

September 2018

Science & Technology

REVIEW

COMBINING LASER CAPABILITIES

Also in this issue:

Machine Learning for Fusion Energy

Metal Hardening Demystified

Insights into Traumatic Brain Injury

About the Cover

An important aspect of inertial confinement fusion (ICF) research at the National Ignition Facility (NIF) is determining what changes occur inside an ICF target struck by NIF's beams, as even seemingly minor variations in the evolution of a shot can affect whether fusion is likely to be achieved. As the article beginning on p. 4 describes, NIF researchers now have the Advanced Radiographic Capability (ARC), a "laser within a laser" that can capture information about previously inaccessible phenomena inside an ICF target. With the high-intensity light it shines on extreme conditions inside these targets, ARC is yielding surprising findings that are having an impact on a broad range of Laboratory missions supported by NIF research.



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Catalysts to Convert Carbon Dioxide

Lawrence Livermore researchers have received \$1 million from the Department of Energy (DOE) to improve the energy efficiency of copper-based catalysts to convert carbon dioxide (CO₂) into methane and other valuable hydrocarbon products. Led by Livermore's Juergen Biener, the project will help meet the nation's future energy needs by converting low-cost, abundant resources into commercially viable fuels. Catalysts play a key role in such efforts, converting CO₂—an industrial waste product—into methane, a versatile fuel that can be readily integrated into efforts to fuel vehicles and power plants. Catalysts can also convert excess electrical energy produced by renewable energy resources, such as solar and wind, into chemical energy, making it easy to store the energy for future use.

However, current electrochemical catalyst technologies are energy intensive and costly and therefore unlikely to be competitive with traditional fuel production methods. The new work is aimed at overcoming the limitations of current approaches that use catalysts to convert CO₂ into fuels.

To optimize the catalysts' performance, the team will fully integrate the Laboratory's unique expertise in the synthesis and characterization of nanostructured dilute alloy transition metal catalysts with atomically precise active sites, along with the multiscale modeling of electrochemical interfaces. This project was funded by the DOE Advanced Manufacturing Office to support early-stage, innovative technologies and solutions in advanced manufacturing.

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Scientists Design Conceptual Asteroid Deflector

Livermore scientists are part of a national planetary defense team that designed a conceptual spacecraft to deflect Earthbound asteroids and evaluated whether the craft could nudge off course a massive asteroid that has a remote chance of hitting Earth in 2135. The design and case study are outlined in a paper published in the February 2018 edition of the journal *Acta Astronautica*.

Dubbed HAMMER (Hypervelocity Asteroid Mitigation Mission for Emergency Response Vehicle), the spacecraft can serve as either a kinetic battering ram or as a transport vehicle for a nuclear device. The possible target is 101955 Benu, which has a 1-in-2,700 chance of striking Earth on September 25, 2135.

The design effort is part of a national planetary defense collaboration between NASA and the National Nuclear Security Administration (NNSA). The Livermore planetary defense team serves as technical lead for threat mitigation and also supports emergency response should mitigation fail. Unlike popular portrayals such as the movie *Armageddon*, the nuclear deflection

approach would involve detonating a nuclear explosive some distance from the asteroid. The explosion would vaporize a layer of the surface, thereby generating rocketlike propulsion as material is ejected from the asteroid.

Because Benu passes close enough to Earth every six years, researchers are able to estimate its orbit with enough accuracy to give a few decades' warning. However, for other objects that do not regularly pass close enough to Earth for radar observations, much more uncertainty exists. The good news is that most of these objects are much smaller than Benu.

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Optimizing Nanoparticles for in vivo Applications

Lawrence Livermore has been developing a novel class of nanoparticles (see image below) for biomedical applications that are highly biocompatible and offer advantages not found in other types of nanoparticles. Termed nanolipoprotein particles (NLPs), the nanoparticles are laboratory-made versions of high-density lipoproteins—or “good cholesterol”—that are used by the body to transport triglycerides and remove harmful “bad cholesterol” in the blood.

The Livermore team recently assessed how the structure of phospholipids used to prepare the particles impacts their stability under physiologically relevant conditions. This key information has important implications for using these NLPs in vivo and would provide insight into how to tune particle stability for applications ranging from diagnostics to drug delivery. The findings appear in the April 26, 2018, edition of the journal *Nanoscale*. The research was supported by the Laboratory Directed Research and Development Program.

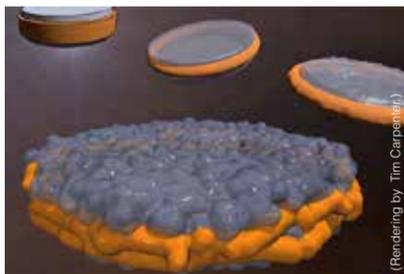
Nanoparticles are nanoscale objects, typically 1 to 100 nanometers in size, that can be used for a variety of purposes, including formulating medicines or vaccines. As of 2016,

51 nanoparticle drugs had already been approved by the U.S. Food and Drug Administration to treat a range of diseases, with another 77 candidates in clinical trials.

Although preliminary studies had previously demonstrated that the type of phospholipid used to synthesize these particles can affect their stability, how specific phospholipid features impact nanoparticle stability under physiologically relevant conditions was previously unclear.

Livermore's results demonstrated that the elasticity of the lipid bilayer—but not lipid surface area or thickness—is a significant indicator of particle instability in the body. These studies provide a foundation for subsequent optimization of NLP composition to tailor stability for the particular in vivo application.

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Emphasis on Learning Empowers the Laboratory's Lasers

THE National Ignition Facility (NIF), a laser the size of three football fields, creates conditions more extreme than those present at the center of the Sun. To build the largest and most energetic laser in world, capable of operating within precise microscopic realms and billionths-of-a-second timescales, required a remarkable series of achievements in design and engineering. NIF continues to grow in capability to support the National Nuclear Security Administration's (NNSA's) Stockpile Stewardship Program (SSP), the Discovery Science Program, and other national security applications.

Drawing on decades of high-energy and high-power laser innovation, Lawrence Livermore commissioned the petawatt-class Advanced Radiographic Capability (ARC) laser in December 2015 for the NNSA as an important counterpart to NIF. As described in the article beginning on p. 4, to become the most energetic short-pulse laser in the world, ARC was not only built on the shoulders of NIF, but was also constructed by sharing components at the heart of NIF. In short, ARC is a very big laser inside the biggest laser of all.

As with NIF, the complexity and sheer magnitude of ARC's energy and power output required much more than a flip of the switch before becoming not merely operational but efficient for its users. NIF operates 24 hours a day, 7 days a week, with a shot rate of more than 400 shots per year because the NIF team never stopped learning or raising the bar. The NIF team had to work hard to perform enough commissioning shots on ARC without disturbing the schedule for all the other NIF deliverables. Now, as the number of ARC shots begins to ramp up, we will see exciting results achieved by ARC applications. We expect ARC to continue to advance and deliver new insights and understanding vital to helping fulfill the Laboratory's missions.

We want to continue improving the quality of the implosions in NIF experiments so that less energy and power are required to achieve ignition. At the same time, we are exploring ways to increase the laser's energy and power. In March of this year, a shot achieved a record-breaking energy of 2.1 megajoules, which was 15 percent higher than NIF's design specifications.

For its part, ARC specifically addresses the effort to improve the quality of NIF implosions. Developed first and foremost for

SSP, ARC will enable us to look at implosions late in time and see what is happening at the final and most critical stages of compression. Only ARC can generate x rays strong enough to produce radiographs on NIF that reveal this information. High-energy backlighting and Compton radiography backlighting are two promising applications of ARC that will let us see more detail than ever before. This learning will continue growing our understanding of what is required to achieve ignition on NIF.

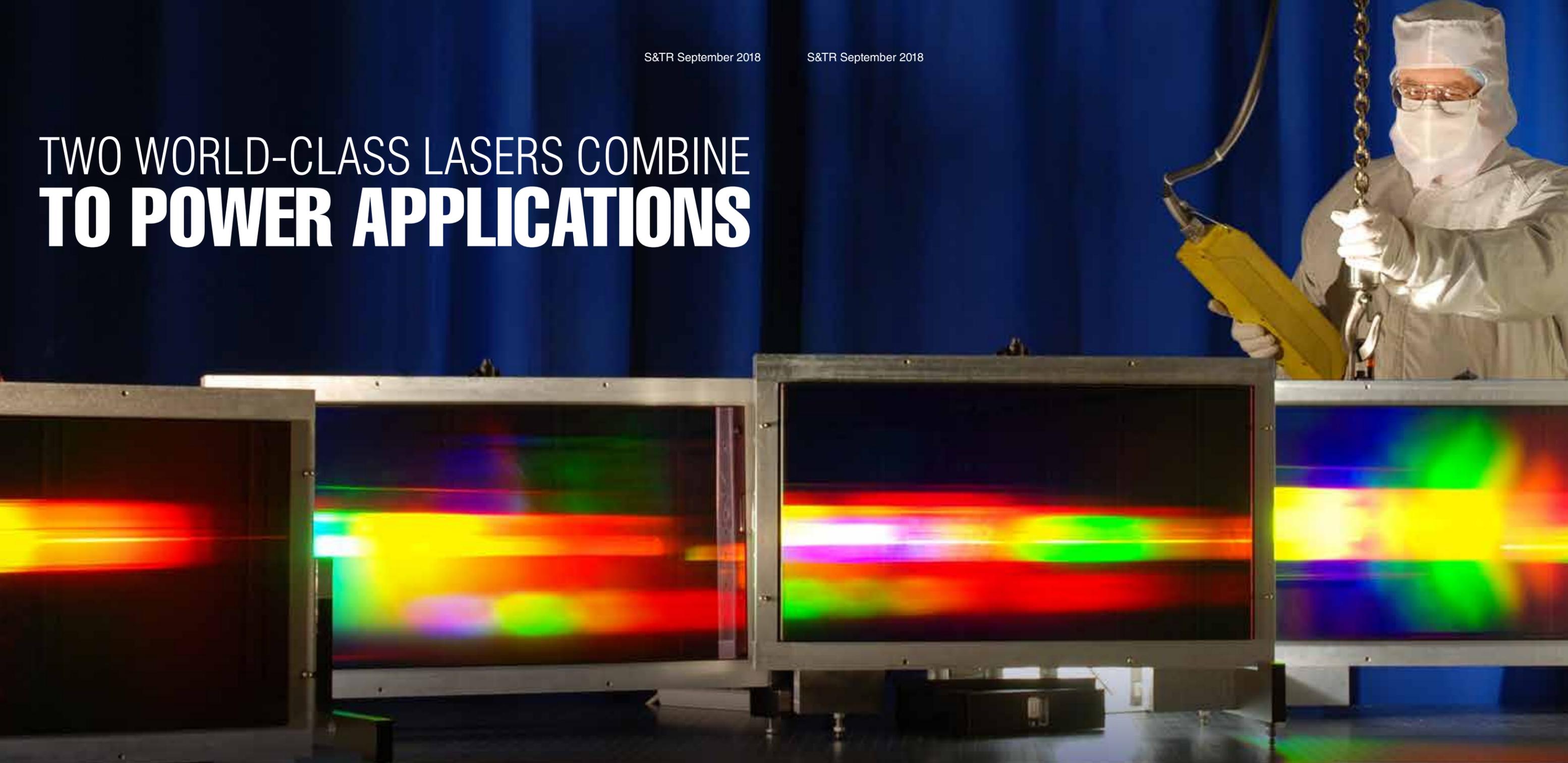
Every program that wants to remain on the forefront of science and technology must frequently infuse new ideas. By also using ARC for Discovery Science experiments investigating fundamental physics, such as proton acceleration and matter-antimatter pair creation, we broaden our expertise in experimental high-energy-density science, our innovations in diagnostics and target platforms, and our insights into the nature of the universe. Time and time again, Discovery Science platforms, diagnostics, and other capabilities have carried over to advancements in SSP.

To advance our laser design and engineering acumen, we continue to develop major new laser capabilities such as ARC. We have also built on our experience with ARC to develop another world-class laser. In June, the Laboratory commissioned the innovative High-Repetition-Rate Advanced Petawatt Laser System (HAPLS) at the Extreme Light Infrastructure Beamlines facility in the Czech Republic. (See *S&TR*, July/August 2017, pp. 4–11.) Taking only three years to design, build, and meet its performance goals, HAPLS pushes the limits of high-repetition-rate, high-average-power petawatt lasers, and again shows that Lawrence Livermore continues to be a world leader in innovative lasers.

As we learn, we want to challenge ourselves to embrace opportunities to learn even more—just what we are doing by developing world-leading technologies such as ARC. Stewardship of NIF means growing the next generation of science, engineering, and operations talent by constantly challenging these men and women to solve hard problems, so they are always ready to support the incredibly important missions with which the Laboratory has been entrusted.

■ Jeff Wisoff is principal associate director for NIF and Photon Science.

TWO WORLD-CLASS LASERS COMBINE TO POWER APPLICATIONS



The Advanced Radiographic Capability laser shines high-intensity light on extreme conditions inside the National Ignition Facility.

PREVIOUSLY, Livermore’s Petawatt laser was built into a beamline of the Nova laser. Today, the Advanced Radiographic Capability (ARC) laser follows the same “laser within a laser” strategy. The most energetic short-pulse laser in the world, ARC resides within the National Ignition Facility (NIF)—the most energetic of all the world’s lasers. Both operate simultaneously during

experiments, and synchronizing the enormous amounts of energy released by the billionths-of-a-second NIF with the trillionths-of-a-second ARC is nothing short of an operational wonder.

A major challenge for researchers using NIF to study high-energy-density (HED) plasmas and inertial confinement fusion (ICF) for the Stockpile Stewardship Program has

been examining the inside of the target to ensure that implosion is occurring in a highly spherical manner. (See *S&TR*, July 2015, pp. 3–14.) The greater the asymmetries and shape swings as the target compresses, the more performance is compromised. Different Laboratory missions require different target materials, and instabilities can adversely impact experiments in a multitude of ways,

A technician prepares four diffraction gratings for installation inside the Advanced Radiographic Capability’s (ARC’s) compressor vessel. The gratings squeeze each ARC beamlet into a high-energy, ultrashort laser pulse.

including reduced fusion yield in the case of ICF. As they strive to improve symmetry and robustness, researchers require a diagnostic tool that can reveal the shape of the target as it compresses, and increasingly ARC is being used to unlock these never-before-measured extremes. “ARC opens up an avenue that we didn’t previously have at NIF,” says David Martinez, a Livermore physicist researching HED science and who heads the team developing ARC for HED backlighting. “As we use NIF’s main laser to drive our targets to higher densities, pressures, and compressions, we now have in ARC a diagnostic that can see through these objects, look at perturbations, and probe further in time.”

X rays image a target’s interior in a manner similar to a doctor taking an image of a patient’s body. To block the x rays from parts of the body not being examined, the doctor has the patient wear a lead-filled apron. However, if lead can stop x rays during a doctor’s visit, how can NIF image the interior of something far denser? For many applications, NIF accomplishes this feat by diverting a small subset of its main laser beams from the experimental target to a separate metal foil target for generating probing x rays of much higher energy. Yet even these NIF-driven x rays are not of high enough energy or flux to probe the target during the final stages of implosion or to see details in lightweight materials such as hydrogen isotopes, an important fuel for ICF. ARC seeks to overcome these limitations.

Since being commissioned in December 2015, ARC has been used in at least 64 shots, including platform-development firings. Beyond backlighting applications, ARC enables exciting new and diverse research into exotic matter and particle generation. Potential studies range from better understanding the nature of the most energetic events in

A diagram shows ARC beamlet path (red) moving from the National Ignition Facility’s (NIF’s) main beamlines to the compressor, parabolic mirrors, and into the target chamber (in cutaway). Some beamlines have been omitted to show ARC’s beam path.

the universe to improving methods for treating cancer.

Powerful Backlighters

In an ICF experiment, up to 192 main laser beams of NIF are fired into the interior of a hohlraum, a 1-centimeter-long, hollow gold cylinder. Inside the hohlraum is a spherical target capsule 2 millimeters (mm) in diameter and filled with a fuel comprising deuterium and tritium, both isotopes of hydrogen. From interactions between the laser beams and the gold, a flux of x rays is formed from all around the curved hohlraum wall, bathing the target capsule in an “oven” of x rays. The high flux of x rays, in turn, transforms the capsule’s outer shell into a rapidly expanding, high-temperature plasma, blasting like a rocket engine. The massive force accelerates the shell inward at a speed reaching over half a million miles per hour, compressing the target capsule to a sphere only 0.05 mm in diameter, or 40 times smaller than its original size. Squeezed at such enormous pressure, the fuel inside the capsule becomes more than 22 times denser than lead, and the resulting central hot spot reaches a temperature exceeding 100 million degrees Celsius. Under these conditions, the hydrogen isotopes undergo nuclear fusion. This is how the energy of a star is born inside NIF.

With early backlighter technology, x rays were generated by up to eight

of NIF’s main laser beams focused onto a small metal foil, delivering as much as 60 kilojoules (kJ) of energy at an intensity of 2×10^{16} watts per square centimeter (W/cm^2). The x rays formed through laser-material interaction in a manner similar to when NIF’s beams strike the hohlraum’s gold wall. The specific energy depends on laser beam characteristics and the material comprising the foil. Metals such as iron, zinc, and molybdenum all emit different line spectra of x rays when irradiated, yielding photon energies ranging between 6 and 18 kiloelectronvolts (keV). However, this x-ray approach allowed researchers to peer inside the target capsule only during the early stages of compression, before the implosion became too dense. (In general, the higher the energy of an x ray, the better the penetration. The more x rays generated, the better the signal-to-noise ratio and clearer the x-ray radiographs of the target.) Furthermore,

these backlighters relied primarily on the target capsule’s atoms absorbing x rays by a process called photoelectric absorption, where the amount of absorption depends on the element and its density—the higher the atomic number (Z) and the more atoms there are, the more x rays are absorbed. With flesh and bone, for example, x rays pass readily through flesh, which is made of

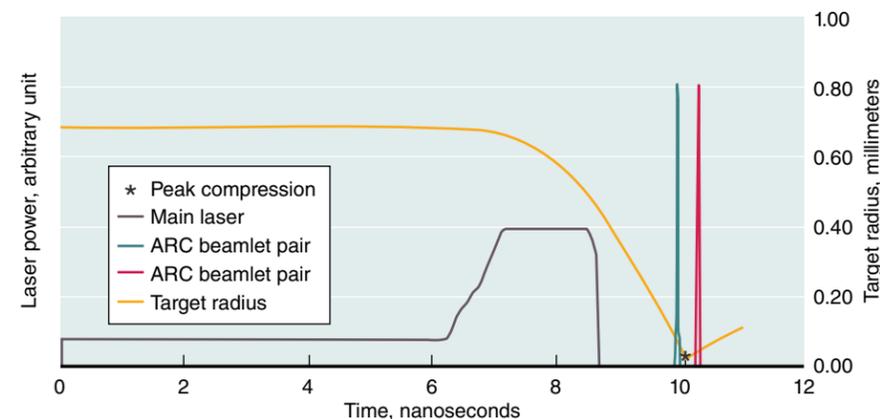
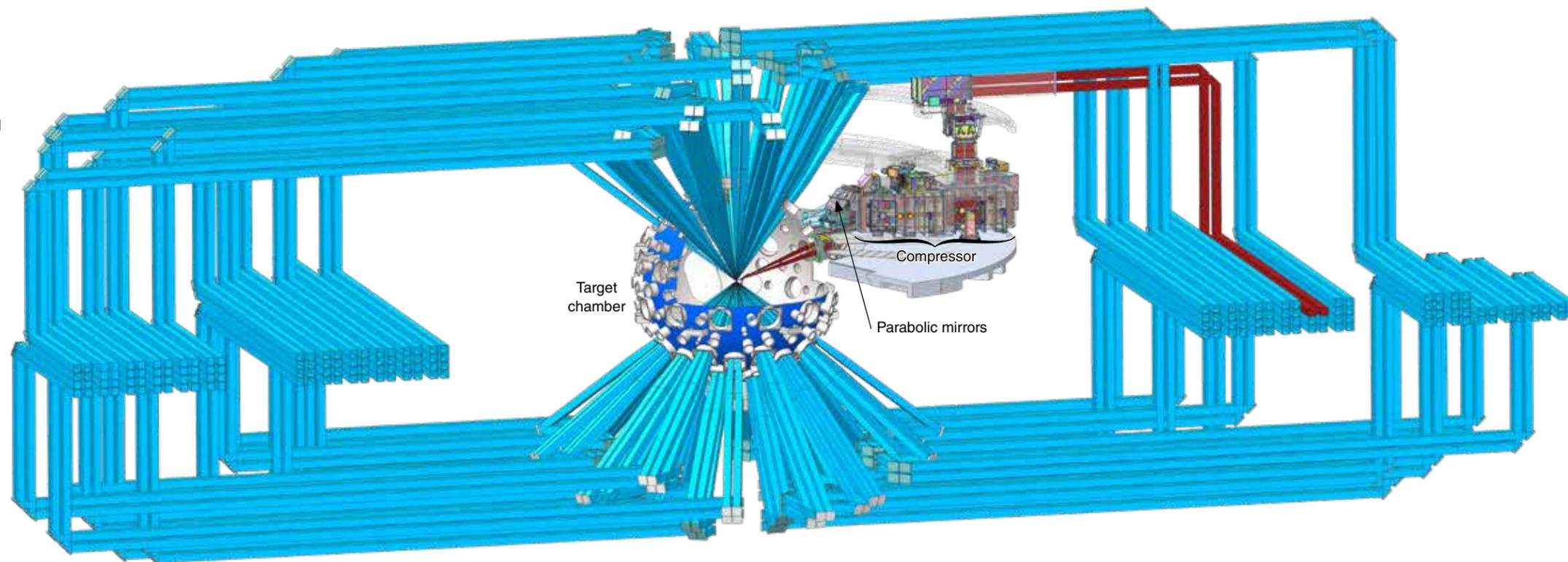
lighter elements than bone, which blocks many more x rays. Explaining the drawbacks of these early backlighters, Martinez says, “Hydrogen is the lightest element and is mostly transparent to x rays even at higher densities. The shell compressing the fuel is higher density, sometimes a metal. So, what we typically observed using those backlighters was only the shell around

the compressed fuel. In addition, an x-ray burst of up to 15 keV is produced by the hot, dense core at peak compression. For the measurements not to be overpowered by x rays from this flash, the backlighter needs to produce stronger x rays, but most of the early backlighters produced x rays below 15 kiloelectronvolts.”

Synergy between Lasers

Incorporating the ARC laser into NIF’s main laser enables x rays of higher energy and flux to greatly exceed previous diagnostic capabilities. ARC uses two beamlines from a single NIF quad (a group of four beamlines). In addition, ARC does not use the entire beamline but instead only the main and power amplifiers, with a specialized front end injecting the

The timings of the NIF main laser and two ARC beamlets are shown in relation to peak compression of a subscale target.



initial laser. In a process called chirped-pulse amplification, ARC's beamlets are stretched in time to spread out the laser energy and injected into the two beamlines in pairs travelling side by side through the amplifiers, after which the four beamlets are diverted from NIF's main laser beam path into a compressor for temporal recompression to provide a shorter pulse. The four resulting short-pulse beamlets are then each independently focused with parabolic mirrors and directed to the target through a dedicated port into the target chamber. (See *S&TR*, December 2011, pp. 12–15.)

The main NIF laser beams are converted from an infrared wavelength of 1,053 nanometers (nm) to an ultraviolet wavelength of 351 nm for better coupling to the hohlraum target. However, ARC bypasses this step both to mitigate the energy loss that occurs during wavelength conversion and to take advantage of target physics in which the conversion of laser energy to high-energy x rays is improved at longer laser wavelengths. ARC also differs

in pulse duration. Whereas NIF runs on the order of nanoseconds (ns), or billionths of a second, ARC clocks in about 1,000 times faster, at 1.3 to 38 picoseconds (ps), or trillionths of a second.

“The ARC beamlets propagate down the beamlines more than 60 nanoseconds before NIF's main laser fires because the longer path through the compressor delays the beamlets arriving at target chamber center,” explains Dan Kalantar, senior target area scientist and co-leader of the integrated product team that helps ARC users develop their target platforms. “For example, setting the timing to view an implosion at 16 nanoseconds after arrival of the main laser beams at target chamber center requires ARC beamlets to precede the main laser by close to 50 nanoseconds. Keep in mind that for some shots, ARC beamlets are typically staggered in pairs with a separation of only 200 picoseconds.” Because of the extremely high energy of both NIF's main laser and ARC, shielding the target

and backlighter from each other and from the side effects of the lasers, plasmas, and other forms of radiation is critical to minimize unintended interactions.

High-Energy Backlighter

Each of ARC's four beamlets can deliver more than 1 kJ of energy at an intensity exceeding 10^{17} W/cm², yielding x rays with photon energies of 10 to 200 keV. “For high-energy backlighting, we use the point projection radiography technique in conjunction with ARC to produce bremsstrahlung radiation,” explains Martinez. “This process generates an x-ray band of about 10 to 100 kiloelectronvolts.” In a typical HED setup to study high-Z materials, an ARC beamlet focuses to a spot of approximately 0.06 mm by 0.12 mm on a 0.01-mm-diameter metal wire positioned side-on to the oncoming laser light, creating a bright source of hard x rays. The diameter of the wire determines the size of the x-ray source—the narrower the wire, the higher the resolution—so

that small details in the target can be captured.

Although the process is still in development, results from recent experiments are highly positive. Martinez says, “We took radiographic images of a driven HED target—a copper foam ball—to see where the shock and ablation surfaces were as a factor of time, something that was very difficult to do with the previous backlighters. In addition, researchers were able to track the shock surface all the way to convergence, which is important because it reveals how well our drive is coupling to the target. We obtained the data we wanted, and they looked good.” Now, the team is optimizing the high-energy backlighter and expanding its use to larger systems and to conditions later in time. Because ARC's beamlets can be focused independently and fired at slightly different times from one another, ARC could enable not just one radiograph but up to four. “We'd like to take multiple radiographs during the same experiment,” says Martinez. “With more beamlets, you can separate them out in space and time, almost like a movie.”

Compton Radiography Backlighting

With ICF targets, radiographs more suited to imaging low-Z materials can be obtained using Compton scattering rather than traditional photoabsorption. Riccardo Tommasini, a plasma physicist working on ICF and leading Compton radiography development, explains, “Compton scattering originates from collisions between an x ray and a bound or free electron. In contrast to photoelectric absorption, which scales as the third power of Z, Compton scattering is sensitive only to the electron density of the material.” This difference makes Compton scattering ideal for probing the dense but low-Z deuterium–tritium fuel in ICF implosions near peak compression. Tommasini



adds, “The radiograph reveals a deficit in x rays traveling through the material, largely because x-ray photons are scattered away from the line of sight by Compton scattering. Being relatively independent of photon energy, broadband detection and the continuum emission of hard x rays of approximately 100 kiloelectronvolts can be used to filter out the x-ray flash produced by the implosion.”

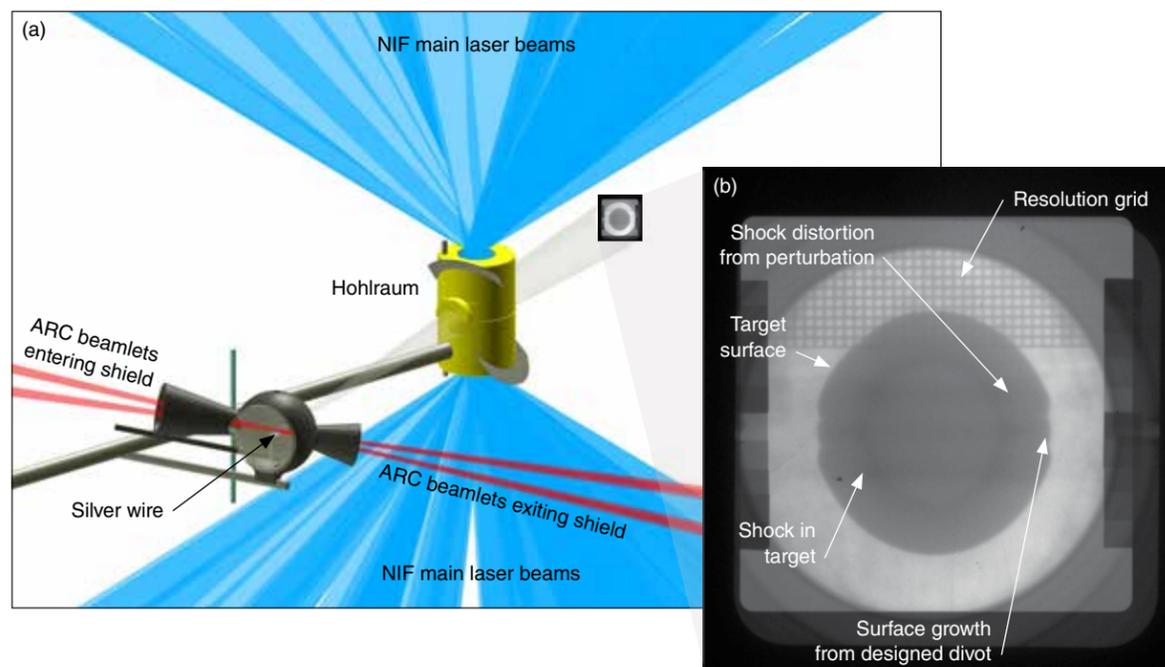
A Compton radiography backlighter involves two ARC beamlets hitting an approximately 1-mm-long, 0.025-mm-diameter gold wire. The wire tip faces the target, acting as a point source. Because the x ray pulse closely follows the ARC pulse in duration, the time resolution is 30 ps or less, depending on laser pulse duration. A filter in front of the detector blocks x rays of less than 40 keV, so that x rays generated by the capsule's hot spot cannot affect the radiographs. An experiment typically uses two Compton radiography backlighters to generate two independently timed radiographs 100 to 200 ps apart.

Any experiment using ARC faces alignment challenges similar to those of

For backlighting using Compton radiography, two pairs of ARC beamlets fire into a shielding cone to generate x rays by striking gold wires contained within plasma mirrors.

other types of high-energy backlighting. Having the ARC beamlets hit exactly the right spot ensures that the maximum amount of laser energy transfers to heating the gold wire that generates the x rays. An improvement to backlighter design positions the gold wire at the bottom of a V-shaped plastic wedge. Acting as a plasma mirror, the wedge not only concentrates the laser light but also mitigates fluctuations in beamlet pointing by redirecting misaligned laser light onto the wire. “Using this plasma mirror around the wire, we have generated backlighters with x-ray yields approximately three times greater than with a bare wire,” says Tommasini. He adds, “Recently, we have tested a parabolic-shaped plastic plasma mirror, which has produced even brighter x-ray emissions from the wire by achieving a higher concentration of laser light.” These backlighters have achieved

(a) An illustration shows the setup for the high-energy ARC backlighter experiment. (b) The work yielded a radiograph of a driven, spherical target.



record-high conversion efficiencies of laser energy into x-ray energy, with the potential of generating radiographs with higher reproducibility and signal-to-noise ratio. This achievement represents a remarkable step for several applications requiring efficient x-ray sources and will be used to generate Compton radiographs of ICF targets at cryogenic temperatures.

Proton Generation

In addition to generating x rays for backlighting, ARC has proven highly promising for producing high-energy, high-flux particle beams. In a project funded by the Laboratory Directed Research and Development (LDRD) Program, plasma physicist and principal investigator Tammy Ma researches proton acceleration. She says, “Because of ARC’s high energy and multipicosecond pulse lengths, we’ve found new mechanisms for accelerating protons to high energies that are efficient and generate enormous numbers of energetic protons.” In two experiments conducted earlier this year, all four ARC beamlets fired simultaneously into

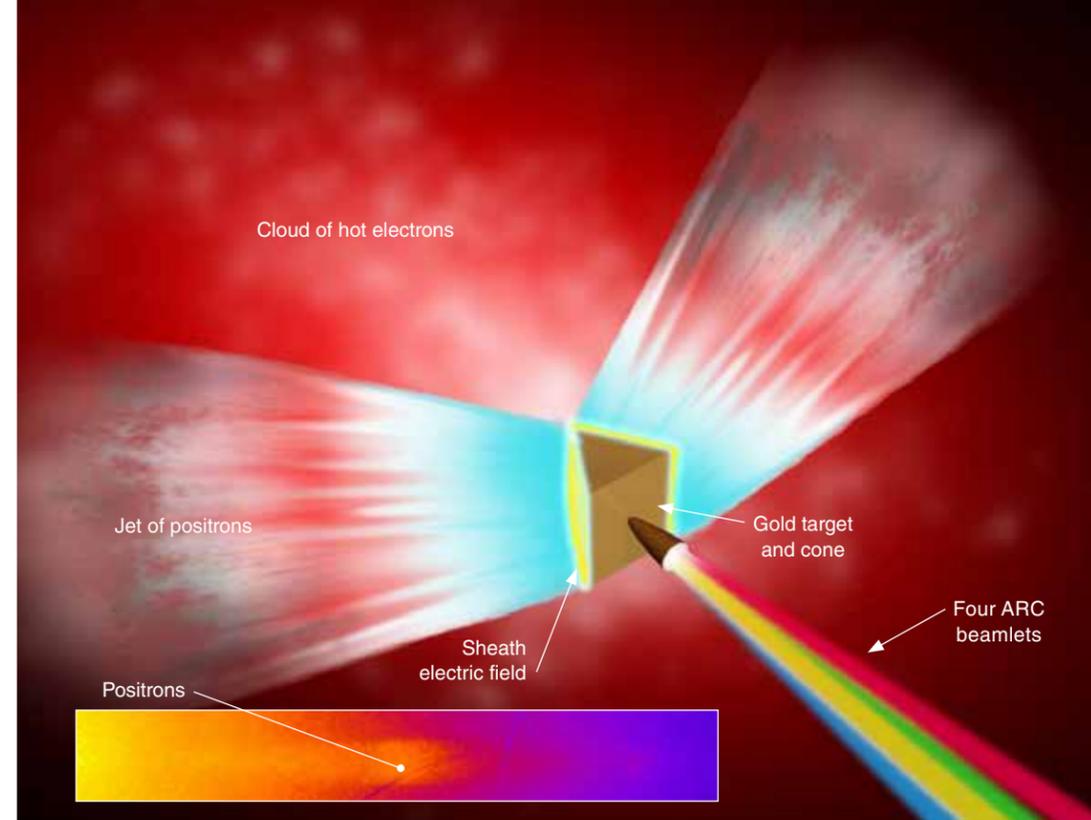
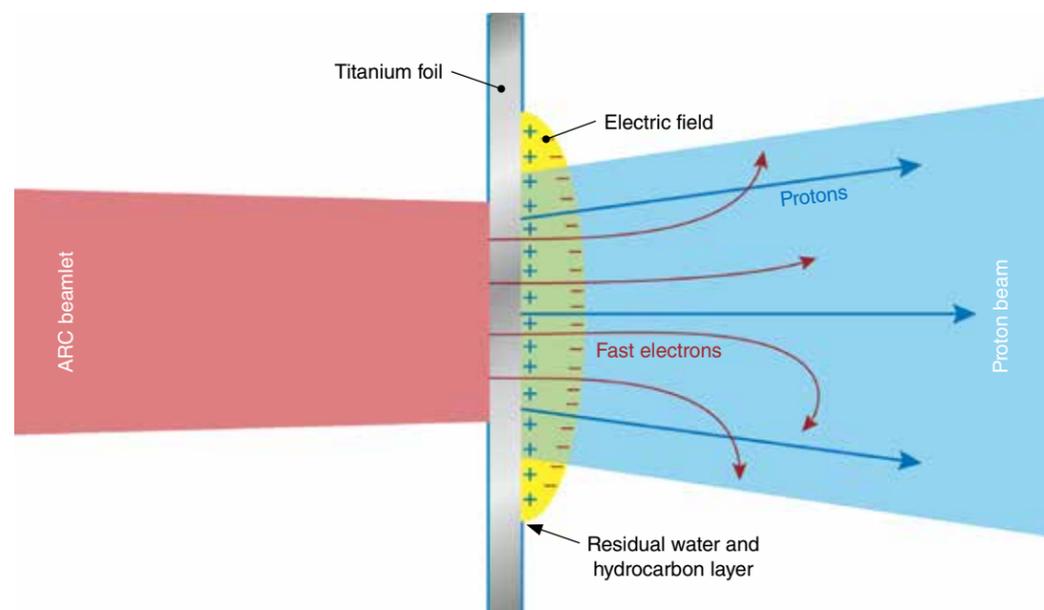
different quadrants of a 0.033-mm-thick titanium foil. With pulse lengths of 10 ps and 1.3 ps—the latter the shortest pulse ever delivered by ARC—total laser energies of 2.4 kJ and 1 kJ, respectively, were achieved. The experiments also reached the highest peak power ever achieved by NIF—more than 700 terawatts (trillion watts).

Upon striking the foil, laser beams quickly ionize the material and accelerate many of the electrons into “fast” electrons that travel rapidly through the foil, exiting out of the rear surface and creating a strong electric field in the foil. Protons from the residual water and hydrocarbon layer on the back of the target then want to follow, and they accelerate in a jet perpendicular to the surface. In these initial ARC experiments, the proton energies peaked at over 18 megaelectronvolts (MeV), and the conversion efficiency—the amount of laser energy converted to proton energy—reached nearly 5 percent, producing a tremendous proton yield of approximately 80 joules (J). “We’d like to use protons to radiograph hohlraums,”

says Ma. “Protons are a charged particle sensitive to electric and magnetic fields, whereas x rays are not. X rays can probe density but not fields.” Protons thus generated have a continuum of energies and so travel at different speeds, enabling temporal radiographs showing how fields change over very short timeframes.

In addition to radiography, proton beams can be used for heating in different NIF applications and other diverse uses. Ma says, “Proton therapy for tumor and cancer treatments would benefit. Protons can deposit their energy very accurately. Unlike chemotherapy or energetic x rays, which irradiate a lot of healthy tissue, protons could target a specific depth.” Other types of particles accelerated by this mechanism will be investigated on ARC soon. For instance, a deuteron beam or other heavy-ion beam can be generated by changing the foil material. Directing this initial particle beam at a secondary target of lithium or beryllium could then produce a neutron beam. Beams of neutrons and other particles can offer researchers more ways to analyze matter under extreme conditions.

Proton beam generation has applications not only in scientific experiments but also medical therapies such as tumor treatment. In the process, an ARC laser beamlet interacts with a thin metal foil to generate fast electrons. These electrons pass through the foil and create an electric field that accelerates protons from the residual layer to form a proton beam.



(top) Four beamlets, guided by the gold cone, strike a triangular solid target. The cone focuses and increases the laser intensity needed to generate relativistic electrons that interact with the gold atoms to produce gamma rays by bremsstrahlung. (bottom) The raw image from a particle spectrometer shows an orange band corresponding to positrons, with a peak number at around 10 megaelectronvolts (MeV) and maximum energy of about 25 MeV. (Illustration by Mark Meamber.)

Matter–Antimatter Plasma

For some ARC applications, using multiple beamlets to strike different parts of a target is sufficient. However, producing matter–antimatter plasma consisting of electron and proton pairs requires more laser intensity than even four separate beamlets can supply. Plasma physicist Hui Chen leads an LDRD project that is using ARC to study, in a laboratory, the most energetic processes in the universe. She says, “Matter–antimatter pairs are abundant in space—as in gamma-ray bursts near black holes and in neutron star collisions—and are an almost fundamental component of matter in the universe.” (See *S&TR*, April 2016, pp. 12–14.)

As part of NIF’s Discovery Science Program, researchers used ARC laser light to generate hot electrons inside a triangular-prism-shaped gold target. The electrons collide with the gold atoms to produce gamma rays, with each massless photon transforming into a positron and electron as governed by Einstein’s famous equation, $E = mc^2$. Some hot electrons depart from the target at relativistic speed and create very strong electric fields near the exit surfaces, which then attract and

accelerate jets of positrons out of the target to mix with a surrounding plasma cloud of hot electrons. The relativistic speed of the positrons and electrons assures very little chance of the two interacting to instantaneously annihilate each other. Instead, the particles coexist as matter–antimatter pairs for a brief moment in time.

The experiments used a specially designed parabolic-shaped gold cone to effectively focus the four ARC beamlets—each 10 ps and 550 J. The resulting electron spectrum indicated a total laser intensity exceeding 4×10^{18} W/cm² onto the target based on scaling from prior experiments. Two high-energy, high-flux positron jets formed, peaking in number at an energy of 10 MeV and reaching a maximum energy of 25 MeV. Refinement of the process is underway to further increase laser intensity and improve positron yield.

Regarding future directions of pair plasma research, Chen says, “With a denser pair beam, we could send the beam into a plasma created by the main NIF laser to simulate astrophysical pair jets flowing through galactic plasma. In addition, once we have a sufficient number of positrons—about 10 times more than

now—we may be able to conduct positron radiography of compressed capsules.” The gold parabolic plasma lens that proved vital to this experiment could also be applied to other uses requiring higher laser intensities or beamlet collimation.

As ARC’s applications advance, not only will each project build on its new knowledge, but the capabilities across all of ARC and NIF will be bolstered through cross-pollinating innovations. This progress will benefit the entire facility, its world-class laser inside a laser, and the broad range of Laboratory missions supported by this diverse research.

—Dan Linehan

Key Words: Advanced Radiographic Capability (ARC), backlighting, Compton scattering, electron–positron pair, fusion, high-energy laser, high-energy-density (HED) science, high-Z material, inertial confinement fusion (ICF), Laboratory Directed Research and Development (LDRD) Program, matter–antimatter pair, National Ignition Facility (NIF), petawatt, plasma, proton generation, relativistic electron, short-pulse laser, Stockpile Stewardship Program, x ray.

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SOLVING THE MYSTERIES OF METAL HARDENING

WITHOUT understanding why, metalsmiths have known for centuries that repeatedly heating and folding a block of metal would strengthen the material. Incorporating this technique into their craft, the master swordsmiths of medieval Japan forged elegantly curved, razor-sharp katanas for samurai warriors—blades exceptionally strong for their light weight. Around the same time, Damascus steel, hardened in similar fashion, became the metal of choice for the fearsome blades used in the Near East. In Russia and other countries, the metal was called bulat steel and formed the weapons carried by Genghis Khan’s armies.

However, an understanding of the science behind this metal-hardening process has only recently begun to emerge, thanks to modern theoretical investigation, observational tools, and computer models. At Lawrence Livermore, materials

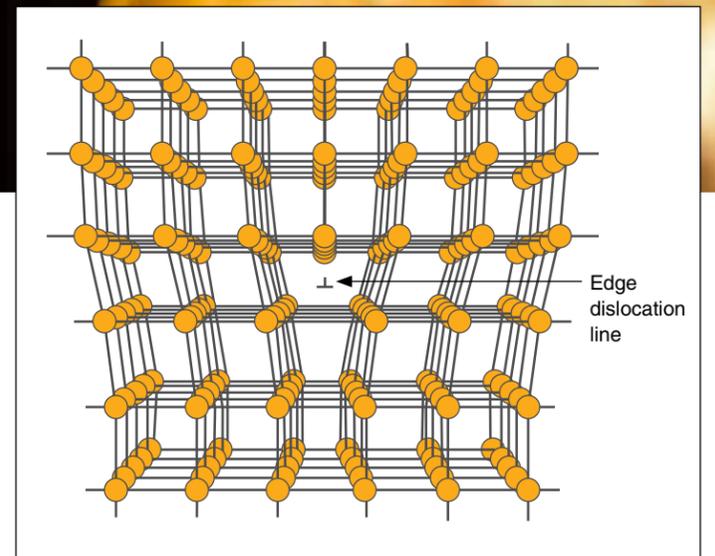
simulations using high-performance computation are peeling back the layers of mystery, revealing some surprising insights into how metals behave under extreme pressure. Driving this research is the Laboratory’s mission of stewarding the nation’s nuclear stockpile. The simulations also contribute to basic science and may have applications in aerospace, astronautics, and other fields where materials are used under high-stress, high-temperature regimes.

Vasily Bulatov, a Livermore computational materials physicist, leads a research team working to simulate how metals behave under high pressure. Bulatov, who has studied the behavior of metals for more than two decades, says, “Our mission is to predict the strength of materials under extreme conditions. We are funded by the National Nuclear Security Administration’s Advanced Scientific Computing Program,

which seeks precise computations instead of some of the measurements previously obtained through nuclear testing.”

The Dynamics of Dislocations

Arriving at the Laboratory from the Massachusetts Institute of Technology in 1999, Bulatov realized that a model was needed to predict metal strength. “None of the existing codes at that time could even form the basis of such simulations,” he explains. He assembled a research team that eventually developed ParaDiS (Parallel Dislocation Simulator), which modeled the dislocation dynamics of metals. Dislocations—irregularities in the crystalline structure of atoms—help explain the strength and ductility of metals. Metallic atoms typically arrange themselves into regular stacks as tennis balls do in a crate, with the centers of the atoms aligning in parallel planes.



This schematic of an edge dislocation in a metal crystal shows how the extra half-plane of atoms interrupts the regular stacking of the crystalline structure. The edge dislocation line is the bottom edge of this extra half-plane.

In one type of dislocation, some planes of atoms are slightly displaced relative to their neighbors such that their centers form a half-plane that displaces the adjacent stacks of atoms to either side. The line formed by the edge of this malformed plane is called an edge dislocation. Another major type of disarrangement is an angular variety called a screw dislocation. Characterizing dislocation patterns is the first step in modeling metals under high pressure.

When a metal is compressed through repeated blows by a metalsmith’s hammer, for example, the force pushes existing dislocations through the material and creates new ones, as well. As these irregularities migrate, some collide with each other, merging or forming junctions that actually strengthen the metal by resisting further strain. Bulatov says, “Take the classic example—an aluminum paper clip. Bend it back and forth a few times, and eventually it starts to harden. The more you bend the

metal, and the more dislocation lines are created and collide with each other, then the harder it becomes for the lines to move. This response to stress defines the material’s strength.”

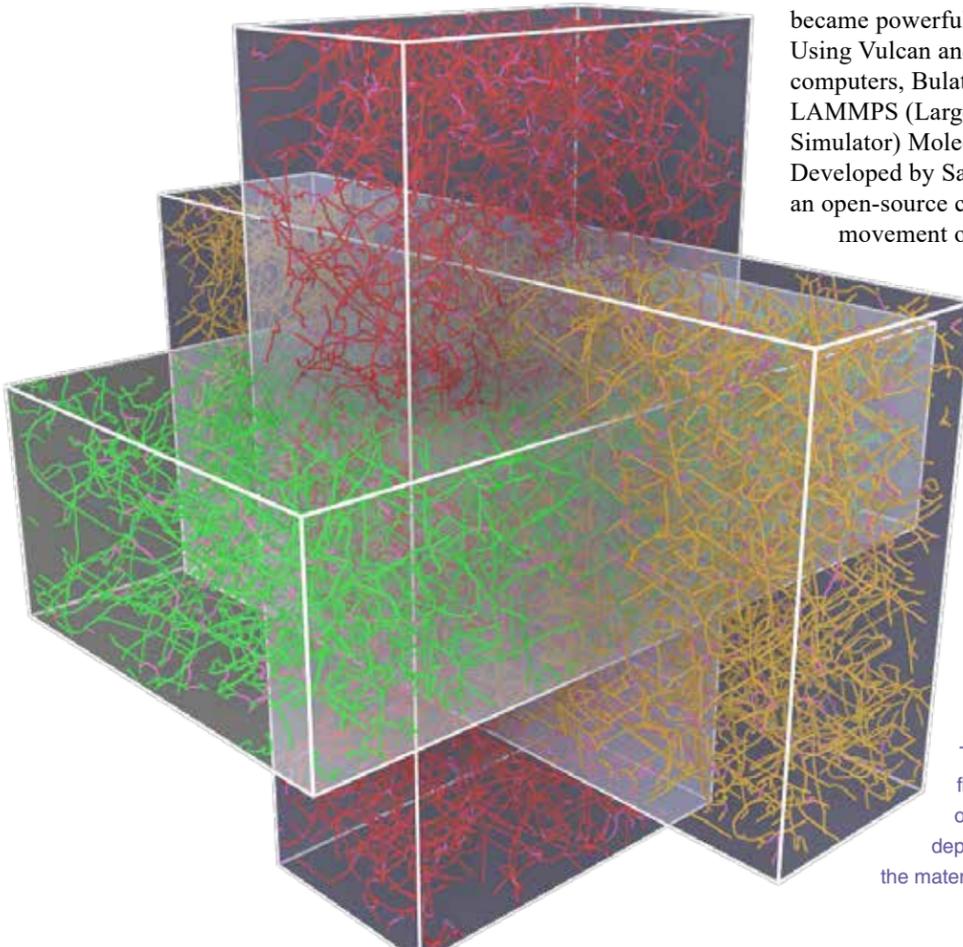
In 2006, Bulatov’s team simulated the element molybdenum. Their results suggested that the behavior of dislocation lines under stress explained the material’s crystal strength, but he more to the story remained—that only an atomistic model could reveal whether any other phenomena influenced hardness. However, even the Laboratory’s fastest computers of the time could not model a large enough number of individual atoms to achieve a fully atomistic simulation of metal strength, also known as a molecular dynamics simulation.

The Need for Speed

“When I began investigating the problem, computers were seven orders of magnitude slower than they are today,” recalls Bulatov. “But a moment came two years ago when computers became powerful enough to make an atomistic model a reality.” Using Vulcan and Sequoia, Livermore’s two most powerful computers, Bulatov and his team began using software called LAMMPS (Large-Scale Atomic/Molecular Massively Parallel Simulator) Molecular Dynamics Simulator for this purpose. Developed by Sandia National Laboratories, LAMMPS is an open-source code that allows users to study the physical movement of atoms and molecules.

The team ran simulations of tantalum (Ta), a hard yet ductile, corrosion-resistant metal with applications such as electronic components, jet engines, and surgical instruments. Starting from atomic configurations generated by Bulatov, Livermore’s Luis Zepeda-Ruiz and Alexander Stukowski of Germany’s Technische Universität Darmstadt ran the simulations. The Laboratory’s Tomas Opperstrup optimized the code and data management. In one of the simulations, rectangular bricks of Ta atoms were compressed serially in three directions—stresses were applied first lengthwise, then

Tantalum crystals can flow indefinitely, similar to a viscous fluid, while remaining stiff and strong and retaining their ordered lattice structure. Three juxtaposed snapshots depict lattice defects—dislocation lines—developing when the material is kneaded like a piece of dough.



along the width, and finally along the height of the blocks repeatedly, “kneading” the metal like a lump of dough. In simulations consisting of up to 268 million individual Ta atoms, the team each day generated approximately five exabytes (10¹⁸ bytes) of atomic trajectory data, comparable to all the data that Google currently has stored on servers worldwide.

A Swift, Distinct Transition

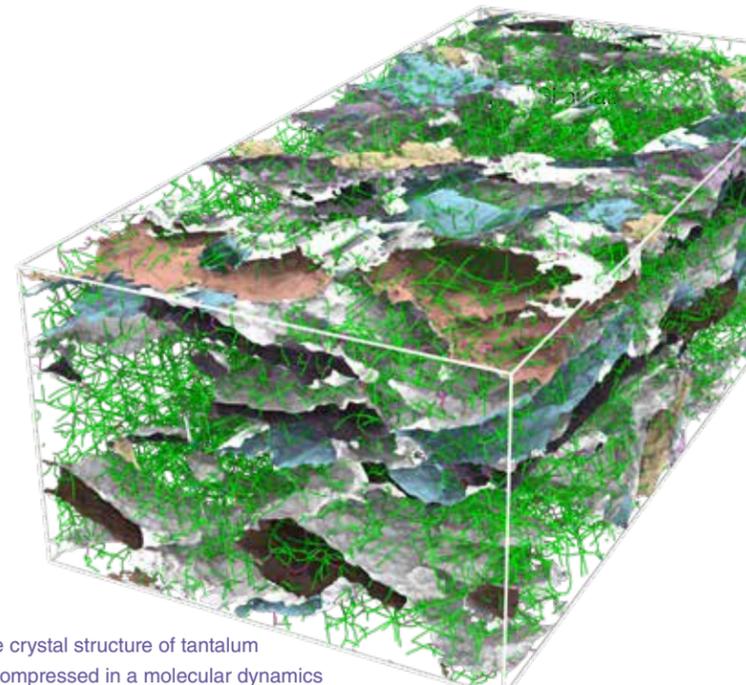
This work, published in 2017, yielded two significant scientific findings. First, the team found that as Ta is compressed, its dislocations extend and collide with each other, moving actively to prevent the metal from breaking. This behavior imparts ductility to the metal—but that was not all. “Something else rather dramatic happens,” says Bulatov. “If you strain the metal very quickly, the dislocations are unable to keep up, and whole chunks of the crystal rotate, a phenomenon called deformation twinning. We showed a very precise threshold where this transition from dislocation to twinning takes place.”

During twinning, planes of atoms do not slide past one another as happens with moving dislocations. Instead, regions of material twist in opposite directions from one another, resulting in volumes with distinct crystal orientations. Scientists had previously theorized that this transition was possible, but simulations by Bulatov’s team revealed the precise atomistic mechanism and the conditions under which the transition occurs.

The second key finding announced in 2017 concerns Ta behavior during slow compression. “When tantalum deforms slowly enough that the dislocations can keep up with the applied forces, the crystal reaches a steady state that persists forever,” explains Bulatov. If the metal is compressed in such a way that the transition to twinning is not reached, dislocations will continue to migrate through the material endlessly, and this mechanism will remain dominant, preventing the metal from breaking. Kneading thus ensures that no other changes will happen, and that the metal will retain the same strength indefinitely. This may be the molecular secret to the famously strong swords.

Even Larger Simulations

Metals subjected to force often harden in stages, undergoing a low level of hardening upon initial compression, then high-strength hardening, and back to low-level hardening until breakage occurs. The reasons for this three-stage process are not fully understood, but further simulations may elucidate what is happening at an atomic level. Since reporting their work, Bulatov’s team has run an even larger simulation



The crystal structure of tantalum is compressed in a molecular dynamics simulation. All atoms are removed for clarity, and the structure is represented by lattice defects—dislocations (green and red lines) and interfaces of twin particles (surfaces of various colors).

involving more than two billion atoms. The results are still being analyzed. Because these simulations generate so much data, Bulatov is planning to use machine learning to identify the significant data and detect patterns in data sets too large for humans to comprehend. Recent simulations have generated a volume of data equivalent to seven to ten times the data on Google’s servers worldwide.

Bulatov is optimistic about solving the remaining mysteries of metal hardening. He states, “As both computing power and the accuracy of atomic models steadily increase and, at the same time, the spatial and temporal resolution of experimental methods in materials science improve, we are increasingly seeing the complete confluence of experiments and atomistic simulations.” For solving the mysteries of their ancient craft, the swordsmiths of yore would be impressed indeed.

—Allan Chen

Key Words: Advanced Scientific Computing Program, bulat steel, Damascus steel, deformation twinning, dislocation dynamics, edge dislocation, high-performance computing, katana, LAMMPS (Large-Scale Atomic/Molecular Massively Parallel Simulator) code, metal hardening, molecular dynamics, molybdenum, Parallel Dislocation Simulator (ParaDIS) code, screw dislocation, tantalum.

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MACHINE LEARNING POINTS

TOWARD NEW LASER TARGET DESIGNS



WHEN the Trinity supercomputer at Los Alamos National Laboratory was first coming online, calls went out for research projects that would test—and potentially break—the new system. Researchers from Lawrence Livermore answered the call, and their work with Trinity and machine learning could disrupt 40 years of assumptions about inertial confinement fusion (ICF).

“The theory of ICF was all done with pencil and paper, assuming a spherical implosion,” says design physicist Luc Peterson. “In many studies, if your implosion isn’t spherical, you’re not getting as much energy out of it as you could.” ICF implosions at Livermore’s National Ignition Facility (NIF) are

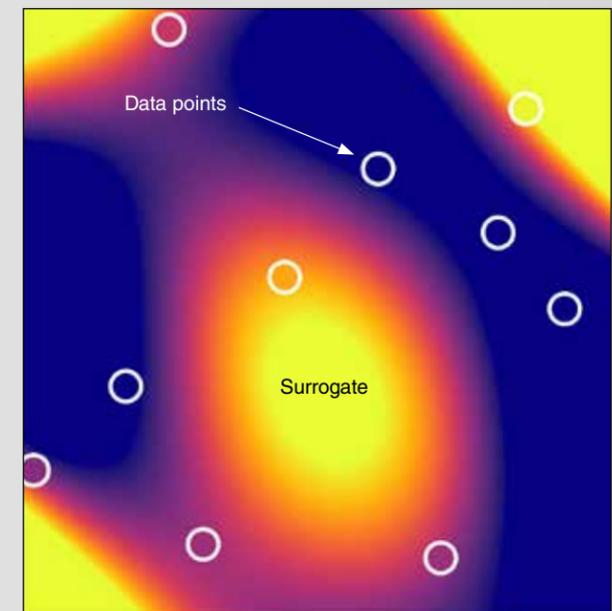
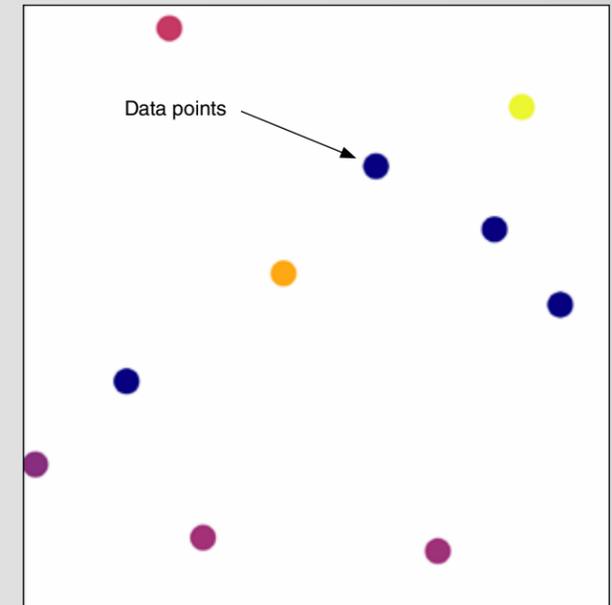
aimed at a spherical target housed in a cylindrical hohlraum, which creates an asymmetrical, preferred axis. To combat this tendency, Peterson was tasked with what he calls an impossible job: either make the implosions more round or create an implosion robust enough to withstand the inherent asymmetries and still achieve high energy yield. “I listed all the ways that NIF could possibly implode something asymmetrically,” Peterson says. “I got a very large number of parameters and realized that to check all the different combinations, I would need to run many simulations—more than had ever been done before.”

The nine parameters included various asymmetries, drive multipliers, and gas fill densities—all factors that affect the

quality of target implosion. Simulating all the permutations would produce 5 petabytes of raw data, which is close to the current limit for Livermore’s parallel file systems. Steve Langer, Peterson’s colleague and a fellow Laboratory design physicist, heard about the effort to map out all nine parameters and conceived of a way to help.

From Supercomputer to Server Farm

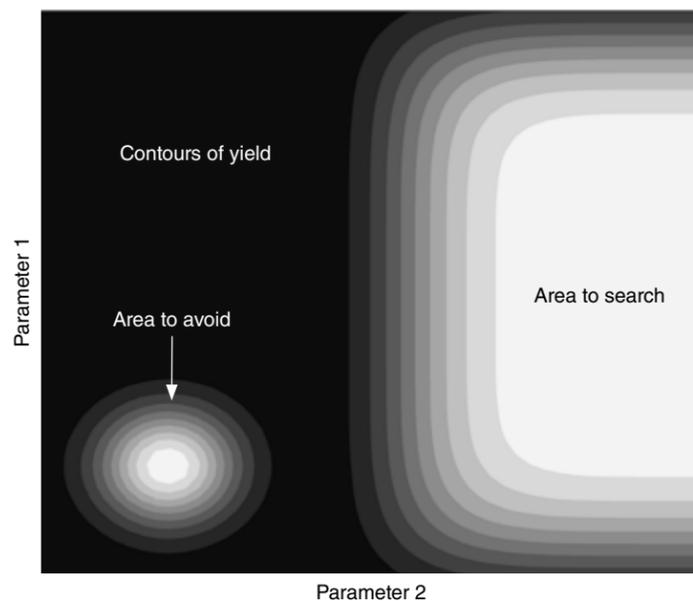
Langer’s idea involved Trinity, then a brand-new Cray XC40 system. Typically, before transitioning a new computer to classified work, a national laboratory holds an open-science period where researchers can “kick the tires” of the new system



(top) Simulations on the Trinity supercomputer produced approximately 60,000 data points, which were then used to train a machine-learning model. (bottom) The model predicted all the points between the simulations to produce a surrogate model across nine parameters, which can be represented by the gradient in any two dimensions of the nine-dimensional space.

by running unclassified experiments. Laboratory technicians can also consult with the computer's vendors as the experiments run and discover ways to fine-tune the system. Langer's plan was to process their raw physics data on the fly, analyzing and deleting files while they were being created, instead of saving all the data. Peterson and Langer pitched their big-data physics simulation proposal to Los Alamos, and a collaboration was born. "We knew we would have to do some distillation to even store the results on disk, which prompted us to create this on-the-fly, in-transit system," says Peterson. "We developed a system to perform the filtering while the simulations are running. The approach is like filling up a bucket with water while making a hole in the side to drain the bucket so it doesn't overflow."

Their project essentially turned Trinity—then a 8.1-petaflop (10^{15} floating-point operations per second) supercomputer designed to run one large simulation at a time—into a giant "server farm" capable of running several thousand simulations at once. The approach was not only necessary for the project but also worthy of the new computer's open-science challenge, stressing Trinity in new, often unforeseen ways that sometimes affected other users. One surprised Los Alamos employee sent out a midnight email asking whether someone was performing large data transfers that had lowered data rates to only 17 gigabytes per second for codes that normally achieved more than 600 gigabytes per second. "Los Alamos put me on



speed dial for what I did to their poor machine," says Peterson. The filtering system managed to trim the expected 5 petabytes of raw data down to 100 terabytes, but transferring the data between the two laboratories still took several months. "We joked that it would actually be faster to rent a van and drive across the desert with a bucket of USB drives," he adds.

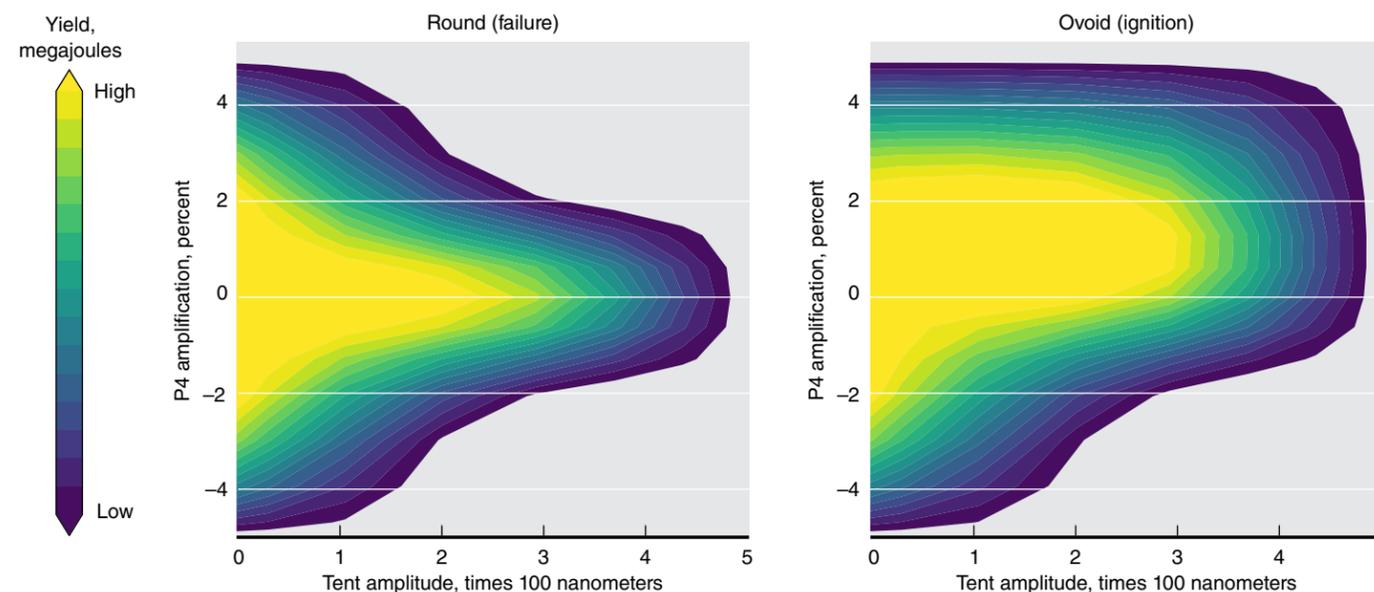
Rise of the Machines

Generating the data was only half of the challenge. The next step was to analyze the data and search for robust designs. However, searching through all the simulations was not sufficient. "We have approximately 60,000 data points, which sounds substantial, but when you consider nine-dimensional space, it's actually pretty sparsely sampled," says Kelli Humbird, a Livermore Graduate Scholar who helped Peterson study the data. "We wanted an algorithm that would interpolate between the points and connect the dots so we could approximate the results of simulations anywhere in the nine-dimensional space."

To fill in the gaps, Humbird used 80 percent of the Trinity simulations to train a machine-learning model, which was then tested on the remaining 20 percent of the data to evaluate its predictive capability. The model—a random forest decision tree method—accurately predicted yield with a less than 10 percent margin of error. Having a trained machine-learning model in hand that closely mimicked the expensive physics code, Humbird began predicting implosion performance between the simulated data points to search for a robust implosion. "This is not something we could have done with just our physics code," says Humbird, whose work with Peterson has led to a machine-learning project under the Laboratory Directed Research and Development Program. "Performing this search through nine-dimensional space would have required something like 5 million physics simulations and 3 billion central processing unit hours. One would never have enough time. However, a rapid, accurate machine-learning model could do the same search in a fraction of the time."

A sort of topographical map of target designs began to emerge as the model filled in additional data points. Some regions of the map represented locations where an implosion

In this two-dimensional conceptual illustration, varying combinations of target design parameters produce high-yield simulations (light areas) and low-yield simulations (dark areas). The larger the light area, the more resistant the target's implosion would be to perturbations.



Researchers discovered a ridge of high energy yield (yellow) that was larger for an ovoid target than for a sphere. Ignition was found to be far more likely with an ovoid, within a broader range of parameters.

would likely produce high energy yield, whereas other areas indicated the opposite. The high-yield areas indicated how robust the implosion was—what Peterson calls "wobble room." A target designed within a broad "plateau" of high-yield implosions would be resistant enough to withstand perturbations unavoidable in experiments, whereas a target based on a narrow peak on the map might be easily disrupted and "fall off the mountain." After searching through the most promising Trinity simulations and the adjacent machine-learning predictions, the model had what looked like an answer. However, this optimum target did not look like the long-desired sphere but rather more like an egg.

Off Target Can Still Be on Target

The topographical map—much more detailed thanks to Humbird's model—indicated that areas representing egg- or football-shaped targets, known as ovoids, were plateaus of stability. Even if NIF could not create an implosion at the absolute center of the plateau, being slightly off-center would still produce a high energy yield. With a better idea of where to look, Peterson

and Humbird ran a more expensive, full-scale physics simulation on the ovoid target, and their predictions were confirmed, although the researchers were initially not sure why.

After puzzling over the contradictions, Peterson realized he was seeing zonal flows in the imploding egg-shaped target. Similar to a spiraling hurricane sucking up neighboring clouds, zonal flows can absorb disruptions caused by target support tents or capsule roughness and incorporate them into a larger, more stable vortex. This incorporation steadies the implosion and allows for greater energy output, the researchers concluded. The next steps are to improve the detail of future simulations and continue the search for the perfect target shape.

"Our codes indicate that other designs could exist out there, which is fascinating because we've been chasing the same design for 40 years," says Peterson. "The crazy thing is, we didn't force the code to produce the data. The code could always have yielded these results if we had just known where to look. Machine learning and data science gave us the power."

—Ben Kennedy

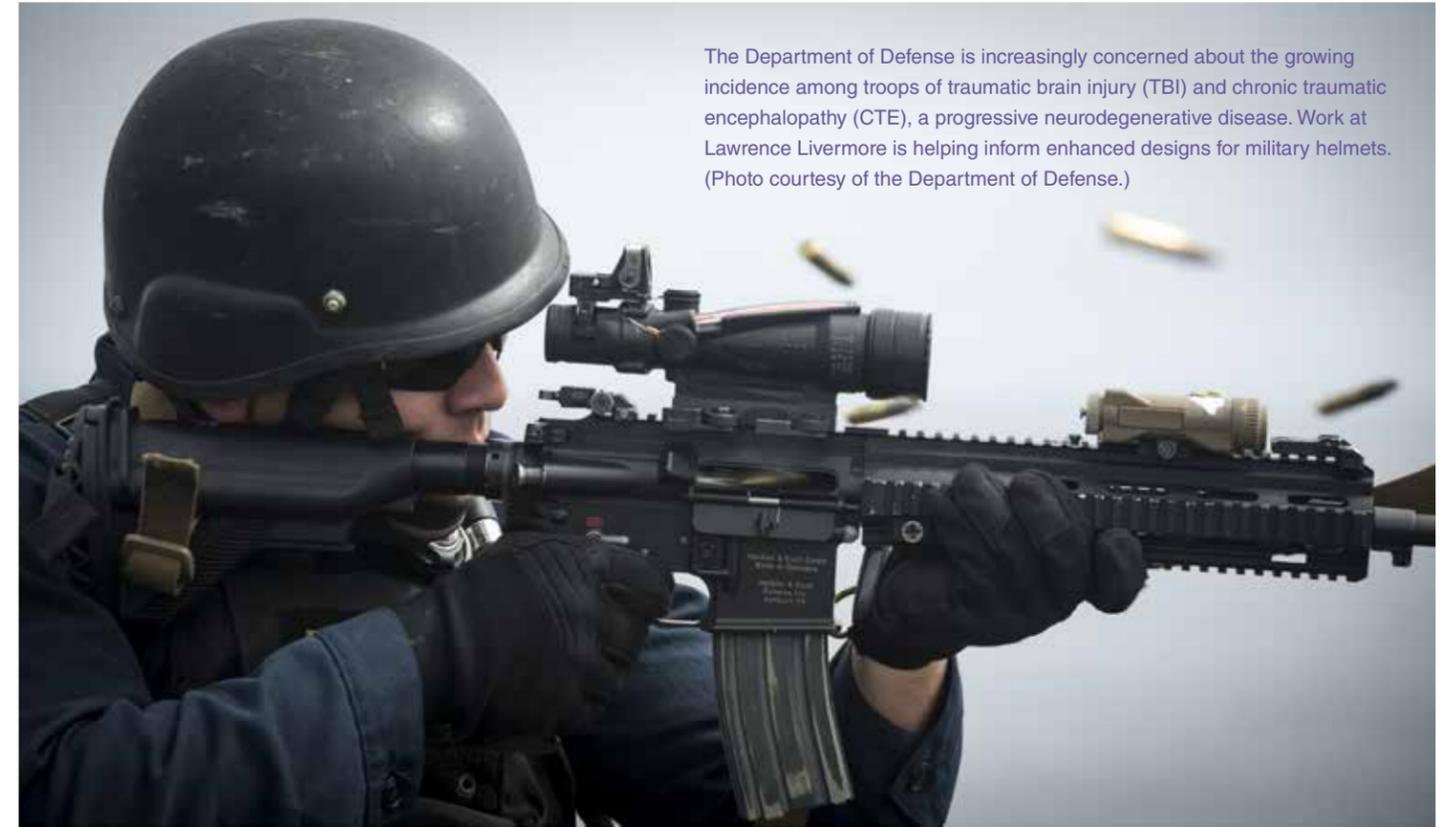
Key Words: inertial confinement fusion (ICF), Laboratory Directed Research and Development Program, machine learning, National Ignition Facility (NIF), supercomputing, target design, Trinity, zonal flow.

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COMPUTER MODELING PROVIDES NEW INSIGHTS INTO TRAUMATIC BRAIN INJURY

SIMULATIONS combining advanced Livermore software with some of the world's most powerful supercomputers have made remarkable strides in furthering stockpile stewardship and enhancing scientific understanding of how materials interact and behave under extreme conditions. For the past decade, Livermore physicist Willy Moss has used the Laboratory's high-performance computing (HPC) resources to help medical researchers and U.S. Department of Defense (DOD) scientists understand and prevent traumatic brain injury (TBI).

Moss's latest simulations, conducted with Livermore computational engineer Andy Anderson, support experimental findings that the neurodegenerative disease known as chronic traumatic encephalopathy (CTE) can result from head accelerations caused by either blasts—from a grenade or improvised explosive device, for example—or impacts such as those in contact sports. Furthermore, the simulations help explain how CTE can occur



The Department of Defense is increasingly concerned about the growing incidence among troops of traumatic brain injury (TBI) and chronic traumatic encephalopathy (CTE), a progressive neurodegenerative disease. Work at Lawrence Livermore is helping inform enhanced designs for military helmets. (Photo courtesy of the Department of Defense.)

even in the absence of concussion, defined as a head trauma that causes immediate symptoms.

The Livermore simulations were part of a large-scale study, funded by several federal agencies and other organizations, in which Moss and Anderson joined more than 40 medical researchers led by Lee Goldstein, associate professor at Boston University School of Medicine. The Livermore researchers used computational modeling to investigate why both impact and blast were linked to CTE, whereas concussion resulted only from impact. The study's results were published in 2018.

Warfighters and Athletes at Risk

TBI and CTE have become of increasing concern to DOD, with some 380,000 personnel affected. Although soldiers serving in combat zones are particularly vulnerable to TBI, earlier this year a study showed that thousands of U.S. troops could suffer TBI from repeated exposure to head trauma while training with high explosives or rocket launchers. Soldiers using these weapons subject their skulls and brains to sudden acceleration and loads (force) below the threshold of a concussion.

CTE is found not only in military veterans but also in athletes such as football players—some as young as 17—and others with a history of repetitive brain trauma, both with and without signs of concussion. In fact, about 20 percent of CTE cases diagnosed in the Boston University brain bank did not have a history of

concussion. CTE is a neurodegenerative disease characterized by abnormal accumulation of a protein called tau, which serves a structural function in normal brains but ceases to perform that function and accumulates around small blood vessels in the brains of CTE sufferers. The disease spreads slowly, killing brain cells and causing behavioral changes and eventually dementia. Symptoms do not usually appear until years after the head trauma, as seen in some National Football League (NFL) players who began to show symptoms only after retiring from the league. In the first part of the study, Boston University researchers examined four brains from teenage athletes who died within four months of receiving a head impact injury. The athletes exhibited a spectrum of post-traumatic pathology, with one case of early-stage CTE and two cases of abnormal accumulation of tau protein. Brains from a control group without recent head injury did not show the same pathological changes.

The researchers also conducted experiments subjecting laboratory mice to the two different injury mechanisms linked to CTE—sports-related impact and military-related blast exposure. The researchers detected the same brain pathology in the head-injured mice as in the injured teenagers. Both mechanisms showed strong evidence linking head acceleration to TBI and early CTE. None of the mice experiencing a blast suffered a concussion. However, some degree of concussion occurred in the majority of mice following impact, despite similar head motion in the two

injury mechanisms—both of which triggered CTE pathology. This result suggested that concussion and CTE might be unrelated. “The findings from the animal experiments were very surprising,” says Anderson. “So, Willy and I turned to supercomputer simulations to take a closer look.” The simulations confirmed that the mechanisms that trigger concussion may be distinct from those that lead to CTE. The simulation results also provided important insights into the origin of concussion.

Code to the Rescue

Moss has used simulations to study head trauma in support of U.S. warfighters for many years. Nearly a decade ago, he and Livermore mechanical engineer Michael King sought to better understand TBI using Livermore’s hydrodynamics code ALE3D, originally developed to model the fluidlike flow and shock responses of materials exposed to a nearby detonating weapon (see *S&TR*, March 2010, pp. 14–17). When run on one of Livermore’s massively parallel computers, ALE3D can simulate how a blast generates waves of pressure and how those waves interact with structures in their path, including helmeted heads (see *S&TR*, June 2017, pp. 20–23).

Using a simplified head model, the three-dimensional simulations modeled the detonation of high explosives and the blast wave’s propagation, revealing that the blast wave was focused by the helmet to cause pressure on the skull exceeding the external

CTE has also been found in the brains of people playing contact sports, even in cases involving no history of concussion. (Photo courtesy of U.S. Air Force.)



blast pressure. The simulation results, published in 2009, further confirmed the utility of using HPC to protect U.S. warfighters and inform helmet design. “Our blast simulations received a lot of scientific, public, and military attention,” says Moss.

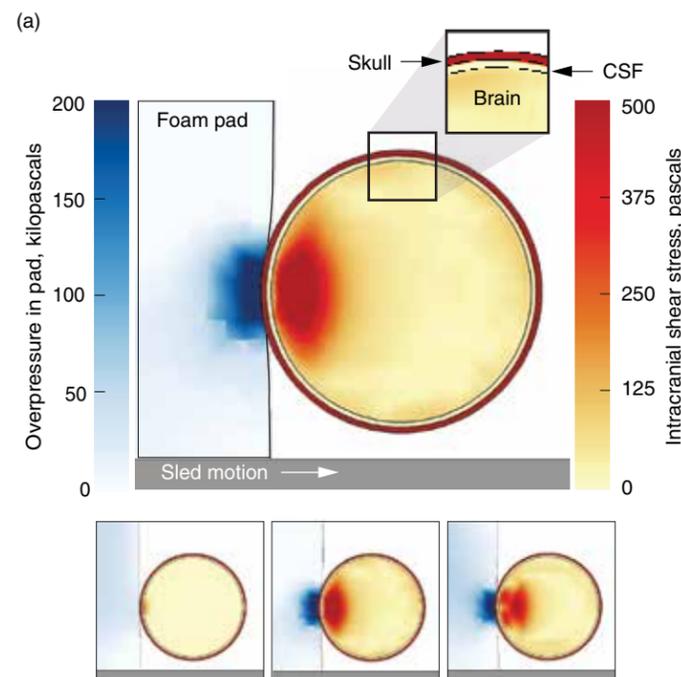
As a result of the 2009 findings, the U.S. Army asked Moss and King to conduct a computational study to determine whether the pads used by the NFL could protect against military-relevant impacts better than foam pads then used in Army combat helmets. The simulations showed that for comparable thicknesses, the NFL pads did not outperform the current Army helmet pads. However, the simulations’ most significant finding was that a slight increase of only one-eighth of an inch in the thickness of Army helmet foam pads lessens the severity of impact by 24 percent (see *S&TR*, April/May 2012, pp. 14–16). “We found an extreme sensitivity to changes in the thickness of the standard-issue three-quarter-inch foam pad,” says Moss. The results of the study are being incorporated into the Enhanced Combat Helmet, the next generation of Army combat helmets.

Goldstein, already familiar with the power of HPC from previous work with Moss and colleagues, asked Livermore to simulate the blast and impact experiments involving laboratory mice. “We needed a way to assess what was going on inside the heads of the mice, and the only way we could probe that space was with computation,” explains Moss. He and Anderson once again turned to ALE3D and Livermore supercomputers to simulate blast and impact-loading conditions. Overall, approximately 100 simulations were performed, repeating the same head motions seen in the mice experiments. Each simulation used 60 to 100 processors and took a few hours to run.

Shear Stress Is Key

“We first looked at pressure fields in the brain resulting from both impact and blast and didn’t see anything surprising or suggestive,” says Moss. “Then we looked at shear stress and saw a clear difference. We suspected we were on to something important.” Closer examination showed that shear stresses occurred before any gross motion of the head occurred. The high-shear region remained nearly stationary and persisted around the point of impact. Even with a low-magnitude concussive impact—one that does not rip or tear brain tissue—shearing can disrupt small blood vessels and nerve fibers in the brain. In contrast to an impact, a blast produces a global effect on the skull and brain, with the pressure wave flowing fairly uniformly around the head and resulting in very little shear stress in the brain.

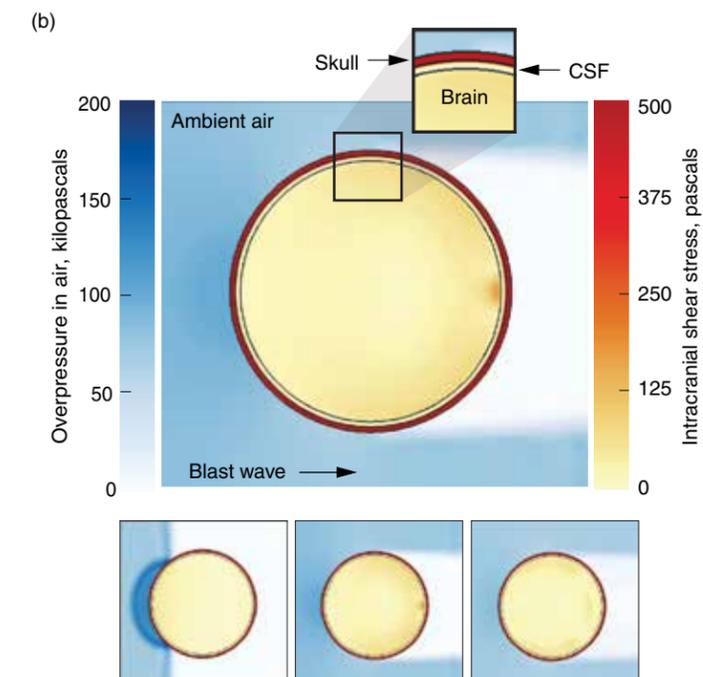
The Livermore investigators surmised that localized loading from an impact, producing a high concentration of shear stress, leads to a concussion, which takes place



in less than a millisecond, before significant head movement. In contrast, CTE seems to be triggered by repetitive impacts to the head from injuries sustained during contact sports and from repeated military blast exposure, both of which involve significant head acceleration. This commonality of impact- and blast-induced accelerations both leading to CTE built on an earlier study by Goldstein, Moss, and others that showed that blast-induced head acceleration caused CTE in mice. The simulation data from the current study, consistent with that from animal experiments, helped the researchers conclude that the mechanisms that cause concussion are distinct from those that lead to CTE. “Someone can develop CTE without ever having been concussed,” states Moss.

The researchers hope the study’s findings will guide the development of new diagnostics, therapeutics, and protective equipment to help people affected by TBI or at risk for CTE. In work funded by the Department of Energy and the Veterans Administration, Livermore researchers, partnering with other national labs and the University of California at San Francisco, are using the Laboratory’s HPC resources to develop precision diagnostics and optimized treatments for TBI patients based on HPC predictive modeling. In addition, Livermore bioengineers are helping develop TBI therapies such as deep brain stimulation (DBS) for DOD. Currently the subject of clinical trials, DBS involves surgically implanting electrical leads to disrupt certain electrical signals with pulses delivered to selected brain tissues (see *S&TR*, June 2018, pp. 4–11).

“We want to help the warfighter with our simulations—help their well-being in combat and for the rest of their lives,” states Moss. As for CTE linked to contact sports, Moss says, “We have



In these samples of Livermore simulations from mouse experiments, two-dimensional slices of the three-dimensional simulations are shown. Circles represent vertical slices of a mouse skull, cerebral spinal fluid (CSF), and brain. (top) The simulations show why overpressure (blue) from both (a) impact and (b) blast caused significant head acceleration—which is linked to CTE—while only impact sometimes resulted in concussion. The key is the clear difference in shear stress (red) caused by localized loading from impact. (bottom) Three time intervals over a 150-microsecond duration show shear stress persisting in the impacted brain but not in the brain subjected to a blast.

a special responsibility not only to our warfighters but to our kids, as well. We have been too focused on concussion. However, concussion and CTE seem to be distinct entities, so we shouldn’t use concussion as the sole criterion for determining whether someone has possibly suffered a brain injury.” He suggests, for example, more research to protect athletes from repetitive hits by redesigning helmets. The Livermore simulations are once again demonstrating that applying advanced simulation techniques originally conceived for stockpile stewardship can be equally useful for protecting people in other ways, too.

—Arnie Heller

Key Words: ALE3D, chronic traumatic encephalopathy (CTE), concussion, deep brain stimulation (DBS), football, helmet, traumatic brain injury (TBI).

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In this section, we list recent patents issued to and awards received by Laboratory employees. Our goal is to showcase the distinguished scientific and technical achievements of our employees as well as to indicate the scale and scope of the work done at the Laboratory. For the full text of a patent, enter the seven-digit number in the search box at the U.S. Patent and Trademark Office's website (<http://www.uspto.gov>).

Patents

Graphene Macro-Assembly-Fullerene Composite for Electrical Energy Storage

Patrick G. Campbell, Theodore F. Baumann, Juergen Biener, Matthew Merrill, Elizabeth Montalvo, Marcus A. Worsley, Monika M. Biener, Maira Raquel Cerón Hernández
U.S. Patent 9,870,871 B2
January 16, 2018

Label-Free Identification of Stem Cell-Differentiated Cells

James W. Chan, Deborah Lieu
U.S. Patent 9,879,224 B2
January 30, 2018

Resonant Optical Transducers for In-Situ Gas Detection

Tiziana C. Bond, Garrett Cole, Lynford Goddard
U.S. Patent 9,880,096 B2
January 30, 2018

Selective High-Affinity Polydentate Ligands and Methods of Making Such

Sally J. Denardo, Gerald L. Denardo, Rodney L. Balhorn
U.S. Patent 9,884,070 B2
February 6, 2018

Awards

Henry Chapman, who worked at Livermore from 1996 to 2007, was presented with an **honorary doctorate** by Sweden's **Uppsala University** for his work on developing techniques for imaging and crystallography with intense x-ray pulses. Chapman is a professor of physics at Hamburg University and director of the Coherent Imaging Division at its Center for Free-Electron Laser Science. He is also the founding director of the Center for Free-Electron Laser Science at the German Electron Synchrotron. The honorary doctorate was awarded for his work in this field, along with his initiatives to bring together and leverage international teams and resources.

During his time at Lawrence Livermore, Chapman helped his team earn an R&D 100 award for a project that put forth novel systems for microelectronics. Chapman later moved into imaging molecules with x-ray free-electron lasers. Before his departure, he also received the Edward Teller Fellowship for his work at the Laboratory.

Explosives Mimic for Testing, Training, and Monitoring

John G. Reynolds, Matthew M. Durban, Alexander E. Gash, Michael D. Grapes, Ryan S. Kelley, Kyle T. Sullivan
U.S. Patent 9,890,092 B2
February 13, 2018

Encapsulated Microenergetic Material

Jeffery James Roberts, Roger D. Aines, Eric B. Duoss, Christopher M. Spadaccini, Kevin S. Vandersall
U.S. Patent 9,896,921 B2
February 20, 2018

K-9 Training Aids Made Using Additive Manufacturing

John G. Reynolds, Matthew M. Durban, Alexander E. Gash, Michael D. Grapes, Ryan S. Kelley, Kyle T. Sullivan
U.S. Patent 9,897,419 B2
February 20, 2018

Hybrid Indirect-Drive/Direct-Drive Target for Inertial Confinement Fusion

Lindsay John Perkins
U.S. Patent 9,905,318 B2
February 27, 2018

Two researchers affiliated with Lawrence Livermore—**Bill Pitz**, a combustion scientist in the Materials Science division, and **Charlie Westbrook**, a retired employee—have been named **fellows** of the **International Combustion Institute**. Both are inaugural fellows and were recognized “as distinguished for outstanding contributions, whether it be in research or in applications,” at the 37th International Symposium on Combustion in Dublin, Ireland, this summer.

A 35-year Livermore employee, Pitz was honored for his work to develop chemical kinetics models for fuels with a large impact on the simulation of combustion in engines. Westbrook, who mentored Pitz for much of his Laboratory career, solved the question of what property of hydrocarbon fuel creates engine knock. Westbrook retired from the Laboratory in 2005 after a distinguished 41-year career. The Combustion Institute—of which Westbrook was once president—is an international professional society for combustion researchers, with 4,267 members from 33 countries.

Abstract

Two World-Class Lasers Combine to Power Applications

The world's most energetic short-pulse laser, the Advanced Radiographic Capability (ARC) laser enables researchers to examine high-energy-density (HED) plasmas and the extreme conditions during implosion leading up to fusion at times later than ever before. Used for diagnostic purposes in conjunction with the National Ignition Facility (NIF) main laser beams, ARC fires up to four high-intensity beamlets at a metal target to produce high-energy, high-flux x rays. When used as a high-energy backlighter, or target illuminator, these x rays have more penetrating ability than current backlighters using x rays from several diverted NIF main laser beams. Therefore, radiographic images from ARC-generated x rays show more detail and can reveal the compression of a target at much higher densities. A second backlighter application, Compton radiography backlighting, relies on x rays generated by ARC and Compton scattering to image low-atomic-number materials, such as hydrogen and its isotopes, inside a target capsule. Besides generation of x rays for backlighting, ARC can be used for a wide range of other applications. Recent Discovery Science Program experiments have produced streams of protons and a possible method for creating beams of neutrons, deuterons, or other particles. Additional experiments have generated matter-antimatter plasma pairs of electrons and positrons, an exotic condition of matter associated with black holes. This work has also led to breakthroughs in target platforms that could be helpful in other HED and inertial confinement fusion experiments.

Contact: David Martinez (925) 422-8113 (martinez264@llnl.gov).

Extending the Life of a Workhorse Warhead



Researchers are conferring another 30 years of life to the W80 warhead.

Also in October/November

- *Seismic hazard program helps countries build stronger infrastructures to resist earthquake damage.*

- *The Improvised Nuclear Device (IND) City Planner Resource (iCPR) offers science-based analyses to U.S. cities to help create emergency plans for the aftermath of IND detonation.*

- *ScrubJay, a Livermore-developed data analysis tool, helps ensure that the Laboratory's high-performance computing center lives up to its name.*

COMING NEXT ISSUE

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