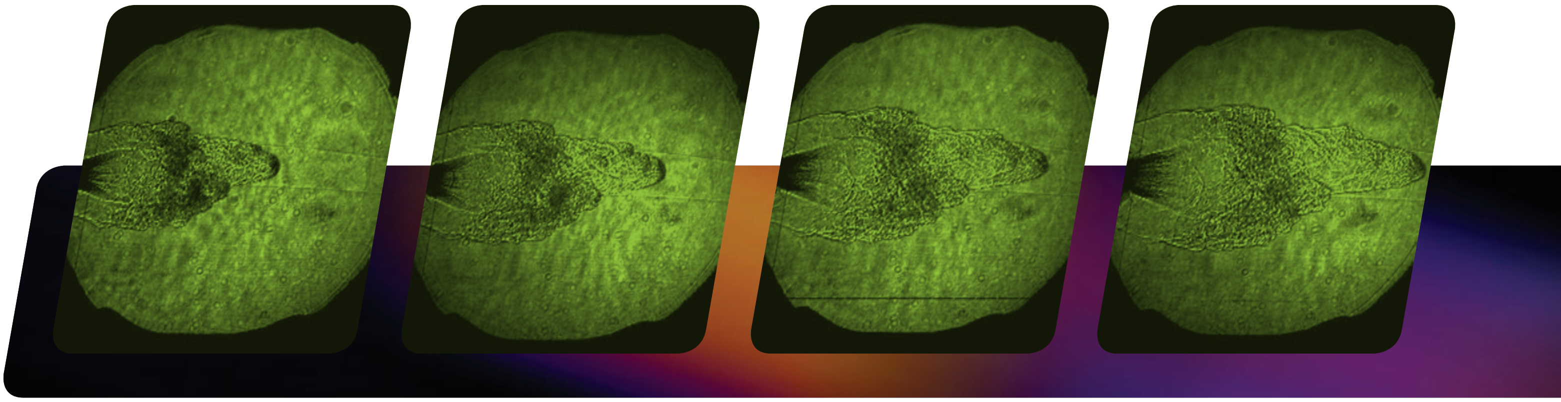
More data are needed to understand why hot-spot formation hasn't worked as simulations have predicted – if instruments can capture them. "You need 10-picosecond resolution," Porter says, and for the UXI, "that's a huge stretch." Light can travel about a foot in a nanosecond; it goes only about a quarter of an inch in 25 picoseconds.

Scientists with British company Kentech Instruments had one idea to get detectors up to speed: the pulse-dilation electron tube, which Hilsabeck describes as "a zoom lens in time" that stretches a signal's temporal information so a slower-speed camera can record it. Light, including X-rays, from an experiment strikes a photocathode, which converts it to electrons. An applied voltage accelerates the electrons but is ramped up over picoseconds so each has a different velocity. The electrons drift down a tube toward a camera



Four images taken at 2-nanosecond intervals by two UXI cameras show the evolution of a blast wave in laser-heated gas. The images provide insight into the early stages of an experimental fusion technique at Sandia.

UXI image sequence of a laboratory astrophysics experiment on Sandia's Z-Beamlet Laser Facility, conducted by researchers at the University of Texas at Austin. The experiment was designed to create and analyze radiative blast waves scaled to reproduce the dynamics of a supernova remnant.



for recording, spreading out and stretching the signal that reaches the detector. The longer the tube, the more the signal is extended, turning a picoseconds-long electron burst into a nanoseconds-long pulse that's easier to capture.

Hilsabeck and Livermore scientists collaborated with Kentech in the late 2000s to deploy the drift-tube technology in the dilation X-ray imager, or DIXI, on NIF. It can capture frames with exposures as short as 5 picoseconds, but its spatial resolution is limited to 10 microns – tiny, but not minute enough to clearly capture needed detail. Imploding material and plasma "move at such a velocity that they blur over 10 microns," Hilsabeck says.

Another disadvantage: DIXI can capture only one frame per experiment. The UXI can capture several but isn't fast enough for experiments measured in picoseconds. The solution, arrived at via a collaboration connecting Sandia, Livermore, General Atomics and Kentech, was to connect DIXI's pulse-dilation electron tube to UXI's hybrid sensor.

The pulse-dilation electron tube "changes the whole landscape," Porter says, turning a 10-picosecond exposure into a nanosecond-scale pulse "that's ideal for our detector. The two together are really powerful."

After four years of work to overcome technical challenges, the team produced the single line-of-sight X-ray imager, or SLOS, in late 2016. The name means it records multiple frames through time of a single image cast on the diagnostic, rather than capturing multiple images cast from slightly different vantage points – often from repeated runs of the same experiment.

The first SLOS imagers were tested on OMEGA, a powerful laser at the University of Rochester's Laboratory for Laser Energetics, and at NIF. Neither was designed to withstand the highest radiation produced in ICF experiments. NIF technicians are now testing a SLOS that adds a curved crystal X-ray optic that will form a narrow-band backlit image of the target capsule with improved contrast and resolution. That instrument, called SLOS-CBI, has limited radiation tolerance and will be used on low-yield NIF shots. A third version, hardened SLOS, should be ready next spring for use on high-yield experiments.

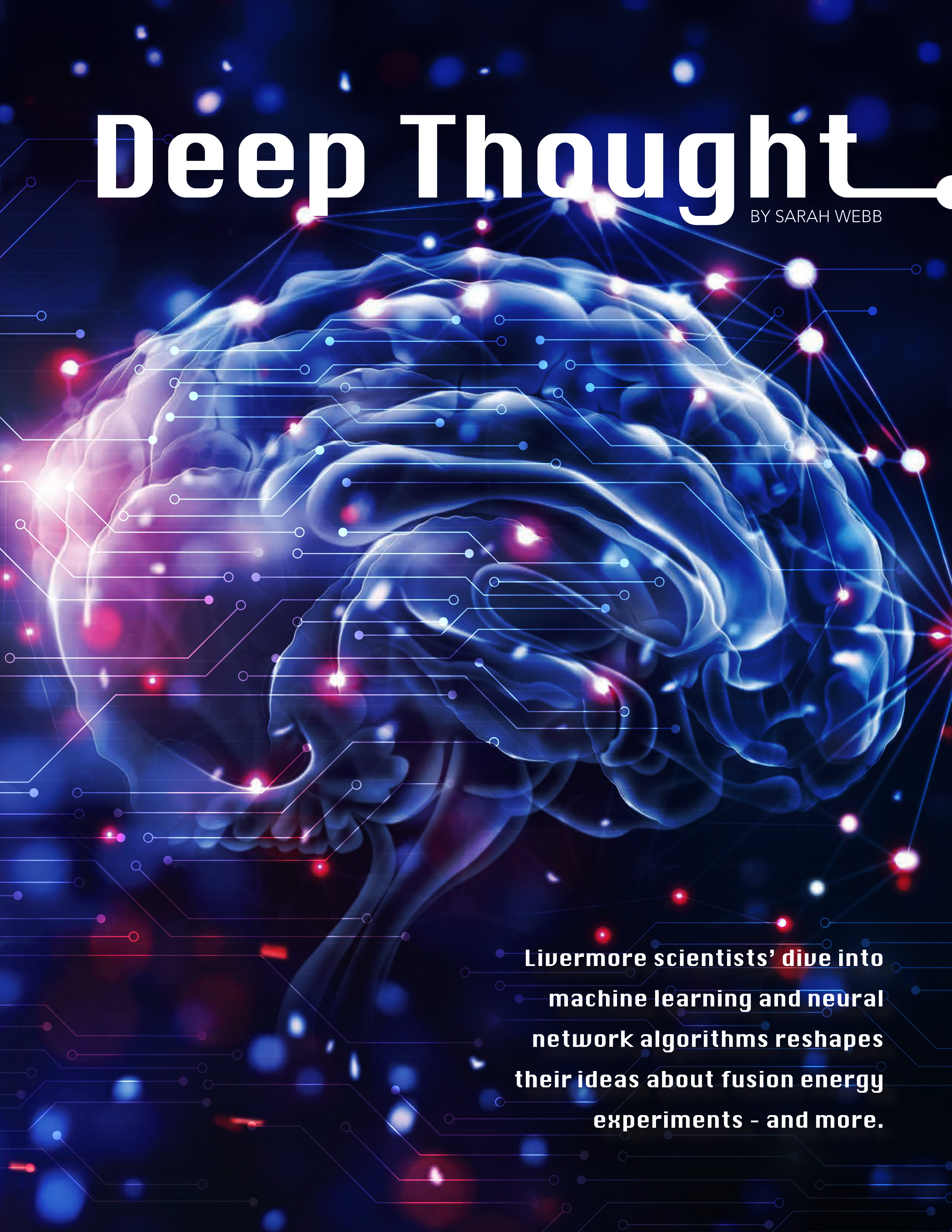
The hardened SLOS will have two UXI sensors, each with two hemispheres that can take four images for a total of 16 20-picosecond frames per experiment. That will let researchers make an implosion movie to monitor hot-spot growth, shape, debris intrusion and other reaction phenomena, Hilsabeck says. Combined with the crystal backlighter, "we're potentially in the position of seeing this late-time shell symmetry that we haven't been able to see before. It could be a big lever on performance."

The UXI and SLOS have yet to achieve their full potential, Porter says, and are on the cusp of helping realize a major advance. For example, researchers could simultaneously field several of these high-speed digital cameras from different viewing angles to produce three-dimensional images of experiments similar to CT scans in medical imaging.

"I'm proud that we're visualizing phenomena that's in many ways never been seen before," he says.

Deep Thought

BY SARAH WEBB



Livermore scientists' dive into machine learning and neural network algorithms reshapes their ideas about fusion energy experiments – and more.

FROM SMART PHONES to driver-assistance systems, artificial intelligence tools are transforming the technology that powers our everyday lives. But these machine-learning algorithms are not only reshaping consumer gadgets; they're also changing how researchers approach scientific questions in high-energy physics and many other fields.

Over the past five years, the newest flavor of machine-learning algorithm, known as deep learning, has come on the scene. Largely developed commercially, these tools can help with a range of optimization problems, and researchers use them to tweak complex systems for new and better solutions.

At Lawrence Livermore (LLNL) and other national laboratories, "we're picking up these tools and we're turning them around onto our stewardship science problems and our physical science problems," says Brian Spears, an LLNL physicist. "We're using them in ways that were not originally intended, but ways in which they're extremely successful."

Since the United States ended nuclear testing more than 25 years ago, stockpile stewardship at LLNL and the Department of Energy's other National Nuclear Security Administration labs has integrated simulations and experiments to understand the high-energy physics of nuclear materials and assure their safety, security and efficacy. To develop predictive computational models, physicists simulate processes and compare results with experimental data. When those outcomes don't match, the researchers go back to examine the code and the physics. By tweaking parameters in computational models to produce results that align with an experiment, scientists explain the discrepancies with hypotheses they can test via future experiments and simulations. This iteration among hypothesis, simulation and experiment helps researchers improve underlying physics models.

This approach has necessitated making one change at a time, Spears says, and can bump up against natural human limitations. These complex computational models can include so many parameters and interactions that even the most skilled physicist can struggle to consider them all at once.

Livermore researchers have recognized that deep-learning algorithms could save a lot of time in addressing these problems, says Katie Lewis, LLNL's Applications, Simulations and Quality (ASQ) division leader. These algorithms allow scientists to survey many complex potential interactions collectively. The algorithms can make small changes to many parameters quickly, often providing a novel combination that matches experiments well.

Spears characterizes the approach as something like a robotic exoskeleton a future firefighter might wear to lift a beam off someone trapped in a burning building. Just as technology can boost a firefighter's strength, machine learning can allow a physicist to explore and navigate a terra incognita of complex interactions. "Machine learning is something like a wrapper for the simulation. I run all of my simulations, and the machine-learning code learns what the simulation thinks about the world. It gives me the lay of the land."

Recently, Livermore physicists used machine learning to glean an unexpected insight into a problem in inertial confinement fusion (ICF) experiments at the lab's National Ignition Facility (NIF), where an enormous network of lasers focuses energy on a tiny gold oven known as a hohlraum.

Inside is a high-density carbon capsule no bigger than a peppercorn that contains reaction fuel, a mixture of the hydrogen isotopes deuterium and tritium. As NIF's lasers heat the hohlraum, it blasts radiation onto the surface of the capsule and it implodes. Pressure and temperature skyrocket as the capsule compresses down to 30 times its initial radius. The reaction fuel heats and densifies, spitting out neutrons. The aim is to reach ignition, a point where the energy created by thermonuclear reactions outstrips all energy losses in the implosion.

Livermore physicist Luc Peterson compares the fusion challenge to a person compressing an inflated balloon by hand. Without applying enough force evenly on all sides, the capsule's contents can bulge out instead of collapse inward. To reach ignition, NIF physicists thought they needed to apply radiation pressure symmetrically, in the shape of a sphere. But perfect symmetry is difficult to achieve, so the system also needs to be resilient enough to account for asymmetries – factors that lead to imperfections in the implosion.

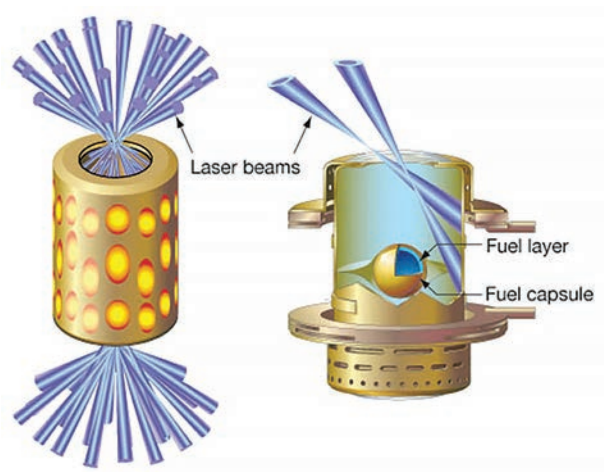
Livermore's Sierra supercomputer.

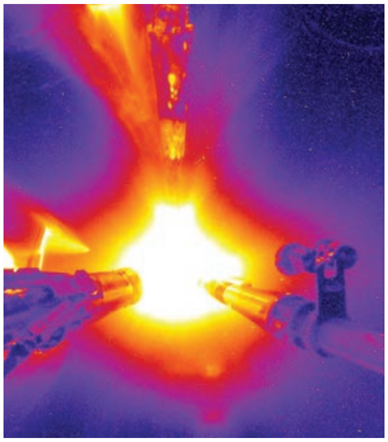
Small changes in energy flow or microscopic flaws in the capsule can throw off an experiment. The NIF team wanted a way to make these systems resilient to subtle variations while keeping the reactions as efficient as possible.

When they started work on these questions, Peterson notes, physicists suggested many solutions, based on their scientific training and intuition. Ideas included making the capsule bigger or changing the laser pulses. Peterson wanted to use computation to survey the options.

Peterson began by designing a run of 60,000 different simulations on the Trinity supercomputer at Los Alamos National Laboratory. Those produced five petabytes of raw data, approximately 33 times the entire content of Apple's iTunes store. Even after initial processing, the data still exceeded 100 terabytes, a huge mountain to overcome. Peterson didn't have the tools to examine all the possible solutions.

That's where machine learning came in. Kelli Humbird, a Texas A&M University graduate student working at the laboratory, built a computational model that helped begin to navigate those simulations. The researchers had two primary questions: Could they find an area within this enormous set of simulations that coped well with asymmetries? And would it lead to a solution they wouldn't have found otherwise?





Above: A gold cylinder known as a hohlraum, the target of the National Ignition Facility's 192 laser beams in inertial confinement fusion (ICF) reactions. Right: An ICF implosion (colorized). Livermore physicists are using machine-learning algorithms to improve these experiments' resilience and efficiency.

The surprising answer came quickly. Instead of an expected spherical compression, the model suggested that pushing on the capsule in an asymmetric ovoid, or egg-shaped, way would be most resilient. The neutron yield was slightly lower, Spears says, but the approach protected the experiment against perturbations from non-uniform X-ray radiation or imperfections in the capsule surface. "It generated something like a flow-driven armored plating that protected the implosion," Spears says.

The team didn't trust the results at first. "No. Wait, no," Peterson remembers thinking. "That's just not right. It has to be round." But the results have held in further simulations, and the scientists plan to test them experimentally. The project taught the team two important lessons, Spears says. "One, our biases can hold us back sometimes. Two, this tool does help us navigate those high-dimensional parameter spaces in a way that would've been really difficult in the past."

To analyze the ICF simulation data, Humbird and Peterson had started with a machine-learning model called random forests, in which programmers devise a map of decision trees to process the data. Building the model is easy, Peterson says, but the results can appear coarse and blocky like a patchwork quilt.

To refine their results, Peterson encouraged Humbird to study neural networks, a computational model designed to loosely mimic how neurons work in the brain. These algorithms form the basis of deep-learning tools. To make predictions, the algorithms first train by analyzing large data sets while defining and refining their own structure. The process is like kneading butter and flour to make pastry, Spears says. "They get stretched and folded, croissant-dough style, and they get mixed and matched until they come up with what we might call a really representative space." All without a baker; no programmer intervention is required. The algorithms incorporate information about the data they're processing and use that to create and optimize the neural network.

Unlike decision trees, however, good neural networks are not always easy to construct, with many parameters that must be chosen. To simplify the problem, Humbird used TensorFlow, Google-developed open-source software, to build an algorithm

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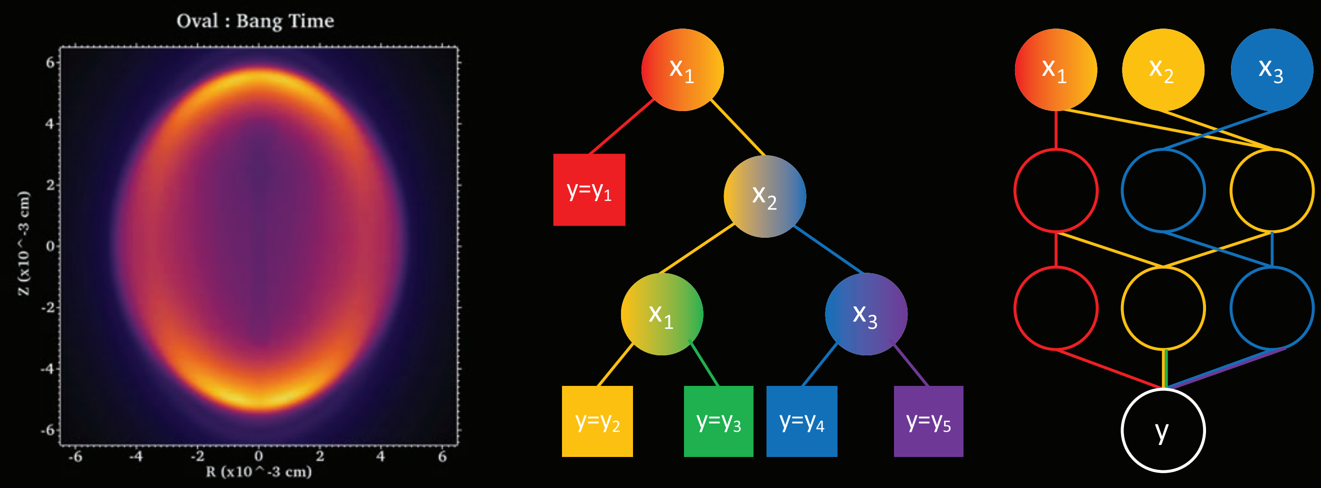


Left: A density map of a novel inertial confinement fusion (ICF) implosion design, via a machine-learning approach physicists used to explore optimal experiment designs. The egg shape defied conventional wisdom that favored spherical implosions. Center and right: At center is an algorithm type called random forests that produced the egg-shaped model above. The diagram on the right is a schematic of the neural network used in deep jointly informed neural networks, or DJINN – Arabic for genie. Among other tasks, DJINN boosts accuracy and calculates the uncertainty in its predictions.

that turns decision trees into neural networks, thereby eliminating the need to choose a good set of parameters. When the researchers tried the approach on the ICF data, it was up to three times more accurate than what they'd used to find the ovoid strategy, Peterson says.

They named the algorithm deep jointly informed neural networks, or DJINN – Arabic for genie. Besides boosting accuracy and calculating the uncertainty in its predictions, this algorithm is also good at handwriting recognition and other, wildly different analysis tasks. It's easy to tweak for other applications, Peterson says.

Neural networks can boost laboratory efficiency in other ways, Lewis says. The ICF project has shown that these algorithms can help physicists seek solutions to problems by new and more productive means. DJINN is also computationally faster and more compact than its predecessor algorithm – trainable in five minutes while occupying just a few hundred kilobytes of memory, compared with 45 minutes and 300 megabytes for a traditional decision tree-based uncertainty model.

Neural networks are still computationally intensive and use hardware differently, but researchers can optimize performance by matching processor types to the appropriate task. Newer supercomputers such as LLNL's Sierra include both central processing units (CPUs) and graphics processing units (GPUs). Although GPUs are ideal for training neural networks, they require more resources to run. Once networks are trained, researchers can transfer the question-posing process to less intensive processors. One such emerging technology is known as a neuromorphic processor.

LLNL has been testing one version of these new chips, IBM's energy-stingy TrueNorth. The chip uses just one ten-thousandth of the power that a GPU does for similar problems, Lewis says. Matching computing resources to specific problems on Sierra, a 10-megawatt system, could cut energy use and help researchers allocate its computational resources efficiently, she says.

One ongoing challenge across all applications: The results from a neural network like DJINN can seem like magic. The algorithms provide predictions, often the right ones. But within all those computational layers, users don't always understand how they work, Spears says. "I really need to understand what this process is doing for me so that it's not just a black box."

Livermore and other national laboratories could assist industry with its research on deep learning, Spears says. Unlike self-driving cars or language recognition, hard sciences like physics rely on mathematical theory and equations to support their experimental results. As such, the LLNL team can directly compare the mathematics their neural networks use to process physics data with the fundamental equations of physical theory to see if they're consistent or differ in important ways.

Livermore also has large physical science data sets – core information that could be fundamentally useful for machine-learning researchers everywhere. "We see that as part of a mission that we have as a national lab," Spears says, "to spread knowledge by offering these data back to the national community." SS

Shattering a Metal Ceiling

BY ANDY BOYLES

ONE FALL MORNING IN 1998, a small group of scientists and technicians met in the New Mexico mountains to test a piece of stainless steel produced using a new manufacturing technique called additive manufacturing, or AM, now widely known as 3-D printing. The team wanted to learn how the AM steel's dynamic strength and ductility (ability to bend or flow) compared with its traditionally cast or wrought counterpart.

Among those present was George T. "Rusty" Gray III, now a laboratory fellow and recently inducted member of the National Academy of Engineering, working at Los Alamos National Laboratory. Gray remembers testing the AM sample on a device called a Split-Hopkinson pressure bar. Under compression, the AM steel "basically fragmented apart" at a low level of strength and flexibility – far below that found in conventional wrought stainless steel, Gray says.

Microstructural analysis revealed why that early AM stainless steel had such poor material properties: Its powder layers were only partially fused.

Since then, AM materials have continued to display inferior properties to standard wrought materials. AM technology and metal alloys made with it lack the history of refinement traditionally processed metals have, and it seemed that AM metals might never match their performance.

But a recent experiment has shattered that notion. John Carpenter, a technical staff member in metallurgy at Los Alamos, was working with his colleagues to compare three cylinders of a stainless steel variety called 316L. The first one was wrought – fabricated traditionally and followed by heat treatment to make the atoms align in a uniform crystal microstructure throughout. The team built another cylinder using AM and heated it to make its microstructure mimic the first sample's. The researchers also made the third cylinder with AM but didn't heat-treat it, leaving it as-built.

The researchers then subjected each cylinder to an impact comparable to a plane crash. They fired a small metal plate from a gun powered by compressed gas. The blow from the plate creates a compression wave that moves through each sample, producing stresses throughout that bend, crack and often shatter it.

Carpenter recalls the crumbling AM materials of 20 years earlier. "In this more recent experiment, we expected similar results," he says. "We were trying to see if an improved understanding of additive processes would have a positive impact on performance."

Indeed, their improved understanding paid off. The first impact opened lengthwise cracks in the wrought cylinder and in the heat-treated AM cylinder. But the as-built cylinder, far from being the weakest, had only a smattering of small cracks inside. The faults had failed to spread and connect into one large fracture. A second, harder impact smashed the two weaker cylinders. The second impact finally cracked the as-built cylinder but didn't break it.

"This behavior was a surprise to us," Carpenter says. "We had hoped to get behavior as good as wrought. We were not expecting the as-built material to behave at a higher performance level."

LOS ALAMOS RESEARCHERS TEST METHODS TO MAKE 3-D PRINTED METAL PARTS THAT RIVAL ONES MADE WITH TRADITIONAL PRODUCTION TECHNIQUES.

The experiment wasn't the first to show that scientists have yet to unlock AM's full potential – to create materials with enhanced properties that no one has achieved using traditional materials manufacturing methods. Similar signs have emerged as AM researchers advance in making products as reliable as traditionally made ones.

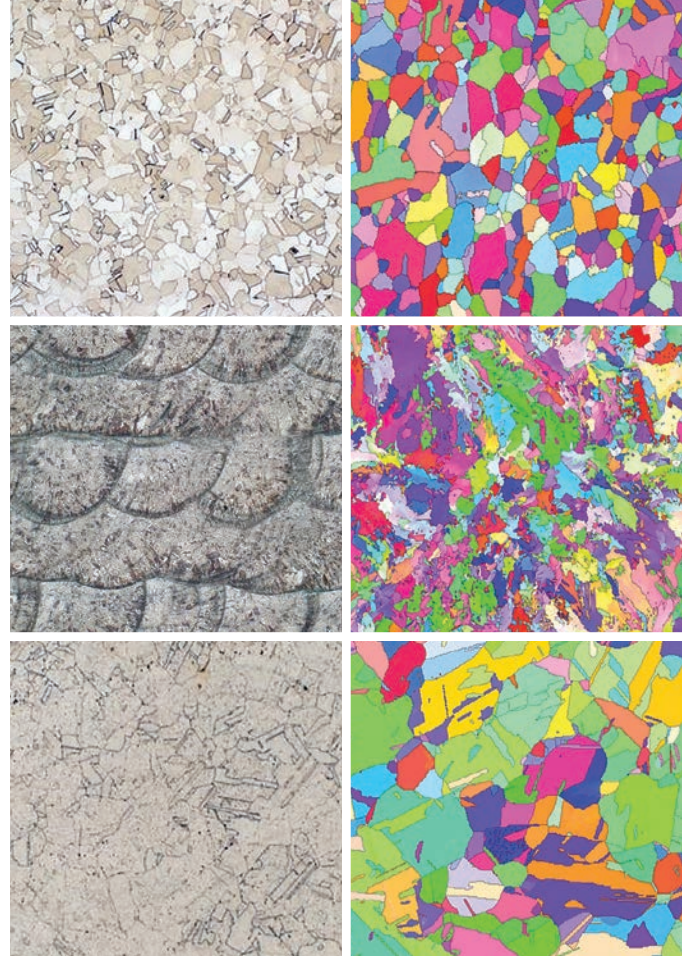
The technology's allure is that it might speed the manufacture and testing of new designs by eliminating the time-consuming process of fashioning each variation from a single piece of metal. "This is the promise of AM from an engineering perspective," Carpenter says. "But many AM metal parts bend, break, wear out or otherwise fail before their time. The materials perspective of AM, therefore, is as much or more promising than simply being able to fabricate complex geometries."

A material's properties arise from its microstructure. Wrought metal is produced via a casting process as a single piece that cools at a rate of 1 or 2 degrees Celsius per second or slower. This gradual cooling can lead to large microstructure volumes called grains in which the atoms align in a similar fashion. Large grains lead to weak materials. Wrought processing, such as blacksmithing, reduces the grain size and makes the material stronger. A blacksmith uses a hammer to break the large grains into finer ones, then heats the metal to settle the atoms into crystal structures that have desirable properties.

By contrast, each AM layer is a small, molten volume element, or voxel, added to a cooler piece of the component under a computer's direction. A voxel can be only about one-third the thickness of a human hair and thus can cool as fast as 1,000 to 10,000 degrees per second, many times faster than cast metal. This rapid cooling means the atoms in each voxel have very little time to align closely with those around them. In addition, as a new voxel cools, it begins to contract while the surrounding cooler metal resists the shrinkage. Microscopic tugs of war ensue, straining some crystals in tension and compressing others. The sum of these residual stresses can distort the shape of an AM part, create weak areas within it, or both. Residual stress shortens a part's life the way a warped floorboard nailed into a straight position is the first to split or loosen.

Before an AM part can replace its wrought counterpart in a car, military vehicle, spacecraft or other machine, manufacturers must show that the new part not only looks like the original but also matches its strength, durability and other essential properties. The drive to qualify AM materials is a major thrust of the Los Alamos group's work, and they've brought in every method at their disposal to probe them. Besides the gas-gun experiments, they use light microscopy, electron microscopy, X-ray imaging, electron backscatter diffraction (EBSD) and neutron diffraction.

The surprising superiority of a few as-built materials has raised tantalizing possibilities for future metals. Carpenter offers the example of lightweight alloys to boost fuel-efficiency in vehicles. Providing designers with AM-produced stainless steel that weighs the same as standard metal but is stronger means they can produce a lighter vehicle that's just as safe



Light optical microscopy (left column) and electron backscatter diffraction (right column) images allowed microstructure comparisons of a wrought stainless steel variety called 316L (top) with an as-built additive-manufactured (AM) version (middle) and a heat-treated AM version (bottom). The as-built AM steel, likely because of its interlocking small-crystal structure, performed well in strength tests.

or safer. "So it's a win for the designers because they use less materials, and it's a win for the consumers because their lighter car requires less gas."

Before AM can render futuristic materials, researchers will have to understand its processes in great detail and then learn how to manipulate them.

Close examination revealed clues to as-built 316L stainless steel's strength. Instead of the widely used AM method of sintering metal powder particles together – a technique known in the field as "powder bed" – the team chose a technique called "directed energy." This approach uses a laser to melt an oval-shaped spot in the material where new metal is to be added. Then the AM device pours metal powder into the pool. After the powder melts completely and rises above the surrounding surface, the laser moves on and lets the new material cool. Carpenter compares the process to building an ice structure by freezing layers of ice cubes in place.

Light microscopy and EBSD showed that directed-energy AM had created a novel crystal microstructure in the as-built cylinder. While the two weaker samples were made of large, granular crystals, the as-built material contained smaller, branching crystals that appeared to interlock. This branching crystal structure with small grains is likely the key to the sample's strength.

Another stainless steel type, 304L, also exhibits remarkable qualities in the as-built state but for different reasons. Wrought samples can withstand 150 megapascals – a force comparable to the weight of a Chevrolet Malibu balanced on a spot one centimeter square. But an as-built AM piece of the same metal can withstand 350 megapascals without significant deformation – stack a Dodge RAM 1500 pickup truck onto the Malibu.

The team knew that neutron diffraction would be their best tool to study this material. Microscopes and EBSD can image only surface details and X-rays cannot penetrate thick pieces of metal. But neutrons pass through stainless steel and come out the other side with information about the spacing and orientation of the atomic nuclei within – that is, the crystal microstructure. The group was ideally positioned to undertake the study, having access to the Los Alamos Neutron Science Center (LANSCE) and its neutron diffraction laboratory, the Spectrometer for Materials Research at Temperature and Stress (SMARTS).

The researchers probed the wrought and as-built metal samples while the materials were in tension (as if being pulled apart) and in compression. The most dramatic difference between the two centered on a feature in the crystal lattice called a dislocation. Bjørn Clausen, a SMARTS instrument scientist who participated in the study, describes dislocation as "basically a fault in the lattice. That means that there's a strain field around that fault that makes it difficult for other dislocations to move through." Donald Brown, who operates SMARTS with Clausen, also participated in the studies. The as-built version of 304L stainless steel had 10 times more dislocations than the wrought version. In this case, the multiple tugs of war within the metal are small and disorganized, pulling in random directions that average out and lend strength to the overall material.

Other studies explore the flipside of AM materials: Why some are weaker than their wrought counterparts. The Los Alamos team chose a type of stainless steel called GP1, which has remarkable toughness and ductility in its wrought form. "What was surprising with the AM version of it was that it did phase transform," Clausen says. "That means that it changed its crystal structure into a different form that turned out to be much weaker."

A piece of AM-built GP1 must be heated and compressed to transform its initial phase, called austenite, to the wrought metal's stronger phase, martensite. The team wanted to know why AM renders GP1 as austenite, not martensite. Perhaps the voxels cool too fast during manufacture, giving them a microstructure that's stable but poised to collapse to another state of lower energy, like a snow pile before an avalanche. Or maybe some other factor is at work.

To capture the transition from austenite to martensite, the team studied small cylinders of as-built GP1 as they were heated and compressed. The samples were about a half-inch long and quarter-inch diameter. Again, for such thick samples, neutron diffraction was the diagnostic of choice. In the probe done before heating and compression, the team found a surprise: high levels of both nitrogen and oxygen in the metal. Now nitrogen also was a suspect because it's known to stabilize the austenite phase in stainless steel.

Next, the researchers probed the cylinders with neutrons as they heated the metal in a vacuum. The microstructure did not settle into martensite but remained austenite. Clearly, the crystals were stable and had not formed due to rapid cooling, but the heat process had depleted nearly 90 percent of the nitrogen. The team now thinks nitrogen determines the microstructure and that there was still enough of it remaining to keep the austenite phase stable. Only under physical stress did the microstructure transform into martensite. Samples that had less nitrogen due to heating made a more complete transition to martensite, acquiring the superior performance of the wrought material.

Ideally, AM will someday be able to directly produce GP1 with martensite microstructure. The key may lie in reducing the powder's nitrogen content and limiting exposure to the gas during AM.

Ultimately, the Los Alamos team wants to understand the AM process from start to finish, at a microscopic level and on fine time scales. In fact, the researchers have developed a unique system to capture the crystallization of voxels as they cool. Traveling to Argonne National Laboratory (ANL), they've used high-energy X-rays at the lab's Advanced Photon Source, or APS. Unlike lower-energy laboratory X-rays, this synchrotron-generated radiation can penetrate a hot droplet of metal 3 millimeters in diameter.

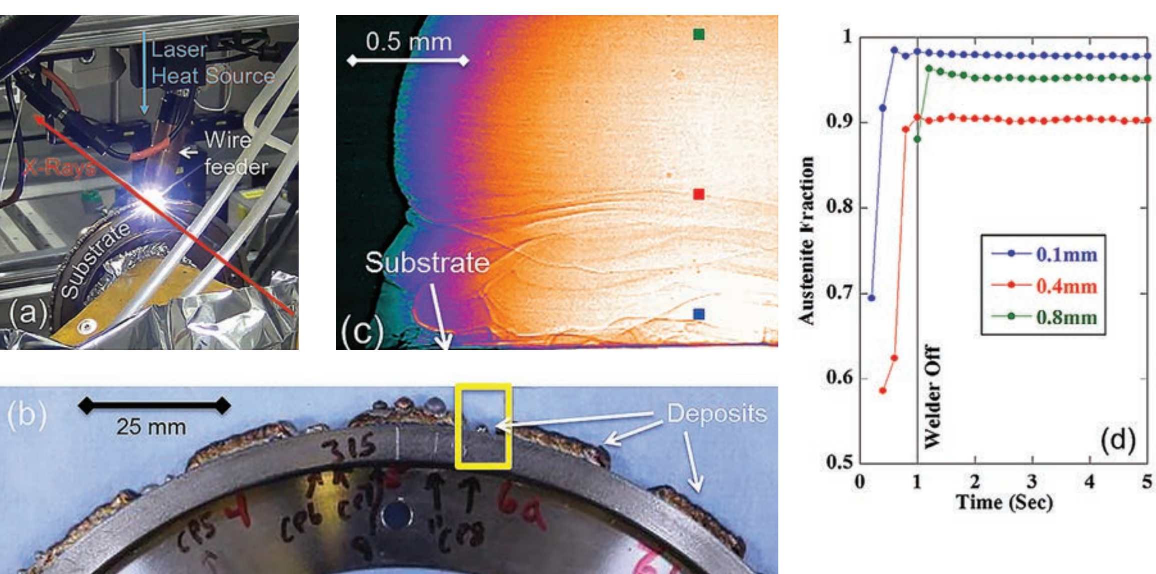
All previous methods have been able to probe only the end point of crystallization, the solidified voxel after deposition. "We have really been able to do something novel and new at the APS," Carpenter says. "We've been able to use high-powered X-rays that can actually punch through metal and allow us to see what's going on in the material as the rapid solidification is occurring."

An early use of the system showed different regions in the same molten voxel forming austenite crystals at different rates, depending on the distance from the solid substrate below.

Future studies will add to the team's understanding.

"Once we start to understand how the material is moving from liquid to solid, then we can start to understand how to manipulate it in order to accentuate certain characteristics," Carpenter says. "Could we produce a material that is even stronger in the additive, as-built material than we currently produce? The answer is likely yes." SS

Andy Boyles is contributing science editor for Highlights for Children Inc. and a freelance science writer and editor.



In tests at Argonne National Laboratory's Advanced Photon Source, researchers used (a) a wire-feeder to deposit stainless steel on a rotating substrate while X-ray data were collected. The yellow box on the substrate (b) marks deposits of interest, imaged via X-ray radiograph (c); the colored dots indicate diffraction collection points, plotted at right (d), showing the fraction of austenite crystals at each spot. The technique enables a glimpse of what happens inside metal as it transforms from liquid to solid – and, ultimately, how to buttress the strength of 3-D printed materials.

'No End to the Problems We Face'

Dimitri Kusnezov is Chief Scientist at the National Nuclear Security Administration in the Department of Energy. He earned A.B. degrees in physics and pure mathematics at the University of California, Berkeley, and did research at the Institut für Kernphysik, KFA-Jülich, in Germany, before earning master's and doctoral degrees in theoretical nuclear physics from Princeton University. After a decade on the Yale University faculty he went into public service in late 2001.

What are your duties?

They're diverse for a number of reasons. The scientific base we oversee is necessarily broader than our mission footprint. We plan through the aperture of nuclear weapons and nuclear security in a number of areas, from counterterrorism and nonproliferation to the U.S. nuclear weapon stockpile, but the science and technology we maintain at the laboratories touches nearly everything. There are national interests, administration priorities, international or urgent matters where our laboratories are involved or could be called on. I look into our network and understand the best opportunities or places where we should be in conversations or can add value, where science can best inform or advise policy or other exigent matters. There is no end to the problems we face and we're always short of solutions, so finding the best way to inject science into conversations in Washington is an important part of my duties.

What made you interested in math and physics?

You could explore the world, and you learn whether your understanding was right or wrong. Math is the language of physics and physics is the way to interpret the natural world. Together they allow you to observe the world with some precision, which fit my temperament at that time. Today, an analytic basis to understand and explore the complex options we face is a luxury we often don't have. But being able to use this training to approach solutions remains important.

What do you like most about what you do?

That almost anything is possible. This is a place where you can have national or international impact, where you can do grand things, where you're not confined to thinking small, and there is latitude to propose possibly transformational ideas. Instead of thinking about narrow physics or mathematics problems, as I did as an academic, I can think more broadly. It's a nice world to be in because you can see cause and effect of science transforming into solutions.

What do you see ahead for stewardship science research?

We have to continue to drive science at a scale no one else can, not for its own sake, but because the problems demand it. We use the DOE national labs because there's no other place to do things – often high-hazard or classified or at unprecedented scales, or with the materials or technologies we need. We use academia and the private sector as needed to draw in or test new ideas or to design and develop technologies, but the focus of delivering against our missions resides with us. For example, we want to build artificial intelligence into our traditional high-performance computing approach and integrate AI with big data from our increasingly instrumented experiments. We need new means to understand uncertainty quantification and prediction with advanced, more cognitive computers. We're also using AI in controlling experiments and integrating it into much of what we do. We'll see this science continue to migrate into other NNSA and DOE missions. We still need higher laser energy, higher power, faster computers, smarter systems, smaller sensors, longer battery lives and more.

How do programs like the DOE NNSA SSGF fit into this?

There are no institutions of higher learning for our missions – for our classes of problems, the materials we use or the environments we investigate. We need students to step into our system and experience it. What we care about is timeless while fields funded by open calls in science tend to follow the latest ideas. In that community what's hot today often is what becomes a funding opportunity, and the metrics often are publications. We do the science because we own the outcomes. We develop tools, practices, capabilities and devices, and we send them into the field. We're not as fluid in funding the next hottest thing. SSGF helps fill the gaps where academic funding streams may miss what we need.

What advice do you have for students interested in stewardship science?

We do science that makes a difference. Our science, our engineering, our technology is purposeful. We can define how it will impact the world and the country. It's not for everybody, but if you want to make a difference, it could be for you.

DOE NNSA SSGF FELLOWS ROSTER

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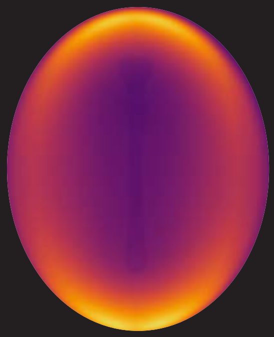

SHAPE SHIFT

When Lawrence Livermore National Laboratory physicists used machine learning to explore designs for fusion implosions, the computer generated this egg-shaped surprise of a density map. They'd been expecting something spherical. Turn to page 16 for more about how machine learning is helping scientists reshape their basic assumptions.

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