HARDENING TARGET

Los Alamos aims protons to see inside solidifying metals

Livermore: Extreme chemistry

Sandia: A new twist on fusion

Plus: Inside explosions, juking joints, final-year fellows’ findings, science leadership at NIF, the stuff of stars
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LETTER FROM NNSA

Nuts and Bolts, Explosions, Lots of Volts and Star Stuff

WELCOME to the fifth volume of Stewardship Science, the annual magazine of the DOE National Nuclear Security Administration’s Stewardship Science Graduate Fellowship. The magazine tells the stories of fellows, former fellows and NNSA national laboratory researchers from diverse technical backgrounds, studying equally diverse topics in experimental and computational science.

Up front, you’ll learn how final-year fellows spent their summer research practicums at national lab facilities, and about researchers at those same places who study chemical processes at the onset of an explosion and others who model the literal nuts and bolts of nuclear missiles. This year’s interview is with Lawrence Livermore National Laboratory’s (LLNL) Marilyn Schneider. Marilyn details her experiences along the way to her leading the radiative properties groups at LLNL’s Physics and Life Sciences Directorate.

You will also find in-depth articles on major research efforts at the laboratories. Our cover story follows the recent work of Los Alamos National Laboratory’s Amy Clarke and colleagues on the experimental observation of alloy-formation at its earliest stages. This work is used to understand the solidification of metals at the mesoscale, knowledge that promises to improve the reliability of metals’ manufacture. We also profile LLNL’s Nir Goldman and his work with carbon and hydrogen atoms’ quantum physical behavior under extreme conditions. His research on water and its superionic phase has been applied to planetary science and to improve the understanding of carbon-based NIF (National Ignition Facility) fuel capsules. And at Sandia National Laboratories, researchers have come up with a concept called MagLIF, in which laser-heated fuel is confined using very high magnetic fields on Sandia’s Z machine. It’s an alternative to laser-based approaches to inertially confined fusion.

In the essay, current fellow Juan Manfredi explores internal conditions of stars via the National Superconducting Cyclotron Laboratory at Michigan State University and outlines his plans to extend his star studies to exotic fissile nuclei when the Facility for Rare Isotope Beams begins operations.

This issue once again reminds us of the importance of the work ongoing at the NNSA national laboratories — and speaks to the importance of the SSGF in developing the next generation of scientists.

Keith LeChien
Acting Director, Office of Inertial Confinement Fusion
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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-NA0002135. Krell is a nonprofit organization serving the science, technology and education communities.

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FERNLIKE METAL FINGERS
This rendering from a computer simulation depicts microscopic dendritic growth competition in an aluminum-copper alloy during solidification. The lighter gray, fernlike dendrites eliminate their darker gray neighbors in the center. This process directly affects grain sizes and boundaries, which control material properties. Read more, starting on page 10, about Los Alamos National Laboratory researchers’ efforts to couple modeling with experiments that glimpse the solidification process in real time so they can predict and control microstructural development.
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Birth of a Blast

Explosives have uses in weapons, construction and engineering, but the extremely fast and powerful reactions they generate aren’t well understood. A better grasp of the initial steps in these complex chain reactions could help with the design of new, safer explosive materials, says Shawn McGrane of Los Alamos National Laboratory. Illuminating how shock waves change material chemistry also could help improve safety, with new types of body armor and methods to improve safety in stored explosive chemicals.

By their nature, explosions are quick and violent. Because heat, mechanical shock or a combination of the two can trigger blasts, shocks provide a useful way to study them. Such shock waves cause drastic changes in a chemical’s temperature and pressure as they run through it.

To mechanically shock explosives and study their chemistry, researchers usually experiment with a gas gun or an explosively driven impact to accelerate a projectile so it impinges on a chemical and generates a shock wave in the target. These devices provide valuable information about explosions on the microsecond or nanosecond timescale, roughly a millionth of a second after detonation, but require a small-building-sized enclosure to deal with the large quantities of energy the blasts release.

Even in that tiny time, a lot of chemistry may already have transpired. McGrane and colleagues use laser-based tools in small laboratory spaces, allowing them to study shock-based chemistry tens of trillionths of a second (tens of picoseconds) after a detonation-strength shock wave.

The Los Alamos researchers have used their experiments to examine how shocks affect a variety of liquids. Unlike solids, liquids don’t have an organized molecular structure, so they’re a simpler test system for understanding intricate chemistry. The scientists place liquids inside a disk, an inch in diameter and a few micrometers thick, behind an aluminum cover. They then focus lasers on the aluminum for 300 picoseconds, generating a small amount of plasma on its surface and producing a shock wave that moves into the chemical sample. The shock penetrates just a few micrometers into the liquid sample, producing pressures hundreds of thousands of times that of Earth’s normal atmosphere and raising the sample temperature to 1,700 degrees Celsius.

McGrane’s group uses optical spectroscopy to study how the shock changes the liquid.

McGrane and colleagues started with a variety of simple hydrocarbon samples to see whether different arrangements of atoms and bond strengths changed the response. They found that many of those arrangements were inert under shocks. The researchers also looked at several liquids with known explosive properties, including acrylonitrile, a compound used in plastics that can detonate under some conditions. Because researchers have studied acrylonitrile with gas guns and computer models, the Los Alamos group has data to compare its results against.

McGrane, Kathryn Brown and their colleagues found that at these very early time points, acrylonitrile’s behavior is consistent with what researchers have seen at time and length scales orders of magnitude larger. “The same chemistry happens, but it just happens faster when you shock it harder,” McGrane says. The results are consistent with computer simulations using quantum molecular dynamics, which previously was the only way to study chemistry at an explosion’s earliest stages.

– Sarah Webb

Explosive Predictions

Until nuclear processes take over, chemical energy primarily powers nuclear weapons. “Igniters, initiators, rocket propellants, boosters, detonators, main charges – everything is chemically powered,” says Lawrence Livermore National Laboratory’s Randall Simpson, associate program leader in Weapons and Complex Integration.

During his career, Simpson has shepherded research, storage and surveillance of Livermore’s chemical energetic material efforts, primarily for the nation’s nuclear weapons stockpile. The major component of Livermore’s Energetic Materials Center (EMC) is continued on page 8
Members of the DOE National Nuclear Security Administration Stewardship Science Graduate Fellowship’s 2014 outgoing class share their national lab research experience.

FELLOWS ON LOCATION

TRACKING THE TURBULENT EDGE

During his 2011 Lawrence Livermore National Laboratory practicum, Evan Davis picked up a computational tool he’s since used for his Massachusetts Institute of Technology research group and his doctoral thesis under Miklos Porkolab.

Davis researches properties of magnetic confinement fusion at MIT’s Alcator C-Mod and General Atomics’ DIII-D reactors. Fusion attempts to recreate the processes fueling the sun and stars by heating hydrogen isotopes to temperatures so high electrons are stripped from atoms. Rapidly moving nuclei in the resulting plasma collide and merge, releasing tremendous energy.

C-Mod and DIII-D are tokamaks, doughnut-shaped chambers that are leading candidates for successful fusion reactors. Powerful magnetic fields hold the searing plasma so it doesn’t damage the tokamak walls. The outer edges are the most critical areas for confinement, but small-scale turbulence there often allows the plasma to escape.

Researchers, including Davis, want to understand this edge turbulence and control it. Working with Xueqiao Xu, a researcher in Livermore’s Fusion Energy Sciences Program, Davis learned to use the Boundary-plasma Turbulence (BOUT++) code to portray edge turbulence using input from C-Mod experiments.

Davis’ BOUT++ simulations showed that a C-Mod operational regime called enhanced D-alpha high-confinement mode becomes unstable when the calculations include realistic values for the plasma’s electrical resistance. The resulting resistive plasma modes may be responsible for controlling C-Mod’s observed edge turbulence.

Meanwhile, Davis also helped improve the BOUT++ algorithm that generates the data-point mesh used to model the plasma. High-performance computers calculate physical changes at each point; drawn together, they portray the plasma’s activity. Each grid must match the unique profile of the plasma experiment that the simulation models. By comparing experimental data with the grids BOUT++ created, Davis suggested and implemented changes to the grid-generation algorithm, leading to more accurate and numerically stable profiles.

GETTING INTO THE MIX

Much of Michael Hay’s Princeton University research has focused on the outcome of inertial confinement fusion (ICF) experiments at the National Ignition Facility (NIF) at Livermore.

During his 2011 summer practicum at Livermore, however, Hay turned to what goes into the experiments – specifically, how mixing between hydrogen isotopes and plastic in the shells holding them affect ICF implosions. Much of his experience was detailed in “Laser Days of Summer” from the 2012-13 Stewardship Science.

Hay worked with Larry Suter, who oversees the Hohlraum Dynamics Group in Livermore’s Theory and Target Design Division. For part of the project, Hay simulated how mixing between the plastic capsule and the frozen deuterium and tritium (DT) fuel affects NIF shots.

The DT capsule sits in a hohlraum, a gold cylinder about the size of a pencil eraser. Pulses from NIF’s 192 intense laser beams enter each end of the cylinder, generating X-rays that burn off the plastic shell, compressing the isotopes to densities 100 billion times that of Earth’s atmosphere. Under compression and heating, the hydrogen nuclei should fuse, releasing tremendous energy.

Using HYDRA, a radiation hydrodynamics code, Hay performed simulations examining how mixing affects the ignition threshold factor (ITF). ITF measures kinetic energy in an implosion relative...
Hay says the practicum suggested new directions for his Princeton research with Nathaniel Fisch, which looked at waves that propagate in NIF compressions and making the waves more effective in driving the ICF reaction.

**ADDITING IT UP IN METAL**

His 2013 Livermore practicum drew John Gibbs into the burgeoning field of three-dimensional printing, also known as additive manufacturing.

Livermore researchers are out to improve 3-D printing processes to make high-quality metal components. Printing parts with metal is relatively easy, Gibbs notes in his practicum review. Livermore researchers are tackling the more difficult task of more quickly certifying such parts for use in critical applications.

Gibbs devised a simulation of selective laser melting, an additive manufacturing process that uses a laser to melt metal powder. The model incorporates laser melting of the metal powder bed, heat transfer, the thermal effects of transformation between solid, liquid, vapor and powder, and tracking the interface between the condensed and vaporized material to determine where the laser energy is deposited.

The model, combined with experiments, will help researchers better understand the physics of metal additive processes, Gibbs’ practicum supervisor, Wayne King, wrote in his review.

In a related project, Gibbs analyzed laser beam speed data, helping demonstrate conditions that enable a transition to what is called “keyhole mode,” in which a laser evaporates metal to form a cavity. That analysis became part of a paper submitted to the Journal of Materials Processing Technology.

Gibbs’ doctoral studies, under Peter Voorhees at Northwestern University, focus on coarsening, in which particles in a multiphase material get bigger while shrinking in number. Gibbs has especially focused on the coarsening rate in liquid-solid metal mixtures.

**CRACKING THE SHELL**

During her 2012 Livermore practicum, Stephanie Lyons turned from her usual nuclear physics research to fusion plasmas, helping simulate spectra from a NIF diagnostic.

The project focused on carbon-12, an isotope used to make the plastic capsules holding the deuterium-tritium (DT) fuel mixture in NIF experiments. Working with practicum supervisor Charles Cerjan, Lyons wanted to understand how existing NIF instruments, especially the Gamma Reaction History (GRH) diagnostic, could track carbon-12’s gamma ray signature in implosion experiments.

Although Lyons says her skills in large-scale computation were rudimentary, she quickly learned MCNP, a Monte Carlo neutron-transport code, and used it to create neutron transport simulations. These calculations analyzed how various configurations of shell deformity, doping and density concentrations affect the down-scattered ratio (DSR) of neutrons, an important DT fuel assembly diagnostic, and the carbon-12 gamma-ray yield generated when neutrons bombard isotope nuclei. This gamma-ray signal provides valuable information about the remaining shell material mass near peak compression.

From those neutron transport simulations, Lyons selected cases with the correct DSR and input them to a GRH model. Discrepancies between the simulated and experimental results will help researchers interpret capsule implosion tests and perhaps help optimize performance, Cerjan says.

The practicum project, Lyons says, was a perfect complement to her doctoral research into nuclear physics. That background helped her understand the project’s gamma spectroscopy aspects while Cerjan helped her grasp the plasma physics components. And after the practicum, she reports, “I am much more confident working with various codes.”

Lyons’ University of Notre Dame research under Michael Wiescher concentrated on the NaNe cycle, reactions in stars...
At a time when the reliability of the nation’s nuclear arsenal increasingly depends on supercomputers’ predictive power, researchers are struggling to accurately model how bolted and screwed joints behave under the stresses missiles encounter when reentering the atmosphere. Correcting these nuts-and-bolts deficits is “high tech and high stakes,” says Daniel J. Segalman, a recently retired Sandia National Laboratories distinguished research engineer who spent the final 16 years of his career working on the problem. “It is part of the broader effort to bring greater physical fidelity into our computational models.” Segalman was among the first to warn that past models weren’t fast enough – the required minimum interval is in the picoseconds – to assess the equations that describe how re-entry vehicle joints dissipate energy and damp vibrations.

Many mechanisms contributing to vibration also occur at tiny length scales “impractical to incorporate directly into structural dynamics calculations,” Segalman says. Even dimensions smaller than a micron can be important, says Matthew Brake, a principal research engineer who recently joined Sandia’s joint modeling research team. Under the high oscillating loads and compressive stresses of atmospheric re-entry, some parts of stuck joints can repeatedly slip to release pent-up energy. But at the same time, joints may remain locked in other places nearest to bolt holes. Under such varied flexing, joint and bolt materials can deform. If dynamic loads on joint structures are sufficiently high, the structures’ metal may start out behaving elastically but “quickly become plastic,” says Brake, who won a 2012 Presidential Early Career Award for Scientists and Engineers. The end result can be permanent deformations and, potentially, failure. Equations describing such behavior can themselves quickly morph from manageably solvable linear ones to difficult-to-impossible non-linear varieties.

“This is like trying to predict how runners will do in a marathon by looking at what shoes they’re wearing.”

Since agreeing to an underground nuclear testing moratorium in 1992, the United States has relied on experiments and computers to ensure the arsenal is safe and reliable. Whereas actual experiments during underground and open-air tests may have proved that our weapons’ joint mechanics can hold up, that “only assured us that those weapons could survive those tests,” Segalman says. “We want to be able to consider other loadings on perhaps other packaging of those weapons. This is one of the ways that computational modeling mitigates the end of underground testing in assuring the safety and surety of the stockpile.”

Advanced research is underway across the world, Brake says. One modeling goal is “to accurately predict energy dissipation by mechanical joints. To do this, we must develop and improve the codes that run on large-scale parallel systems.” Technical advances, Segalman says, have allowed “what used to be heroic calculations to become more day-to-day exercises” that run on comparatively modest computers. But “full-scale structural dynamics calculations of weapons, using the nonlinear models we have devised for some of the joints, employ the most advanced, massively parallel computing available.” Sandia’s contribution has enlisted as many as 15 researchers since 1998, Segalman estimates. Still, Brake says, “even as a new generation of researchers pick up this cause, the ultimate goal of developing predictive, physics-based models is something we don’t expect to come during our lifetimes without large collaborations.” - Monte Basgall

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This intentionally crude mesh simplification shows multiple components of a nuclear weapon body on atmospheric re-entry. Each part is comprised of numerous subcomponents, fastened together with screws, nuts and bolts, jar-lid-like screwed fittings and more. Joints modelers are particularly interested in understanding these connections.
that convert four hydrogen atoms into an alpha particle and are important for synthesizing neon, sodium and magnesium isotopes. She also was involved in the construction and commissioning of Notre Dame’s new St. Ana 5U accelerator, which she will use to perform her thesis experiments.

DETECTING DIVERSION

David Reyna and his fellow researchers at Sandia National Laboratories’ California campus want to detect when a nuclear reactor is used for nefarious purposes. During his 2012 practicum, Thomas Saller was able to set their minds at ease about some scenarios while confirming their notions about others.

Operating reactors generate copious amounts of antineutrinos, counterparts to the chargeless, nearly massless neutrinos that pass through the Earth and us each second. How many antineutrinos a given reactor produces depends on the isotope the device is splitting and other factors. Variations in antineutrino signal can point to changes in the reactor fuel or operation – including changes designed to help divert plutonium, a byproduct used in nuclear weapons.

Sandia researchers are developing antineutrino detectors to monitor reactor functions. Saller’s job was to model reactors to see how different operating and fuel scenarios affect antineutrino signatures.

Using the reactor physics codes HELIOS and PARCS, Saller did three-dimensional simulations that included mixed oxide (MOX) fuel. He ran eight possible scenarios for plutonium diversion and benchmarked his PARCS output against results from Los Alamos National Laboratory’s MCNPX neutron transport code.

Saller says the practicum was a good extension of his work with Thomas Downar and Edward Larsen at the University of Michigan. Saller regularly uses HELIOS, PARCS and MCNPX as he investigates ways to improve the accuracy with which reactor models portray neutron interactions.

– Thomas R. O’Donnell
What prompted you to pursue physics?

When we were in third grade my twin sister was in a play called _Children of the Sun_. It mentioned the discovery of Neptune using calculations of the orbit of Uranus. That inspired my interest in astronomy and in predicting things from calculations. I love the idea that you start from Newton’s Law – force equals mass times acceleration – and derive things like a planet’s orbit. My mind works in that logical fashion. I’m not very good at analyzing literature or languages. I love the logic of physics.

How did you end up in the area of high energy density plasmas?

Before coming to the lab, I used optical techniques to study fluid. When I interviewed for a job at the lab, I was told that my background matched their projects. I was involved in only one project that related to my background. But I’ve taken image processing from the optical to the X-ray, and it evolved into studies of high energy density physics.

You have a long title. Just what do you and your groups do?

The radiative properties group in Physics and Life Sciences is small. We use X-ray spectroscopy to measure opacities, X-ray line shapes and X-ray cross-sections, and to measure material properties of plasmas. It’s a pretty diverse group, with people matrixed into other lab projects. The NIF group is new and will grow by developing and implementing spectroscopic techniques at NIF.

Why is spectroscopy important for NIF? What kinds of things can spectroscopy tell us?

It’s a non-perturbative technique. Sometimes we add a dopant, but the system isn’t really perturbed. We can deduce plasma conditions, such as temperature and density, from the measured spectra. In some cases, this benchmarks how well computer codes are modeling the plasma. There’s also a mystery in the gas-filled hohlraums: We can’t explain where 15 to 20 percent of the laser energy is going. If we could do some spectroscopy on the plasma in the hohlraum, we might be able to balance the energy.

It seems like there’s a lot of engineering that goes into these diagnostic devices. How hands-on do you get in that?

I don’t do hands-on things anymore. I mainly calculate and analyze. I calculate the spectrometer designs, their throughput, their alignment tolerances and so forth, then I analyze the data. It’s a little frustrating not to be able to tinker. Earlier in my career, I did all these things. I believe training at small-scale facilities, where you do everything, is really, really important. In your career, you need to understand all the details of an experiment so that when you’re supervising scientists and technicians at larger facilities, you thoroughly understand what’s involved.

Your primary mission, I take it, is to help advance national interests in stockpile stewardship. How does that affect or influence the research you do? Do you ever feel constrained?

It hasn’t frustrated me. I like solving problems and I like analyzing data, so I’ve always found something engrossing to do. The whole field of opacity and radiative transport is fascinating.

What do you find most engaging about what you do?

The problems are intriguing and the people are really fantastic. NIF has large groups and each person is an expert in his or her own field. When there’s an issue to address or when NIF is moving in a new direction, it’s a lot of fun to sit down with a group of such highly gifted people and figure out a path forward.
With proton radiography, Los Alamos researchers can glimpse metals changing from liquid to solid and other previously unobservable phenomena in real time.
MORE THAN A CENTURY after X-rays peered inside the human body, a new radiation beam is poised to make its mark in the physical sciences. Aiming a focused stream of protons at molten metals has let Los Alamos National Laboratory scientists create motion pictures of the solidification process. And just as the first X-rays uncovered our bodies’ hidden anatomy, these images are revealing in never-before-seen detail the inner structure of metal alloys as they transform while hardening.

Los Alamos materials scientist Amy Clarke is the force behind a research team that uses proton radiography to study the physical and chemical properties of metal alloys. The experiments, begun in 2011, are conducted at LANSCE, the Los Alamos Neutron Science Center, home to a powerful 800 mega-electron-volt (MeV) proton linear accelerator that provides the proton beam. Completed experiments have captured metals changing phase from liquid to solid, followed two immiscible liquids interacting, and recorded metal alloys filling a casting mold. With each new experiment, the researchers record events in real time in bulk samples at the unprecedented level of detail made possible by proton radiography.

“What’s really exciting about this work is that each time we do one of these real-time imaging experiments we almost always see something we didn’t expect,” Clarke says. “We make new discoveries with almost every experiment that we do.”

The research group describes some early experimental results in a June 2013 online paper in the journal *Scientific Reports*, published by Nature Publishing Group. These tests provided proof of principle that proton imaging could capture metal solidification in real time.

“When we first started down this path we tried to choose an alloy that would give us large density differences so that we could see contrast in the imaging,” Clarke says. She and her team worked with an aluminum-indium alloy that when heated separates into two immiscible liquid phases, like oil and water, with different densities. They chose a relatively thick sample size of 6 mm, allowing them to examine behavior in bulk and at the intermediate scale, or mesoscale, that has been difficult to observe because no tools were available to enable real-time imaging.

Up to this point, the theory underpinning metal solidification has relied on data collected from destructive processes, such as crosscutting through metals, and modeling the process with transparent organic analogs – waxy materials that solidify at near room-temperature and have microscopic features closely mimicking solidifying metals. At the microscale, scientists have used penetrating X-rays to study metal alloy structures in thin foils.

But X-rays can’t penetrate thicker sections and don’t work well for heavy metals. Properties of the comparatively massive and charged proton beam allow it to probe relatively dense objects, such as metals, that X-rays can’t penetrate. The advent of proton radiography now allows materials scientists to gather data at the mesoscale,
the intermediate dimension between microns up through millimeter-sized samples that bridges microscale and bulk scale. This intermediate range is where impurities and imperfections form as metal alloys cool into solids. It deals with grain size, solid-liquid boundaries and interfaces in composite materials that affect that material’s behavior. Solving these mesoscale issues could make major contributions to materials science and engineering, allowing improved manufacturing processes that result in more reliable products, ranging from sheet metal to turbine blades.

“These techniques using X-rays and protons are nondestructive and allow you to see inside of a metal without having to cut it up after the fact,” Clarke says.

“Proton radiography is allowing us to probe inside of metals in real time and actually see and understand how they evolve. We think by linking these two methods together, X-rays and protons, we will ultimately be able to predict and control metals during solidification.”

In the Scientific Reports alloy experiments, the researchers recorded the sample melting from the top down. They observed as indium-rich droplets were released during liquefaction of the surrounding solid aluminum. And although the primary purpose of these initial experiments was to examine metal solidification physics, Clarke says they also observed behavior that’s common in industrial processing. For example, the researchers recorded the denser, indium-rich liquid raining down through the majority liquid phase and settling at the bottom of the experimental crucible. This phenomenon of gravity-induced sedimentation is common in casting processes and causes difficulties in casting many alloys, including some under development for industrial production. With proton radiography, issues such as casting conditions and structure development can now be studied under realistic bulk scale environments. Clarke and her team have demonstrated that the technique can bridge that gap in understanding.

“If you can understand what’s happening at the microscale and mesoscale, it can afford the opportunity to control what’s happening on the macroscale,” she says. “This understanding across different length scales could be very powerful.”

**THE NEXT PHASE**

The strength of Clarke’s early experimental work with proton radiography earned her a 2012 Department of Energy Early Career award. The five-year grant will

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Karyn Hede is a freelance journalist whose work has appeared in Science, Scientific American, New Scientist, Technology Review and elsewhere.
allow researchers to continue focusing on proton and X-ray radiography of an expanded array of metal alloys and to combine that work with theoretical modeling of melting and solidification. Team members include postdoctoral scientists Seth Imhoff and Paul Gibbs, Los Alamos physicists Christopher Morris and Frank Merrill, and collaborators Kamel Fezzaa at Argonne National Laboratory and Wah-Keat Lee at Brookhaven National Laboratory.

The research team also has forged a collaboration with solidification physics and modeling experts Alain Karma and Damien Tourret of Northeastern University in Boston. Karma has developed a multiscale model of the growth dynamics of highly branched dendritic structures that can form as metal solidifies under certain conditions. Controlling the growth of these tree-like patterns has many practical applications in metallurgy. For example, turbine engine blades are cast to induce dendrite formation in specific arrays that increase the blade’s strength. Materials scientists want to improve predictions about dendrite formation under various casting conditions and in alloys of varying composition. Karma, Tourret and Clarke’s groups are coupling proton radiography with computational modeling to predict dendrite growth.

“We are working with them to design a grain-boundary grooving experiment,” Clarke says. “We are interested in the details of what happens when you have two grains meet. We’re also looking at what’s called hot-tearing, when you have liquid flowing between solidifying dendrites. The liquid feeding can have an effect on forming cracks in zones between dendrites, so we are trying to design some experiments where we try to promote hot-tearing to better understand how that occurs.”

Because nearly all metals used in industrial processes at some point are cast into molds, the group also has extended its research to include watching how liquid alloys behave as they fill various mold geometries.

“In some of our imaging we see features that evolve that could be considered defects in casting,” Clarke says. “And what’s great is we can actually control the local conditions to understand better how they evolve and also look at strategies for controlling those defects and where they end up. We can melt and erase them and start all over. There’s really a lot of opportunity in processing to control the way microstructure evolves.”

In a recent experiment designed to look at solidification from the bottom up, for example, the researchers observed a dendritic structure getting trapped in the solidified material.

Defect-free mold design combines experience, simulations and trial and error. To cut time and cost, researchers employ proton imaging of instrumented casting experiments to gain quantitative information to improve models. Left: a two-dimensional section of a three-dimensional casting simulation, where molten liquid metal is filling a mold cavity. The color represents temperature (degrees Kelvin). Right: a proton radiograph from a real-time casting experiment of a mold filling. The simulation and the experiment share the same geometry and thermal conditions.

Solidification structure development at different length scales in an aluminum alloy with 10 percent indium by atomic percentage. The left image highlights the use of protons to examine a large sample volume during solidification; the inset, right, shows a representative sample volume probed using X-rays.
OS ALAMOS NATIONAL LABORATORY scientists first aimed a focused beam of protons at a high-explosive sample in 1996 to study its ignition. The physics group at Los Alamos, charged with evaluating different configurations of composite explosives used to initiate nuclear reactions, developed proton radiography to record dynamic data as part of the National Nuclear Security Administration’s mission ensuring the safety of the nuclear stockpile. These experiments, over in a blink, required a technology capable of penetrating a thick sample and generating an image every hundred nanoseconds or so.

“What makes protons useful is they are highly penetrating,” says Chris Morris, one of the physicists who invented the technique and now a lab fellow. “The idea that makes proton radiography work is that you put a magnetic lens between the object you are looking at and the detectors that make an image of what you are looking at. You can focus those particles like a camera and the detectors are like film.”

To make a series of images, the protons collide with a plate coated with cesium-iodide crystals, which emit light when the proton radiation excites them. The light signals are transmitted to a digital camera similar to those found in any smartphone. A computer can reconstruct the series of images into a movie.

Once it became clear that proton radiography could faithfully record data from complex explosives experiments, other applications soon became apparent. The technique can accommodate samples up to a few centimeters in size, with widths ranging from aluminum foil to a deck of cards for solidification experiments.

Materials scientist Amy Clarke recognized the technique’s potential to probe metals’ internal structures. Her experiments occur on a much slower time scale: a few seconds to about half an hour. Individual images also are captured on a longer time scale, allowing the scientists to eliminate stray radiation defects that can mar images.

“We can eliminate all the extraneous radiation defects by delaying the camera image capture until those stray protons are gone, so we get much higher quality pictures than with our dynamic experiments where we have to capture images on a much shorter time scale,” Morris says.

The LANSCE facility has three lenses: a 1X lens that can resolve down to 0.25 millimeters, a 3X lens that can resolve images to 80 microns and a 7X lens that can resolve images to 20 microns.

“This particular dendrite was something we didn’t expect to see,” Clarke says.

“We saw an aluminum-rich dendrite growing in the melt. Then it floated up to the solid-liquid interface.”

In this case, a dendrite could be considered a casting flaw, Clarke says. In an industrial-scale process, the casting could be designed so these dendrites float to the top, where they could be cut off after the casting is solid. The idea is to predict defects and use processing as an advantage in eliminating them.

“The link between processing and structure is important because structure profoundly affects the properties of engineering materials,” Clarke says. “The as-cast structure is important because it also follows throughout the downstream processing as well. The as-cast microstructure is difficult to erase – that’s why it’s so important to try to get it right. If we can get the as-cast structure right, we can improve properties and performance of materials.”

EXTENDING KNOWLEDGE

As part of that Early Career Award, Clarke plans to look at the interaction of fluid metal with mold walls. She’s also interested in modeling fluid flow and turbulence using the proton radiography platform.

For instance, upcoming experiments will examine casting metals within a magnetic field.

“A magnetic field can influence the turbulence of the flow,” she says. “We think there is a lot of opportunity here to advance solidification technology.”

Recently, the team also has pushed the limits of proton radiography spatial resolution, imaging higher-density metals and large samples.

“We think there is a lot of opportunity for application to heavier metals, which can have national security applications,” Clarke says.

Proton radiography is seen as a core technique in Los Alamos’ long-range plan supporting NNSA’s Stockpile Stewardship Program. As a DOE-designated national user facility, the proton source also is available to researchers from U.S. universities, industry, and other government laboratories. Given its unique imaging capabilities, it shouldn’t be long before proton radiography finds many innovative applications.
Goldman’s work helping achieve nuclear fusion has its conceptual roots in table tennis.

The intellectual lineage of his new, world-leading model of carbon and hydrogen atoms’ quantum physical behavior under extreme conditions goes back 20 years, to when Goldman, a staff scientist at Lawrence Livermore National Laboratory, imagined the perfect flight of a pingpong ball.

As a Yale undergraduate chemistry student in the mid-1990s, Goldman took physicist Bill Bennett’s popular Computer as a Research Tool course. Bennett, co-inventor of the helium-neon laser, was legendary for his class demonstrations and project assignments, like in-class laser wart removal and calculating how long it would take monkeys sitting at a typewriter to produce phrases from classic literature.

“We had to write a computer program to calculate how much backspin you need on a pingpong ball to create the perfect shot, one that would bounce over the net and then bounce back over,” recalls Goldman, a staff scientist in the lab’s Chemical Sciences Division. “It was so much fun. I grew up playing pingpong and I wanted to know how to do that shot. We determined it was impossible to do it, at least by hand.”

When Goldman arrived at Livermore in 2003 with a physical chemistry doctorate from the University of California, Berkeley, he’d graduated from imaginary pingpong balls to considering the atomic interactions under extreme temperature and pressure that are essential to stockpile stewardship research.

His latest extreme computational chemistry models, developed on Livermore’s supercomputers, can predict how carbon atoms behave under a vast range of thermodynamic conditions — including temperatures from near...
absolute zero to those inside stars – thousands of times faster than previous models.

“Matter behaves very differently under those extreme conditions,” says Goldman, 38. “Part of the fun is coming up with chemical computational models that can capture the weird and interesting behavior that you see.”

Predictive computational models of extreme chemistry are central to designs for a new generation of nanodiamond-coated fuel capsules for the Department of Energy’s National Ignition Facility (NIF).

In a twist Professor Bennett would appreciate, Goldman’s also working on a shocking approach to understanding the origins of the chemical complexity that fueled life’s emergence on Earth (see “A Shocking Start for Life on Earth,” page 17).

THE EXTREME CARBON CYCLE

We think we know carbon. We know this six-electron element at room temperature and pressure. We know carbon as the slippery graphite in pencils and as the sparkling, super-hard diamond of engagement rings. And of course, we owe our basic chemistry to carbon as the atomic backbone for DNA and proteins.

Ratchet up the temperature and pressure, though, and carbon transforms into states alien to daily life.

“The more you squeeze it and the pressure increases, carbon atoms jostle to form an atomic configuration that best relieves the pressure,” Goldman explains.

At these extremes, carbon can transform into a metallic liquid and take on exotic solid phases. That includes BC8 (body-centered cubic), a structure predicted to form at above 1,075 gigapascals – more than three times the pressure found in Earth’s core – in which carbon atoms arrange in a cubic lattice of eight atoms per cell.

These unusual forms fall under carbon’s equation of state, which characterizes a material’s state of matter under particular physical conditions. Modeling elements’ full range of equations of state informs a range of science applications related to the U.S. Stockpile Stewardship Program, including understanding matter’s behavior in planetary interiors, says Laurence Fried, scientific capability leader for Livermore’s Chemistry Under Extreme Conditions group in the Chemical Sciences Division.

“Our view of matter is skewed by the fact that we live here on the surface of the Earth,” Fried says, noting that we also need to pay attention to matter inside planets.

Since Goldman began at the laboratory as a post-doctoral researcher, he and Fried have improved computational methods for modeling matter under extreme conditions. In 2005, their first joint paper used ab initio, or starting from basic conditions, quantum molecular dynamics calculations to verify theoretical predictions of what happens to water when it’s squeezed in a planetary gravitational vise.

They found that at pressures like those within Uranus and Neptune – and now in possibly hundreds of Neptune-sized exoplanets – water forms an exotic superionic phase. In this hot ice, water’s oxygen atoms form a stationary lattice, while hydrogen protons zip through the material.

Here on Earth, this quantum molecular modeling prowess could provide an unprecedented view of the physical transformations occurring in carbon-based NIF fuel capsules.

“The capsule candidate material of choice is often dependent on the results of recent simulations,” says Goldman, whose father, Bob, is a retired theoretical plasma physicist at Los Alamos National Laboratory.

NIF capsule candidate materials are primarily carbon-based, including conventional plastic polymer ones and new and promising nanodiamond coated ones, or high-density carbon (HDC) capsules.
IN blockbuster movies, cosmic collisions always threaten to end life on Earth. But Lawrence Livermore National Laboratory computational chemist Nir Goldman has shown that early comet impacts might have provided just the right stuff to begin terrestrial life.

Ancient cometary crashes into Earth’s surface could have transformed the simple molecules in these dirty ice balls into more complex life-precursor molecules, including the structural sub-units of DNA and amino acids, Goldman’s recent computational simulations suggest.

“That’s the surprising conclusion” of results that in 2013 made the cover of The Journal of Physical Chemistry A, Goldman says. “We found that the shock conditions of a cometary impact provide a unique set of thermodynamic conditions, ones that increase the level of chemical complexity rather than reduce it.”

In the late 1980s, astrobiologists led by Carl Sagan suggested that rather than pulverizing Earth’s natal biochemistry, asteroid and cometary impacts fueled it.

Goldman’s findings both support this cosmic delivery hypothesis and extend it. Not only do comets contain life’s simplest molecular components, Goldman’s detailed quantum mechanical molecular dynamics simulations on cometary impacts show that there is “shock synthesis” of more complex organic molecules.

The simulations, run on Livermore’s RZCereal and Aztec supercomputers, start with a molecular cocktail typical of comets: water, carbon monoxide, carbon dioxide, ammonia and methanol. In the simulations this mix was computationally shocked to mimic the conditions of a glancing impact, producing lower pressures and temperatures than a head-on collision.

Crucially, Goldman greatly extended the time frame of his previous shock synthesis simulations, published in 2010 in Nature Chemistry. The earlier impact model simulated up to 30 picoseconds of impact chemistry, whereas the latest, developed with post-doctoral researcher Isaac Tamblyn, went to hundreds of picoseconds – much closer to chemical equilibrium.

The longer time frame revealed that what’s key to cometary chemical shock synthesis is cycling the material through an impact’s three thermodynamic stages: shock compression due to impact, followed by expansion, and then cooling to ambient conditions. This process forms complex carbon- and nitrogen-containing molecules, including amino acids and ring-shaped aromatic molecules that are essential to life on Earth.

When Tamblyn, now an assistant professor at the University of Ontario Institute of Technology, first looked at the simulation results and saw aromatic compounds such as benzene made from a shock wave, he thought, “Wow – you could start to form lots of different structures through this process,” he says.

There’s a close overlap between this chemical origins of life modeling and stockpile stewardship research, says Laurence Fried, who leads Livermore’s Chemistry Under Extreme Conditions group.

“The cometary impact simulations and stockpile stewardship high-explosive models have approximately the same mix of elements: carbon, hydrogen, nitrogen and oxygen,” Fried says.

“For stewardship we want to have models that are more predictive so that if a change is observed in an organic high-explosives stockpile component we can predict how that would affect performance.”

Just months after Goldman and Tamblyn published their results, a British-led experimental group confirmed their simulation predictions by firing steel projectiles at cometary ice analogs to produce amino acids.

Goldman has applied for a second round of NASA astrobiology support to further pursue the research, and notes that his simulations have added depth to the search for the prebiotic origins of life. “We’ve put impact synthesis out there as a possibility that needs to be seriously considered.”

Finessing fuel capsule dynamics is essential to achieving fusion. At NIF, lasers instantaneously heat a capsule, causing its outer shell to ablate, or blow off explosively. The reciprocal internal shock compresses the hydrogen isotope fuel, triggering a fusion reaction like those found in a star or a detonating nuclear weapon.

In 2012 NIF scientists imploded a nanodiamond capsule to achieve a record yield of neutrons from the reaction. But for developing predictive models for HDC capsule design and experiment configurations (such as power of the laser pulses), there’s still significant uncertainty in their equations of state.

Capsule scientists, Goldman says, “really need an accurate prediction for how the materials behave over an extremely broad range of pressures and temperatures, and there are very few models that can cover this broad range accurately.”

TWO STEPS FORWARD

Goldman’s new carbon-at-the-extreme computational model arose from three years of intensive effort with colleagues to make existing quantum molecular computer codes more efficient, so they can capture time scales relevant to experiments.
At its core, Goldman’s new model is based on the Density Functional Tight Binding (DFTB) method. DFTB is a more computationally efficient variant of Density Functional Theory (DFT), the well-established quantum molecular materials modeling method. DFT has accurately reproduced carbon’s extreme temperature and pressure phase boundaries.

“The problem with DFT is that it’s too computationally intensive and can’t be used to model the necessary experimental timescales,” Goldman says. “Even with a supercomputer you have to work pretty hard to get a short trajectory that spans only 10 picoseconds. The experiments, on the other hand, tend to span much longer time scales. They can be nanoseconds long, a thousand times longer.”

To achieve greater computational efficiency, DFTB uses an approximate quantum mechanical description of electron states to model atomic interactions. Instead of explicitly calculating electron interactions from scratch during the simulation and then performing quantum mechanical operations, the model uses a previously created library to compute the quantum mechanical electronic states – an on-the-fly, off-the-shelf approach.

In 2011 Goldman gave the then-seminal DFTB method a dry run on Livermore’s supercomputers to model diamonds under extreme shocks.

“It was horribly inaccurate for all kinds of reasons,” Goldman says. “It just didn’t work at all under high thermodynamic conditions.”

Developing a next-generation DFTB model meant going back to basics to understand the carbon inter-atomic dance at extreme pressures and temperatures. It turned out there were two more key steps the model needed.

The first involved how carbon’s electrons behave under duress. High school students learn that carbon’s six electrons occupy the lowest-energy s- and p-orbitals. “When you get to really hot, compressed conditions, carbon forms a liquid metal,” Goldman says. “The atoms rearrange in such a way that the higher energy d-orbitals start getting occupied as well. You have to have some mathematical representation of those d-orbitals in your calculations to really get accurate properties out.”

During developmental runs on the laboratory’s massively parallel computers, the researchers found that adding d-orbital electrons greatly improved the model’s accuracy. Yet even with d-orbitals in the quantum mix, something was missing.

“We were having this trouble with our model development,” Goldman recalls. “We dug around in the literature and found this idea about including electrostatic screening in these types of models to moderate atomic interactions.”

Like two basketball forwards along the court baseline with an opposing team’s player between them, in extreme conformations three carbon atoms can be thought of as lying side-by-side in a row. In this formation the interaction of the outer two atoms is screened, or weakened, by their interaction with the intervening one.

“Including screening enables much better prediction of known experiments because it prevents overestimation of the atomic interactions due to the approximate quantum mechanical approach,” Goldman says of work done primarily by Sriram Goverapet Srinivasan, a summer student at Livermore in 2012 and 2013.

“Without the addition of that screened interaction, it wasn’t possible to get to the level of accuracy that we needed.”

The resulting model is called DFTB-p3b, in which p stands for the polarizable d-orbitals, and 3b for the three-body repulsive energy of the in-line carbon atoms.

DFTB-p3b “yields approximately two orders of magnitude increase in computational efficiency over standard Density Functional Theory while retaining its accuracy for condensed phases of carbon under a wide range of conditions, including the metallic liquid phase at conditions up to 2,000 gigapascals and 30,000 Kelvin,” the authors wrote in *The Journal of Physical Chemistry* in 2013.

Goldman says his ultimate goal is to run a new generation of NIF fuel capsule simulations. “With the new code we can get closer than ever to experimental nanosecond time scales and actually tell experimentalists what it is they’re seeing,” he says.

Fried agrees. “This model could eventually enable us to use quantum mechanics to explore the NIF capsule experimental time scale and allow us to see whether there are any slow kinetic processes that you don’t see at a picosecond but we would at a nanosecond.”

Inspired 20 years ago by the ideal pingpong serve, Goldman’s latest model might one day help achieve the perfect shot that will make controlled nuclear fusion a reality.
ON THE LAST DAY OF FEBRUARY 2013, word of a strange and surprising research result began to spread through a large building at Sandia National Laboratories in New Mexico. The experiments had merely tested a newly installed instrument. No one had expected it to produce dramatically different results, especially at the relatively weak magnetic fields of these first tests.

One and two at a time, scientists congregated around a monitor at the imaging laboratory to see new pictures from Sandia’s giant Z machine that had just been processed. The researchers marveled at the digitized depictions. “We were all looking at these pictures and saying, ‘Wow,’” recalls Stephen Slutz, a Sandia theorist and originator of Magnetized Liner Inertial Fusion (MagLIF), the concept behind the new instrument.

Sandia’s Z machine delivers the world’s most powerful jolt of electrical current and, as a result, creates a brawny azimuthal magnetic field. Often called just plain Z (without the “machine”), the instrument is used for a variety of research purposes. One, as on this February day, is to compress nuclear fuel and trigger fusion reactions, a process called inertial confinement fusion, or ICF. Not all ICF technologies use magnetic fields to crush the fuel, however.

When Z, 6 meters tall and 33 meters in diameter, was set into action, a 20-million ampere current raced through a liner, a metal can the size of a pencil eraser. The liner contained deuterium, a hydrogen isotope used as nuclear fuel. In just 100 billionths of a second, the machine produced a crushing magnetic grip called a Z pinch. It imploded the tiny container and its contents, reducing the fuel to just twice the thickness of a human hair or less. In response, the fuel emitted a smattering of neutrons, a sign that deuterium nuclei had fused to create helium.

Scientists have imploded liners of fusion fuel before, but this trial was different. Just before the implosion, the installed instrument – two magnetic coils, one above the liner and another below – created an additional, weaker magnetic field. The instrument, specially adapted to the Z machine, is called ABZ for Applied B-field on Z. ABZ generated an axial magnetic field – magnetic field lines through the length of the liner.

The plan was to move a step closer to achieving self-heating, self-sustaining nuclear fusion ignition by trapping heat inside the fuel during implosion. As the fuel temperature rose, field lines would rein in the outward movements of electrons and newly formed alpha particles. The restrained particles would be forced to dump their energy into the fuel instead of carrying it away.

By the time the Z machine was activated, everyone had evacuated the enormous room housing it. The device’s current rushed to the center from all sides. When Z fires, it sends palpable vibrations through the ground and into the surrounding buildings.

A twist in research at Sandia National Laboratories called MagLIF – magnetized liner inertial fusion – amps energy yields and portends promise for both stockpile stewardship and nuclear fusion energy.

By Andy Boyles
The implosion rewarded the research team with a burst of about 5 billion neutrons. But the experiment also held a surprise – one that convened a spontaneous scientific conference in the imaging laboratory.

X-ray images showed the liner had imploded in a remarkable way. Unlike in previous experiments, this liner did not develop familiar and frustrating instabilities along its length. These magneto-Rayleigh-Taylor instabilities, which often look like an alternating series of bulges and pinches, can quash fusion, ripping a liner open and stopping reactions as they begin.

Instead, the image showed the instabilities were reduced to crisscrossing helices weaving a mesh around the liner.

**JOULES IN THE BILLIONS**

Since that day, MagLIF has had greater neutron yields. It also has stimulated new research to understand how MagLIF stabilizes imploding fuel liners and to tune this unexpected property for greatest effect on both nuclear fusion energy and stockpile stewardship.

“Single-shot high-yield fusion targets would have a profound effect on stockpile stewardship,” says Sandia physicist Thomas Awe, who led the February 2013 experiment. Shots producing energy in the millions or billions of joules “would generate radiation fluxes and neutron yields that would allow unprecedented materials-science and radiation-effects testing for stockpile stewardship.” But such implosions are “likely beyond the capability of any stockpile stewardship facility existing today, and a good understanding of the relevant physics will be required for us to justify building a facility capable of achieving it.”

Commercial energy generation from fusion would require not only a high-yield target, Awe says, but also imploding many such targets in rapid succession. “For inertial fusion energy (IFE) production, the need for repetitive high yield introduces an extensive list of additional challenges.” Some fusion power models call for 10 implosions per second, with each producing tens of megajoules. Others aim for an implosion every 10 seconds at more than a gigajoule each.

That means building new lasers or pulsed-power machines (like Z) capable of repeated operation, with the device and surrounding power-plant infrastructure shielded from shock waves, intense radiation and extreme neutron fluxes, Awe says, plus the capacity to produce thousands to nearly a million fusion targets per day.

“Developing a single-shot, high-yield fusion target would undoubtedly be useful toward solving many of the challenges associated with high-rep-rate IFE.”

These visions of inertial fusion power were seeded six years ago, when Slutz began considering novel ways to make ICF work. His contribution came about partly through inspiration, partly through necessity. Before he took on the problems of imploding liners, the Sandia team was studying the ICF method under investigation at Lawrence Livermore National Laboratory’s NIF (National Ignition Facility) and elsewhere.
In the NIF approach, researchers put deuterium or both deuterium and tritium, another hydrogen isotope, into a spherical capsule and then place it in a small metal can similar to a liner. This container, called a hohlraum, is designed to emit or reflect X-rays under certain conditions. The X-rays inside a hohlraum bombard the fuel-containing capsule, converting its outer layers into plasma. The plasma shoots outward in all directions like rocket exhaust, and the resulting inward inertia implodes the plasma and its fuel. In recent trials at NIF, new approaches to this form of ICF produced more energy than that entering the fuel. (See sidebar, “A Shot at History,” page 23.)

Whereas the NIF team used lasers to make X-rays in its experiments, the Sandia group used the Z pinch to produce them. In the mid-2000s, administrators decided Sandia research should seek an ICF path markedly different from that at NIF since NIF was better able to demonstrate the relevant capsule physics than Z.

Slutz knew Sandia had not yet tried one possible tack. Instead of using X-rays to implode a capsule of fuel, the group might use the Z pinch’s magnetic fields to crush the fuel directly.

One potential advantage to this approach is an enormous savings in energy lost when compressing the fuel in the hohlraum-and-capsule system. In methods that rely on X-rays, energy losses mount with each level in a cascade from magnetic or laser energy to X-ray energy to the kinetic energy of the plasma that pushes inward on the fuel capsule. Using the Z pinch itself to crush a liner filled with fuel would skip two levels in the cascade and thus funnel more of the initial energy directly into the implosion.

But researchers have focused on magnetically driven implosions for decades without achieving self-heating – when helium nuclei, also called alpha particles, created in the reaction contribute their energy to sustaining and boosting the reaction. Before and apart from the Sandia work, a joint team of researchers at Los Alamos National Laboratory and the Air Force Research Laboratory, both in New Mexico, also has been moving toward using magnetically driven implosions to crush nuclear fuel and generate a self-heating bounty of alpha particles.

Like the Sandia’s Z-pinch team, the Los Alamos/Air Force group is experimenting with additional magnetic fields that run through the fuel, trapping heat by containing electrons and alpha particles. But the Los Alamos/Air Force group’s implosions are comparatively slow, taking 10 millionths to 20 millionths of a second on the Air Force’s Shiva Star pulsed-power facility. As a result, this group uses liners that are fairly large – about 30 centimeters long and 5 centimeters in diameter. Liners of this size implode efficiently at Shiva Star’s implosion speed.

CHARGED PARTICLES PULL A U-TURN

Inside these liners, the Los Alamos/Air Force group has employed an established magnetic field set-up called a field-reversed configuration, or FRC. The goal is to constrain the fuel within a configuration of magnetic field lines that are closed loops. Once an FRC is deployed, charged particles flowing along the field lines can’t go out the ends of the liner. Instead, they’ll each perform a U-turn at the end of the liner and plunge back toward the center. The more alpha particles an FRC can retain, the closer the implosion will get to a self-heating state.

But the FRC cannot take form inside the liner. “They have to make this field-reversed plasma configuration outside of the liner and then transport it inside the liner – push it down a tube, kind of like toothpaste – then implode it,” Slutz says. Such a feat is hypothetically possible, he says, but quite difficult. “I got interested because I saw that is a hard problem, and I started thinking, ‘What can we do at Sandia?’”

In contrast to the Shiva Star, the Z machine implodes its target in 100 billionths of a second.

To implode efficiently in such a short time, fuel-filled liners compressed on the Z machine have to be much smaller than those used on Shiva Star. A smaller space makes the transport of an FRC into the liner that much more difficult. “We needed a much simpler field,” Slutz says.
He reasoned that a field line arrangement that doesn’t curl up inside the fuel might work, as long as the liner was long enough and the fuel was dense enough. Open field lines that run the length of the liner would still stop charged particles from shooting out at right angles to the field lines, but they would not restrain any material from flowing out the ends. The liner had to be long enough and the fuel had to be dense enough that energy-bearing electrons and alpha particles moving at their usual pace would not escape before fusion reactions could take place. Luckily, Z’s shorter implosion times allow higher fuel densities and, Slutz’s calculations showed, a length of 0.5 cm to 1 cm would be sufficient.

Slutz realized the group could improve its results further by preheating the fuel. Cold fuel would have to be compressed to such an extent that an overwhelming number of instabilities would emerge and tear the liner apart.

Slutz recalls thinking about these problems seriously for the first time during Christmas vacation in 2007. He began the new year by taking his ideas to Mark Herrmann, who now directs Sandia’s Pulsed-Power Science Center, and physicist Roger Vesey. The three share a commitment that has helped sustain the work, Slutz says.

Since this early work, Slutz and physicist Adam Sefkow have been running simulations of the implosions – Slutz using the Lasnex ICF design code and Sefkow using Hydra, a 3-D ICF radiation hydrodynamics design code – to refine understanding and determine the best working parameters. This work set the stage for installing ABZ and the remarkable modification to the observed instabilities.

No one knows how or why this striking change occurs. Until physicists understand how the helices form, they won’t know if they can ramp up the power to give the liner even more stability.

**FINE-TUNING Z APPROACH**

Matthew Gomez, a former Department of Energy National Nuclear Security Administration Stewardship Science Graduate Fellowship recipient, has taken on the role of lead researcher for more recent experiments. Gomez did an internship at Sandia while he was an undergraduate at the University of Michigan. With SSGF support, he served a practicum at Sandia and received a 2011 doctorate in plasma physics and fusion from the same university. “I learned enough about Z to know that that was what I wanted to do,” he says.

Under Gomez, the MagLIF program has moved into a new phase of research, with fuel preheating added to the system. The implosion is done as before except that a laser shines through a window in the liner’s top and heats the fuel just as the Z machine begins to crush the container. The goal is to hit a temperature of 100 electron volts before compression.
As in prior MagLIF experiments, Gomez and his colleagues use only deuterium. Using all three aspects of the technique – the Z pinch, the axial magnetic field and laser preheating – two recent trials yielded 500 billion and 2 trillion neutrons, respectively. In other words, adding laser preheating increased the yield by 100 to 500 times. If they used deuterium-tritium instead of deuterium, the yield would increase by another factor of 80.

The MagLIF team has a number of goals. It’s working to increase the Z machine’s current, the strength of the axial magnetic field, and the heat the laser delivers. These steps, planned for the next two years, are predicted to increase yield by as much as 100 times.

The group also intends to develop better ways to measure how the liner changes shape and the instabilities on its inner wall as the fuel pressure peaks. Finally, the researchers want to measure leakage of the axial magnetic field out of the liner during compression and to discover how effective the axial magnetic field really is at trapping heat within the fuel.

“Of note is the fact that Congress wants an evaluation of the prospects for inertial confinement fusion from the NNSA by the end of fiscal year 2015,” Awe says. “A magnetically driven implosion (such as MagLIF) is one of three mainline approaches to inertial confinement fusion being pursued by the United States.” The other two are indirect drive, using a hohlraum container and fuel-containing capsule, and polar direct drive, a means of using lasers instead of X-rays to implode a fuel-containing capsule. “Our high-level goal is to demonstrate enough understanding of MagLIF by then in order to assess whether this is a promising path forward worthy of continued investment by the taxpayers.”

A year after Sandia National Laboratory physicists stumbled on a discovery representing a step toward successful inertial confinement fusion (ICF), Lawrence Livermore National Laboratory researchers reported hitting another milestone on the journey.

The team at NIF, the National Ignition Facility, that triggered fusion reactions generating more energy than had entered the fuel includes Laura Berzak Hopkins, an alumna of the Department of Energy National Nuclear Security Administration Stewardship Science Graduate Fellowship. Berzak Hopkins was one of 22 coauthors who published the results in the Feb. 13, 2014, Nature. She received a doctorate in plasma physics from Princeton University in 2010 and completed her practicum at Sandia. Sandia’s experiments use its massive Z pulsed-power machine to generate magnetic fields that crush hydrogen isotopes – typically deuterium – in an attempt to force the atoms together so they fuse, releasing tremendous energy.

NIF uses lasers in an indirect-drive fuel compression technique. In recent experiments, the NIF team began with a 2 millimeter-diameter plastic capsule containing a mixture of deuterium and tritium, another hydrogen isotope. The capsule is held in a gold can, or hohlraum, measuring about 1 centimeter long and 0.5 centimeter in diameter. NIF fired 192 laser beams into the top and bottom of the hohlraum, where they interacted with the gold, converting laser energy into X-rays that bombarded the capsule.

The X-rays rapidly burned away the capsule’s outer layers, converting them into plasma that was propelled outward in all directions. The resulting inward inertia imploded the fuel, creating extreme heat and pressure that fused the deuterium and tritium nuclei, forming helium nuclei and releasing large amounts of energy.

But ICF faces a stubborn problem: The capsule tends to become unstable as it collapses, deforming into non-spherical shapes or even breaking apart. Either of these events will foil an efficient collision of fuel nuclei at the center.

Berzak Hopkins, a Livermore design physicist, worked closely with experimental physicist Sebastian Le Pape in the lead-up to the new experiments. “My role is to take the as-shot laser pulse, study the shock structure it delivers to the capsule and tune the shocks,” she says. “We want them to merge at very specific points within the capsule.”

She also is part of the larger team that determines adjustments to the frequency of the laser beam bundles so energy is redistributed between beams to improve implosion symmetry. The result is a hotter, shorter burst of laser energy at the beginning of each shot, leading to an improved distribution of X-rays and a record-breaking generation of ICF energy.
Starstruck

BY JUAN MANFREDI

The first moments of our universe still are mysterious, but we know that in the beginning there was the Big Bang. We also know that after a millionth of a second, protons (hydrogen atoms) and neutrons formed. Two hundred million years later, these particles began condensing into massive balls of plasma, commonly called stars.

Inside stars’ nuclear furnaces, protons and neutrons fuse to form the two-proton atom helium, slightly heavier than the single-proton hydrogen. As stars produce more helium, it reacts with other neutrons and protons to make even heavier elements, like carbon. After a few billion years, stars explode as supernovae, firing up their internal nuclear combustion engines enough to create heavier elements (like gold, titanium, lead, calcium, and many others we can’t imagine living without). Over the eons, myriad supernovae have spread these particles across the universe, where they became the seeds for planets and more stars. Nuclear reactions, in other words, tell the story of the cosmos.

Stars, light-years away, do not make for an ideal laboratory setup. Here on Earth we do our best to simulate their internal conditions on a smaller scale. I do my research at the National Superconducting Cyclotron Laboratory (NSCL) at Michigan State University, where we accelerate nuclei to half light speed before smashing them to pieces against a foil target. (Many of these pieces are rare nuclei that naturally exist only in the thermonuclear guts of stars or supernovae.) From there, magnets transport the nuclei to any of several experimental stations, where scientists reproduce and analyze the actual reactions that form and destroy stars. These reactions often produce nuclei that decay so quickly we can detect only their remains. Just as collecting debris from a car accident can help determine what the vehicles originally looked like, the products of a nuclear reaction or decay can help us piece together the structure and behavior of the rare parent nucleus. Specifically, we can deduce its weight, how it decayed, and how the protons and neutrons were arranged inside it. This information then helps us determine when, and how quickly such reactions occur in the cosmos.

To probe stars’ inner workings further, my thesis project studies fission – splitting heavy nuclei into two smaller chunks. An important example of this process is uranium fission, a reaction that has powered every nuclear plant in the country for decades and that scientists have studied for even longer. The breakup of heavy, exotic nuclei (which have a remarkably high or low ratio of neutrons to protons) taking place in stars is much more complicated than splitting uranium. There are lots of theories on how fission in this region works, but we need data to test them.

In pursuit of such information, my thesis experiment at NSCL next year will study lead-196, one of many exotic fissile nuclei within our lab’s reach. By measuring its products, we’ll reconstruct the parent lead-196 nucleus and determine its fission barrier – how much energy is needed to split it. We’ll compare that with the fission barriers of more common lead isotopes to see how fission changes for rare nuclei.

Although experiments like this are exciting and full of possible discoveries, more powerful equipment is needed to truly understand the way fission of heavy exotic nuclei works. The Facility for Rare Isotope Beams (FRIB, also at Michigan State) will be complete in 2022, allowing scientists to explore questions about this special type of fission. FRIB will accelerate nuclei to 57 percent of light speed, allowing for the production of more than 1,000 new isotopes. My thesis project will be the first experiment in an international campaign to study exotic fissile nuclei. This program will continue once FRIB opens, expanding the fission frontier into unexplored territory. FRIB also will collect unused isotopes for medical treatment and research as well as generate thousands of construction jobs and an estimated local economic impact of $1 billion over 20 years.

But there lies a deeper, more instinctual drive behind nuclear astrophysics, one going beyond intellectual curiosity and the practical benefits. Studying reactions that create basic elements answers the question of where we and our planet came from. It’s as grand an origin story as humanity has ever seen: In the blazing fires of exploding stars, components of life were forged and launched across the universe. These scattered components clumped together into stars and planets, including Earth, where humanity emerged as a way for the universe to study itself. The same sense of wonder that for thousands of years drove humans to look up and ask why inspires scientists to look inward and ask how. In this evolving quest for answers, we are finally on the verge of fully simulating and studying our true birthplace: the stars.

Juan Manfredi

The author is a second-year fellow at Michigan State University. “Starstruck” won first place in the 2014 SSGF Essay Slam.
DOE NNSA SSGF FELLOWS

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SSGF PROGRAM
Researchers experimenting at the National Ignition Facility can infer pressure-temperature-density properties, but they have no way of probing what’s happening on the atomic scale. Calculations like the one visualized here, which calculates the chemistry of diamond compressed and heated to about 12,000 degrees Kelvin, allow Lawrence Livermore National Laboratory researchers to infer atomic details. For more on the chemistry of extreme pressure, see page 15.