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July/August 2017

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Also in this issue:

Nanoscale Details of High-Explosive Detonations Computational Tools for Materials Discovery Insights into "Relics" of Merging Galaxy Clusters

#### About the Cover

In 2013, the European Union's Extreme Light Infrastructure (ELI) Beamlines facility contracted with Lawrence Livermore National Security (LLNS), LLC, to deliver a petawatt laser capable of firing 10 times per second, with each pulse delivering 30 joules of energy in less than 30 femtoseconds (30 quadrillionths of a second), for a peak power of 1 petawatt. In November 2016, the High-Repetition-Rate Advanced Petawatt Laser (HAPLS) reached its first commissioning milestone and had set a world record for diode-pumped petawatt lasers, achieving 16 joules of energy and a 28-femtosecond pulse duration at a repetition rate of 3.3 hertz. The system, featured on the cover, has recently been delivered to the ELI Beamlines facility, where it will be installed and further ramped to its design specifications.



#### About S&TR

At Lawrence Livermore National Laboratory, we focus on science and technology research to ensure our nation's security. We also apply that expertise to solve other important national problems in energy, bioscience, and the environment. *Science & Technology Review* is published eight times a year to communicate, to a broad audience, the Laboratory's scientific and technological accomplishments in fulfilling its primary missions. The publication's goal is to help readers understand these accomplishments and appreciate their value to the individual citizen, the nation, and the world.

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# Science Technology

#### July/August 2017

Lawrence Livermore National Laboratory

## **Contents**

#### Feature

- 3 A Powerful Petawatt Laser for Experimental Science Commentary by William H. Goldstein
- 4 Advanced Laser Promises Exciting Applications The High-Repetition-Rate Advanced Petawatt Laser System (HAPLS) is designed to fire 10 times per second, which represents a major advancement over existing petawatt lasers and opens the door to new scientific discoveries.

#### **Research Highlights**

12 Detonation Science Blasts into a New Frontier Using an advanced experimental facility, scientists gain insight into the nanoscale processes of high-explosive detonations.

#### 16 Computation Boosts Materials Discovery

Livermore scientists and engineers join forces to accelerate materials synthesis and optimization using machine learning and big data analytics.

#### 20 Shocking Collisions of Cosmological Proportions

An international team including Livermore scientists uncovers evidence that merging galaxy clusters paired with supermassive black holes deliver an unprecedented "boost" to cosmic particles.

#### Departments

- 2 The Laboratory in the News
- 24 Patents and Awards
- 25 Abstract

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#### **Clearing up Clouds' Effect on Global Warming**

Clouds influence Earth's climate by reflecting incoming solar radiation and reducing outgoing thermal radiation. As Earth's surface warms, the net radiative effect of clouds also changes, contributing either a dampening (negative, cooling) or amplifying (positive, heat-trapping) feedback to the climate system. The amount of global warming from increased carbon dioxide ( $CO_2$ ) is critically dependent on the cloud feedback.

In research appearing in the October 31, 2016, edition of *Nature Geoscience*, Lawrence Livermore researchers identified a mechanism that causes low clouds—and their influence on Earth's energy balance—to respond differently to global warming depending on the spatial pattern of the warming. The researchers showed that the strength of the cloud feedback as predicted by a climate model fluctuates depending on the observed time period. Despite having a positive cloud feedback in response to long-term projected global warming, the model exhibits a strong negative cloud feedback over the last 30 years. At the heart of this difference are low-level clouds in the tropics, which strongly cool the planet by a reflecting color rediction to constant.

by reflecting solar radiation to space.

The feedback from low-level clouds in tropical regions between the 1980s and 2000s was found to be substantially more dampening compared to long-term cloud feedback. "With a combination of climate model simulations and satellite observations, we found that the trend of low-level cloud cover over the last three decades differs substantially from that under long-term global warming," says Chen Zhou, lead author of the paper. The

results imply that studies relying solely on recent observed trends may underestimate how much Earth will warm from increased CO<sub>2</sub>. **Contact: Mark Zelinka (925) 423-5146 (zelinka1@llnl.gov).** 

#### Mineral Surpasses Silicon's Solar Cell Efficiency

Organic–inorganic halide perovskite materials have emerged as attractive alternatives to conventional silicon solar cell technology. Their high light absorption and long diffusion lengths result in high power-conversion efficiencies. New research led by Professor Alex Zetti from the University of California at Berkeley, in collaboration with Lawrence Livermore research scientist Marcus Worsley, shows that using the mineral perovskite in graded bandgap solar cells achieves record-setting parameters, including an average steady-state efficiency rate of 21.7 percent. The study appears in the November 7, 2016, online issue of *Nature Materials*.

The new solar cell configuration contains two perovskite layers (incorporating gallium nitride), a monolayer hexagonal boron nitride, and Livermore-developed graphene aerogel. "The graphene aerogel is incorporated in the hole transport layer under the perovskite absorber layer and serves several critical roles in enhancing the performance of the solar cell," says Worsley. The study demonstrated that the graded bandgap perovskite device achieved a 18.4 percent steady-state efficiency rate and a peak rate of 26 percent. Typical silicon solar panels have a maximum efficiency rate of about 20 percent.

In addition, unlike silicon cells, which require expensive, multistep processes involving a clean room and high vacuum, perovskite cells can be made in traditional wet chemistry laboratories. "These advantages have made perovskite solar cells commercially attractive alternatives to silicon-based solar cells," says Worsley. "If perovskite cells reach their potential in terms of efficiency and can be reliable and produced at large-scale, they could ultimately displace silicon."

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#### Synthesizing a Five-Ring Nitrogen Compound

Lawrence Livermore scientists, in collaboration with theorists at the University of South Florida (USF), recently reported the synthesis and equation of state of a long sought-after five-



membered ring nitrogen  $(N_5)$  compound. (See image at left.) The ring-structure compounds, known as pentazolates, are the last all-nitrogen members of the azole series. The research appears in the December 6, 2016, online edition of *Chemistry of Materials*.

Starting from a mixture of cesium azide  $(CsN_3)$  and molecular nitrogen  $(N_2)$ , the Livermore scientists synthesized a stable cesium pentazolate salt compound at pressures just

above 40 gigapascals (400,000 times atmospheric pressure) and temperatures near 2,000 kelvins. Surprisingly, the experiments revealed that  $CsN_5$  is stable at room temperature down to much lower pressures. USF theorists used evolutionary structural search algorithms to generate the roadmap required for the Livermore experimentalists to synthesize and verify the ring-shaped molecular structure. "This work provides critical insight into the role of extreme conditions in exploring unusual bonding routes that ultimately lead to the formation of novel high-nitrogen-content compounds," says Elissaios (Elis) Stavrou, the lead Livermore physicist for this study.

Understanding the chemical processes governing the synthesis of single-bonded, nitrogen-rich compounds is one key required to unlock viable production strategies of high-energy-density chemical propellant and explosive formulations. Stavrou says, "The knowledge gained through this study brings our community closer to understanding how to make stable nitrogen-rich energetic materials. We aim to pursue alternative synthesis routes derived from our recent results."

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### A Powerful Petawatt Lase for Experimental Science

OR more than 40 years, Lawrence Livermore researchers have been developing cutting-edge laser systems, technologies, and optics. Today, the Laboratory is known internationally for designing, building, and reliably operating complex lasers that are aimed at advancing high-energy-density science, national security, inertial confinement fusion, and U.S. industrial competitiveness. Many of these systems have broken world records in laser energy, power, and brightness.

Recognizing Livermore's preeminence in high-power laser technology, in 2013, the European scientific community engaged with the Laboratory to design and construct the world's first laser capable of generating 30-femtosecond (30 quadrillionths of a second) pulses with peak power of more than 1 petawatt (1 quadrillion watts, or  $10^{15}$  watts) 10 times per second. Called the High-Repetition-Rate Advanced Petawatt Laser System (HAPLS), this machine will be a major resource for the European Union's Extreme Light Infrastructure (ELI) Beamlines facility, located in the Czech Republic.

As the article beginning on p. 4 describes, an exceptionally dedicated team of Livermore physicists, engineers, materials scientists, computer scientists, and technicians worked with their colleagues from ELI Beamlines to design, develop, and build HAPLS. In only three years—an extremely short time considering the technology advances that were required—HAPLS went from concept to a fully integrated system, becoming the world's highest repetition-rate petawatt laser. To meet its unique design goals, the HAPLS team incorporated Livermore advances in optics, integrated control systems, modeling and simulation, materials science, thermal management, pulse compressor gratings, systems engineering, and project management. Remarkably, this extraordinary machine can be operated by only two people, as the team demonstrated last year.

The Livermore–Czech partnership was made possible through an agreement for commercializing technology (ACT)—a new technology transfer mechanism piloted by the Department of Energy (DOE). This mechanism was conceived to help national laboratories form research partnerships using contractual terms better aligned with industry practice. Under an ACT, national laboratory contractors may take on financial risk that the U.S. government cannot assume. The Board of Governors for Lawrence Livermore National Security, LLC, which manages the Laboratory for DOE's National Nuclear Security Administration, elected to enter into the largest ACT agreement within the DOE national laboratory family to make HAPLS a reality. In agreeing to a fixed-price contract at its own financial risk, the board expressed confidence in the team's ability to complete the assignment on time and on budget and meet all technical milestones. The board also recognized the project's importance in maintaining the Laboratory's preeminence in high-average-power laser expertise.

HAPLS represents a new generation of high-energy and high-peak-power laser systems. HAPLS's designed firing rate—10 times a second—is a major advance over current petawatt systems, which can fire a maximum of only once per second because of their reliance on traditional flashlamps to pump their amplifiers. To overcome that serious limitation, HAPLS features the world's highest peak-power laser diode arrays. These arrays, developed through a Livermore partnership with the U.S. firm Lasertel, Inc., earned an R&D 100 Award as one of the top technology breakthroughs of 2015. HAPLS's unprecedented repetition rate will improve the signal-to-noise ratio in experiments and thereby enable groundbreaking research in basic physics, materials science, biomedicine, laboratory astrophysics, and industrial processes.

HAPLS passed its final commissioning milestone at Lawrence Livermore in December 2016, some 20 years after Livermore's Nova Petawatt laser became the first system to achieve peak power greater than 10<sup>15</sup> watts. After completing its qualification testing, HAPLS was disassembled and shipped to the ELI Beamlines facility in June. This fall, Livermore staff will be on hand to install and commission the system in the Czech Republic. I look forward to the results achieved from the first experiments conducted on HAPLS, which are expected to begin in 2018. In the meantime, Lawrence Livermore will continue to seek collaborations that leverage our expertise and technology. Such collaborations provide the Laboratory with opportunities to carry on its tradition of more than four decades pushing the frontiers of science.

<sup>■</sup> William H. Goldstein is director of Lawrence Livermore National Laboratory.

# Advanced Laser Set Control of the set of the

The extremely powerful High-Repetition-Rate Advanced Petawatt Laser

System (HAPLS) is poised to be an important tool for scientific research.



Inside the European Union's Extreme Light Infrastructure (ELI) Beamlines facility in the Czech Republic, Livermore's High-Repetition-Rate Advanced Petawatt Laser System (HAPLS) will be available to the scientific user community for a broad range of research.

N 1996, Lawrence Livermore scientists ushered in an age of new laser technology with the Nova Petawatt, the first system to generate a peak power greater than  $10^{15}$  (1 quadrillion) watts. Livermore scientists quickly discovered they could use the machine to create a source of radiation and subatomic particles, such as high-energy x rays, gamma rays, electrons, and proton beams, for experiments that were the first of their kind.

Twenty years later, Livermore researchers set a world record for average-power lasers and delivered a system to the European community capable of firing petawatt pulses 10 times per second (10 hertz). The High-Repetition-Rate Advanced Petawatt Laser System (HAPLS) is a major advancement over current petawatt lasers, which cannot fire more often than once per second. (See S&TR, January/February 2014, pp. 4–11.) "The high repetition rate of the HAPLS system is a watershed moment for the research community," says Constantin Haefner, HAPLS project manager and the program director for Advanced Photon Technologies in Livermore's National Ignition Facility (NIF) and Photon Science Principal Directorate. "HAPLS is the first petawatt laser to provide applicationenabling repetition rates."

HAPLS's pulses are designed to be of such intensity (up to 10<sup>23</sup> watts per square centimeter) that laser–matter interactions can generate intense beams of radiation and subatomic particles. These laser-driven secondary energy sources are compact and versatile and, together with a high repetition rate, will enable many applications in physics, materials science, medicine, biology, and industry. (See the box on p. 11.) In addition, the technology will contribute to the Department of Energy's research portfolio and its National Nuclear Security Administration's (NNSA's) Stockpile Stewardship Program.

Haefner explains that while scientists are currently performing experiments with powerful single-shot lasers, the possibility of repeating experiments 10 times per second—and for hours at a time—is unprecedented. "What the research community needs is reliable laser drivers that deliver the same precise performance pulse after pulse with high photon flux," says Haefner. Proof-of-principle experiments with single-shot lasers have provided a glimpse into new applications, but a high-repetition-rate petawatt laser with high pulse-to-pulse stability and minimal required maintenance is needed to explore these promising research areas and make possible transformative scientific discoveries.

Physicist Andy Bayramian, HAPLS systems architect, points out that researchers using single-shot systems must select experiments with anticipated high signal-to-noise ratios, since each shot is unique and the characteristics of the laser vary from one shot to another. In contrast, HAPLS is designed to repeat an experiment 10 times per second in a steady state mode and is automated to provide closed-loop stability. As a result, researchers can detect subtle reactions in a timely fashion that are typically overshadowed by other physics. In 1996, Lawrence Livermore's Nova Petawatt became the world's first laser to generate a peak power greater than 10<sup>15</sup> (1 quadrillion) watts.

Bayramian says, "HAPLS enables a truly exciting new regime in science and technology exploration."

#### A Record-Breaking Achievement

In 2013, the European Union's Extreme Light Infrastructure (ELI) Beamlines facility contracted with Lawrence Livermore National Security (LLNS), LLC, which manages the Laboratory for NNSA, to deliver a petawatt laser with performance far exceeding current lasers. The system had to be capable of firing at 10 hertz with each pulse delivering 30 joules of energy in less than 30 femtoseconds (quadrillionths of a second) for a peak power of 1 petawatt per shot. The system also had to have low power consumption. For comparison, a modern-day flashlamp-pumped laser system with similar specifications to HAPLS running at 10 hertz would draw 2.2 megawatts of electrical power. HAPLS consumes less than 130 kilowatts.



A team of researchers from Lawrence Livermore and the ELI Beamlines facility was at the Laboratory to mark HAPLS's milestone achievement. Researchers included (front left) Bedřich Rus from ELI Beamlines and (front right) Livermore's Constantin Haefner. (Photo by Jason Laurea.)



Conceptual work on HAPLS began in the fall of 2013. By 2016, an enterprising band of Lawrence Livermore physicists, engineers, materials scientists, and technicians, along with their visiting European colleagues, completed construction and final testing of HAPLS in a laboratory at Livermore. "HAPLS was a very fast-paced project," says Haefner. "In three years, we went from concept to a fully integrated and recordbreaking system with unprecedented capabilities. During that time, we pushed the cutting edge in high-average-power petawatt lasers more than tenfold."

On November 29, 2016, HAPLS reached its first commissioning milestone and had set a world record for diodepumped petawatt lasers, achieving 16 joules of energy and a 28-femtosecond pulse duration (equivalent to about 0.4 petawatts per pulse after compression) at a repetition rate of 3.3 hertz. The system was operated for more than 1 hour. An independent international committee reviewed the results and confirmed the record-setting performance. The test showed that the HAPLS design is sound and that the system can eventually be ramped to 10 hertz once installed at ELI Beamlines.

Following the historic test, Lawrence Livermore Director William Goldstein



said, "The Laboratory takes pride in pushing science and technology to new regimes." Goldstein noted that the Nova Petawatt was the first laser to achieve a peak intensity exceeding  $10^{21}$  watts per centimeter (compared to HAPLS's expected intensity of  $10^{23}$  watts per square centimeter). HAPLS's potential repetition rate is also substantially greater than the Nova Petawatt, which could fire only once every few hours.

HAPLS was disassembled in early 2017 and delivered in late June to the ELI Beamlines facility in Dolní Břežany near Prague in the Czech Republic. The laser will be integrated into the facility's laser beam transport and control systems. Both Livermore and ELI personnel will oversee ramping of the laser to design specifications. ELI Beamlines plans to make HAPLS available in late 2018 to the international scientific user community.

#### Showcase of Livermore Technology

HAPLS embraces a host of groundbreaking methods and technologies developed largely at Livermore, including arrays of laser diodes that replace less efficient and bulky flashlamps; advanced gratings for compressing high-peakpower and high-average-power laser light without damaging optics; automated control systems to continuously monitor components, minimizing the need for human intervention; and advanced optics and optical coatings. The system also uses a Livermore-developed heliumgas cooling method for laser amplifier components. Together, these advances contributed to making HAPLS the most compact petawatt laser ever built.

During HAPLS's development, Livermore personnel worked closely with industry to advance the state of the art. Several innovations driven by HAPLS's subsystem technology, including advanced laser diodes as well as industrial pump lasers and optical coatings, are already on the market. Roman Hvězda, the ELI Beamlines project manager, said, "Given the design requirements, nobody else could deliver this system in such a short time on schedule and on budget." He added that the venture with Lawrence Livermore "will be a basis for continued cooperation in the future."

Development of HAPLS's major systems was organized into several phases that were set forth in the ELI Beamlines–LLNS agreement. Performance milestones mimicked technical progress in research and development, integration, and commissioning, which provided ELI Beamlines with the confidence that the project was on track. The intermediate performance level, achieved in November, demonstrated that HAPLS's systems worked together and that the laser will meet its final design performance once installed at ELI Beamlines.

Chief mechanical engineer Dan Mason was responsible for delivery of laser hardware. "HAPLS required vast amounts of custom hardware that needed to be designed, fabricated, and assembled," he says. Engineers also conducted a great deal of thermomechanical analysis to ensure components and systems would not be unduly stressed. According to Mason, working on a first-of-a-kind laser typically



The exceptional stability of the diode-pumped HAPLS system is reflected in the measurement of the pulse duration. In one test, HAPLS fired 3.3 times per second for more than an hour, with the laser pulses (more than 12,000 total) showing remarkable uniformity. The average pulse duration was 28 femtoseconds (fs), well below the 40-femtosecond requirement. Colors depict the temporal pulse shape for all 12,000 pulses, with yellow and blue representing the highest and lowest peak power, respectively.

requires a laser technology development program, which leads to production of a prototype followed by additional testing. "For HAPLS, we had little prototyping. The schedule was extremely aggressive. We had to identify technology risks as early

#### "HAPLS is the first petawatt laser to provide applicationenabling repetition rates?"

as possible and conduct thorough analyses up front to ensure success. We could not let the system fail in the integrated testing phase and have to start all over again."

#### Working alongside ELI Researchers

In all, about 100 Livermore engineers, physicists, and technicians collaborated on HAPLS. Livermore laser physicists and engineers worked closely to design the system architecture and assemble it into an integrated system. Individual subsystems were developed and assembled by mechanical, electronic, optical, and control systems engineers. Approximately 10 scientists from ELI Beamlines and the Czech Academy of Sciences traveled to Livermore to train and collaboratively commission and operate this new complex machine.

"From the beginning, this collaboration provided hands-on training and expertise, helping to ensure operational success once the laser is installed at ELI Beamlines," said Bedřich Rus, scientific coordinator for laser technology at ELI Beamlines. "We never had a standard client–supplier relationship," he said. "It has been a great experience for our researchers and has supported their careers and professional development."

Bayramian observes, "Our Czech colleagues, mainly young scientists and technicians, saw how Laboratory personnel attacked problems and managed technical risk. They were introduced to our operations and safety culture and were attentive, inquisitive, and hardworking." Jeff Horner, HAPLS chief engineer and project manager for the system's installation at ELI Beamlines, remarks, "We trained ELI staff how to run high-average-power lasers. They were well educated in laser physics, but they had limited hands-on experience." Haefner comments, "Technology transfer does not happen through sharing of manuals, but through sharing of minds."

#### Laser Features Advanced Diodes

HAPLS consists of two interconnected Livermore-designed laser systems that



require a combined space of about 4.6-by-17 meters, plus a 4-square-meter footprint for the laser pulse compressor. Horner says, "One of the great things about HAPLS is its compact design. Laser systems of much less capability exist that are several times larger." One of the keys to the compact size is Livermore inventions in beam transport and amplifier gain balancing.

The first system—a diode-pumped, solid-state pump laser—energizes the second system—a short-pulse laser. The pump laser is designed to deliver 200 joules of energy at a repetition rate of 10 hertz for an average power of 2 kilowatts. The pump laser incorporates many examples of Livermore intellectual property.

The pump laser's amplifier uses two amplifier heads containing many neodymium-doped glass slabs, similar to those used at NIF but much smaller. Helium gas streams through the gaps between the amplifier slabs at almost ultrasonic velocities to remove heat inherently deposited in the gain material as part of the pumping and lasing process. The gas is invisible to the laser beam because of helium's low refractive index, which is close to that of a vacuum. Helium-gas cooling was invented by Livermore scientists George Albrecht and Steve Sutton in the 1980s. This method is an established one for heat removal in Livermore's high-energy, high-average-power laser systems and has been adopted by other groups as well. Gas cooling allows HAPLS to run continuously, firing 36,000 times per hour with high repeatability and stability.

Current petawatt laser systems barely operate at 1 hertz because they use flashlamps to energize their amplifiers. "We are at the limits of flashlamp technology," says Bayramian. "Laserdiode arrays enable a far more capable class of high-energy laser systems." At the output end of the pump laser, a frequency converter doubles the pump laser frequency from infrared to green to match the absorption band of the short-pulse laser.

Essential to HAPLS's remarkable repetition rate are the highest peak-power

The pump laser that energizes the short-pulse amplifier delivers pulses with energy greater than 100 joules and an energy stability of 0.7 percent. As shown in this graph, during a test, the pump laser was ramped in energy to approximately 100 joules in less than 5 minutes and then operated for 1 hour.



HAPLS consists of two interconnected Livermore-designed laser systems—a diode-pumped, solid-state pump laser and a short-pulse laser. At the pump laser output, a frequency converter doubles the laser energy from infrared to green. The short-pulse laser features custom Livermore alpha and beta amplifiers. The Gigashot-HE laser is used as a pump source for the alpha amplifier and delivers 2 joules of green laser energy per pulse at a repetition rate of 10 hertz. The entire laser system measures just 4.6-by-17 meters, plus a 4-square-meter footprint for the laser pulse compressor. (Rendering by Paul Bloom.)

laser-diode arrays in the world. Diode technology was first demonstrated on Mercury, a high-average-power laser built by Livermore researchers in the late 1990s. For HAPLS, the team partnered with Lasertel, Inc., of Tucson, Arizona, to develop advanced arrays of laser diodes with an emitting area of 5.6-by-13.8 centimeters and that produce a peak power of 800 kilowatts each. Diodes are approximately 20 times more efficient than conventional flashlamps, consuming less electricity and generating less heat in the laser.

The Livermore–Lasertel team combined advanced laser diodes and a Livermoredesigned pulsed-power system to produce the High-Power Intelligent Laser Diode System (HILADS). This system delivers two-to-threefold improvements in peak output power and intensity over flashlamp technology in a 10-times-smaller footprint. Four HILADS devices were integrated into the HAPLS pump laser. The four devices together contain more than 400,000 diodes, the largest number ever assembled, and produce a combined 3.2 megawatts of diode power. Extensive testing indicates that the HILADS lifetime will exceed 2 billion pulses. The HILADS development team won an R&D 100 Award in 2015. (See *S&TR*, January/February 2016, pp. 16–17).

"Combining Lasertel's diode technology with Livermore's highly compact and efficient pulsed-power system is the enabling technology to drive high-energy lasers at faster repetition rates," says Haefner. "Our collaboration has allowed several new benchmarks for laser performance to be set in a remarkably short period of time," says Lasertel President Mark McElhinney.

#### **A Delicate Process**

HAPLS's short-pulse laser converts the energy from the pump laser to 30-joule, 30-femtosecond pulses of 820-nanometer laser light with a peak power exceeding 1 petawatt. This laser uses titanium-doped sapphire (Ti:sapphire) as its amplification medium. For short-pulse laser systems, Ti:sapphire is a popular gain material because of its high optical quality, large bandwidth, and large crystal size (up to 20 centimeters in diameter). The 200-terawatt Callisto laser designed by Livermore scientists in the 1990s was used to generate intense beams of protons and is considered the grandfather of Ti:sapphire disk lasers. Although Ti:sapphire has a high thermal conductivity, it suffers from a large quantum defect, converting almost half of the pump power into heat. Thus, it also requires gas-cooling of the amplifier faces, similar to the method used in the pump laser. Mason says specially prepared slabs of Ti:sapphire for HAPLS's short-pulse power amplifier required more than two years to produce, including growing the boule (the initial crystal ingot), followed by months of machining, shaping, edge-cladding, and applying antireflection coatings. The slabs were then integrated into the gas-cooled

amplifier package for installation. "From start to finish, the process was an extremely delicate one," says Mason. "We had only one chance to get it right."

The short-pulse laser features two custom Livermore amplifiers, an alpha and a beta. The Gigashot-HE, a diodepumped solid-state laser developed for HAPLS by Northrop Grumman Cutting Edge Optronics, is used as a pump source for the alpha laser. The Gigashot-HE laser delivers 2 joules of 532-nanometer (green) laser energy per pulse at a repetition rate of 10 hertz, with each pulse lasting less than 10 billionths of a second.

The short-pulse laser incorporates chirped-pulse amplification, a process pioneered at the University of Rochester in the mid-1980s. This technique first stretches a short pulse of light in time from femtoseconds to nanoseconds  $(10^{-15} \text{ to } 10^{-9} \text{ seconds})$  by passing it through an optical device using finely etched diffraction gratings, thereby applying a frequency chirp. This "stretcher" converts the pulse into a



HAPLS's short-pulse laser incorporates chirpedpulse amplification, a process pioneered at the University of Rochester in the mid-1980s. This technique stretches a short pulse of light in time by passing it through a "stretcher" using finely etched diffraction gratings (shown here). The stretcher converts the pulse into a lower-intensity, longer pulse. Following amplification, two pairs of diffraction gratings are used to compress the pulse in time. lower intensity, nanosecond-long pulse in which shorter wavelengths lag behind longer wavelengths. "Without chirpedpulse amplification, the laser beam would very quickly destroy the short-pulse laser optics during this stage," says physicist David Alessi. Following amplification up to 10 billion times higher energy, the pulse is compressed in time by two pairs of diffraction gratings (the compressor), in which shorter wavelengths catch up with the longer wavelengths to achieve a cohesive, short-duration, high-peak-power pulse that can be focused at ultrahigh intensities onto a target. The Livermoredesigned gratings for both the stretcher and compressor were manufactured in-house by physicists Hoang Nguyen and Jerry Britten. The gratings feature hundreds of kilometers of precisely inscribed gold-coated lines that measure less than a micrometer wide and feature a new design that enables these gratings to be operated at high-average power.

#### Control System Keeps Watchful Eye

HAPLS also features an automated, integrated control system such as the one operating at NIF. The control system features multiple ultrafast diagnostics that continuously monitor the health of the laser. "Each shot gives permission to the succeeding shot," explains Daniel Smith, a controls engineer for HAPLS. The sophisticated control system has a high level of automation including an auto-alignment capability and immediately stops the laser if any component is out of specification. Front-end processors are tied to 85 cameras, 24 motors, and numerous diagnostic instruments. The system's high level of automation is largely responsible for allowing the laser to be operated by as few as two people, meeting an operational requirement.

In addition, adaptive optics help produce a high-quality beam a few micrometers in diameter, which when focused on a target will eventually enable HAPLS to generate intensities of  $10^{23}$  watts per centimeter. These optics correct for distortions in the



Samuel Buck from ELI Beamlines and Livermore's Shawn Betts monitor HAPLS's system function and performance during operations. HAPLS's high level of automation allows the laser to be run by as few as two people, which meets an operational requirement. (Photo by Jason Laurea.)

laser beam, providing experimenters with the highest quality laser beam profile.

#### **Pushing the Boundaries**

"It has been an incredible experience pushing the boundaries of laser technology," says physicist Tom Spinka, commissioning manager of HAPLS's shortpulse laser. "The brief time from conceptual design to commissioned hardware was remarkable." Horner cites the support provided by groups throughout NIF and Livermore's Engineering Directorate, such as optics fabrication experts, who helped make HAPLS a reality.

"An incredibly committed team, working long days and weekends, pushed the state of the art by 10 times," says Haefner. "People were inspired by the idea and the technology. Every milestone was completed on schedule, on budget, and within specification. We started with an empty room and ended with a world-record product."

For the Laboratory, the HAPLS project provided several opportunities, including the ability to participate in an international effort to deliver a cutting-edge laser for a flagship research facility. "This project allowed us to advance Livemore knowledge and expertise and push the frontiers of science and technology," says

#### A New World of Applications at ELI Beamlines

The Livermore-designed High-Repetition-Rate Advanced Petawatt Laser System (HAPLS) will be a key component of the European Union's Extreme Light Infrastructure (ELI) Beamlines facility, which was built for the international scientific user community to study laser–matter interactions. Coordinated by the Czech Republic's Institute of Physics, Academy of Sciences, ELI Beamlines is the largest scientific project in that country. Construction of the facility began in October 2012 and was completed in early 2017, although key systems are still being installed. The first experiments are scheduled for late 2018.

Although ELI Beamlines will house at least two other large lasers, HAPLS is expected to be the "workhorse" laser and will be known as the L3 laser system. The facility will include seven experimental chambers located in the basement, including a large experimental chamber dedicated to academic research of laser plasma. Scientists will be able to direct the output from any laser to whichever experimental chamber is needed.

The facility was officially dedicated on October 19, 2016. Patricia Falcone, Lawrence Livermore's Deputy Director for Science and Technology, attended the ceremonies along with Constantin Haefner, HAPLS project manager and program director for Advanced Photon Technologies in Livermore's National Ignition Facility and Photon Science Principal Directorate. "We are excited to be working with our colleagues on realizing new capabilities for lasers and are also looking forward to great scientific results from this wonderful facility," says Falcone.

Other dignitaries described the aim of the facility as attracting the best scientists in the world to perform experiments at the frontier of science to make ELI Beamlines the "CERN of laser research." Bedřich Rus, scientific coordinator for laser technology at ELI Beamlines, noted that several world records already were broken during the development of the project's laser systems, including the world's highest-peak-power laser-diode arrays developed for HAPLS.

HAPLS is expected to drive laser-accelerated sources of electrons with energies of several tens of gigaelectronvolts, as well as protons and ions with energies reaching several megaelectronvolts. Such a capability will make possible new investigations into atomic physics, time-resolved proton and x-ray radiography, nuclear physics, high-energy-density physics, plasma physics, chemistry, biochemistry, and medicine.

As one example, extremely short and bright pulses of x rays are needed for exploring phenomena that take place over very short time and length scales. Streams of extremely bright and short x rays for imaging cells and proteins at unprecedented spatial and temporal resolution will be used to study biochemical reactions and the formation and dissolution of chemical bonds. ELI Beamlines has already established the ELIBIO center, which will exploit some of the world's most powerful photon beams to perform breakthrough studies in life sciences. HAPLS could also be applied to explore treatments for deep-seated tumors using high-quality beams of protons.

Secondary-source applications include advanced imaging and nondestructive evaluation of materials. Other industrial applications include laser peening, nondestructive evaluation of parts and products—for example, to identify defects in aircraft turbine blades—and generating drugs and tracers for medical diagnostics. HAPLS could also force scientists to radically rethink the need for kilometers-long particle accelerator

facilities that require large amounts of real estate. Haefner says, "HAPLS will be able to shrink a 1,000-meterlong accelerator to tens of centimeters."

Haefner. Such knowledge can only serve to benefit the Laboratory and its missions.

Haefner is optimistic the project will also help energize U.S. short-pulse and high-average-power laser research efforts. He notes that several nations in Europe and Asia are planning advanced high-repetitionrate lasers such as HAPLS because of their potential to revolutionize fields ranging from medicine to clean energy. He adds that a valuable aspect of HAPLS's design is its scalability. As Livermore scientists help to integrate the laser system into the ELI Beamlines facility, Haefner and other Laboratory researchers are looking to develop the next generation of HAPLS-type lasers and advance several technologies originally developed for the laser system. Haefner says, "We want to continue to engineer technologies important to U.S. economic competitiveness, national security, and entirely new applications."

—Arnie Heller

Key Words: chirped-pulse amplification; diffraction grating; Extreme Light Infrastructure (ELI) Beamlines facility; flashlamp; Gigashot-HE; High-Power Intelligent Laser Diode System (HILADS); High-Repetition-Rate Advanced Petawatt Laser System (HAPLS); laser diode; Lasertel, Inc.; Lawrence Livermore National Security (LLNS), LLC; Mercury laser; National Ignition Facility (NIF); Nova Petawatt laser; petawatt; titanium-doped sapphire (Ti:sapphire).

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# Detonation Science

IGH-EXPLOSIVE (HE) detonation events unfold in a few millionths of a second. A high-voltage current vaporizes a thin metal foil within a specialized detonator, which throws a tiny plastic flyer—traveling around 2 kilometers per second into an explosive. The impact shock initiates a detonation whose front propagates supersonically through the material as the explosive rapidly decomposes. After the energy release and associated chemical reactions conclude, many HEs leave behind excess carbon that condenses into solid soot.

At Lawrence Livermore, a key aspect of stockpile stewardship includes fine-tuning and experimentally observing HE detonation processes and developing computer models to predict the behavior of different HEs. Over the last several decades, HE detonation science has progressed toward higher Livermore researchers (from left) Ralph Hodgin, Lisa Lauderbach, and Michael Bagge-Hansen prepare a high-explosive (HE) target at Livermore's High Explosives Applications Facility. (Photo by Randy Wong.)

resolution experimental and modeling capabilities that explore initiation processes, the precise chemical reactions involved and how quickly they occur, and the specific temperatures and pressures attained.

Accurate computer modeling of a detonation depends on understanding how quickly the carbon condensates, or allotropes (such as graphite and diamond), form within HE detonation soot. Previous research into this process has focused on validating microsecond phenomena. However, recent computer simulations have modeled the formation of carbon condensates at nanosecond timescales—an uncharted territory experimentally.

To validate the model predictions, a Livermore team led by physicist Trevor Willey has been investigating detonation processes using the intense, pulsed x rays at Argonne National Laboratory's Advanced Photon Source (APS) in Lemont, Illinois. "Detonation experiments produce so much visible light, and solid explosives are generally opaque. Therefore, determining what is happening—for example, optically—is difficult," explains Willey. "X rays help us penetrate deeply into the detonation with wavelengths conducive to observing nanoscale phenomena."

Livermore's multipronged approach marks the initial application of three-dimensional (3D) reconstruction algorithms to detonation systems involving an exploding foil initiator (EFI, or slapper). The effort also inaugurates the use of smallangle x-ray scattering (SAXS) for detonation experiments in the United States. Willey says, "For the first time, we can experimentally interrogate detonation phenomena on nanometer

The custom-built detonation tank developed at Livermore provides a safe, reusable venue for conducting HE experiments. (inset) During a detonation, an ultrafast pulsed x-ray beam is fired onto the target at 153.4-nanosencond intervals. The scattering patterns for individual x-ray pulses are recorded and used to ascertain information about shapes and sizes of carbon condensates.

(billionths of a meter) and nanosecond (billionths of a second) scales." Initially funded by Livermore's Laboratory Directed Research and Development Program, the team's work has transitioned into small-scale detonation science experiments supporting various programmatic activities, including stockpile stewardship and defense nonproliferation.

#### Targets, a Tank, and Technology

Computer simulations of the performance of energetic materials rely on accurate input data related to the timedependent shock initiation, the detonation process, its energy release, and formation kinetics of the resulting carbon condensate. The Livermore team designed small-scale detonation experiments to observe both detonator behavior and carbon condensate formation using a chemically diverse range of HEs. These experiments initially used cylindrical targets of HNS (hexanitrostilbene) and Composition B, which consists of RDX (trimethylenetrinitramine) and TNT (trinitrotoluene), fabricated at the Laboratory's High Explosives Applications Facility (HEAF). Target size varied by material, from a few hundred milligrams to a few grams, based on the minimum amount needed to maintain a self-propagating detonation.

To conduct repeated experiments, the team developed a mechanism for containing gas, soot, and other debris from the explosion. With the help of other HEAF colleagues, Lisa Lauderbach and Michael Bagge-Hansen outfitted a 120-liter steel



tank with a target platform, a vacuum-handling and exhaust system, and x-ray ports, while Ralph Hodgin, Chadd May, and others built the firing system. Meanwhile, the Dynamic Compression Sector (DCS), an intense x-ray beamline funded by the National Nuclear Security Administration and managed by Washington State University, was commissioned at APS. "The Dynamic Compression Sector provides an ideal place for dynamic shock and detonation experiments on fast timescales," says Willey, citing the facility's synchrotron radiation capabilities, which produce 50-picosecond x-ray pulses every 153.4 nanoseconds.

The researchers first conducted a series of EFI imaging experiments at APS. Subsequently, they installed their new tank at DCS, where they performed small-scale detonation experiments to better understand carbon condensate formation. The team collaborated with Los Alamos National Laboratory and National Security Technologies, LLC, who had been performing similar x-ray imaging tests. A four-camera array developed by Los Alamos was used to capture individual snapshots of x-ray pulses during the experiments.

#### Game-Changing Results

During the EFI experiments, APS's ultrafast pulsed x-ray beam provided high-resolution images measuring 1.5-by-1.5 millimeters at 153.4-nanosecond pulse intervals. EFIs were positioned at angles of 0, 15, 30, 45, 60, 75, and 90 degrees relative to the x-ray source and fired in these orientations. The

(a) An artist's rendering shows the setup for an experiment using an exploding foil initiator (EFI). A timing pin measures the time of the shock wave's arrival at the top of the charge. (b) A series of time-elapsed scatter-beam images, captured with the Dynamic Compression Sector's four-camera array, shows the upward progression of the detonation front.

resulting two-dimensional x-ray images, acquired at multiple angles, were input into a homegrown software package called Livermore Tomography Tools (LTT), which allows scientists to reconstruct 3D images of the EFI flyer at the pulse intervals. LTT's advanced iterative algorithms build 3D images of the object of interest from just a few views, in comparison to the typical thousands of views needed for computed tomography scans. As a result, the team captured the first detailed 3D images of flyers' kilometers-per-second motion during EFI operation.

Livermore's series of experiments on carbon condensates at DCS was no less compelling. Using the SAXS technique, the team resolved nanoscale details of the detonation. In this type of experiment, an intense but thin x-ray beam (approximately 50-by-100 micrometers) is fired directly through the sample. Scattering patterns for individual x-ray pulses were collected at 153.4-nanosecond intervals. Whereas previous studies showed condensate particle growth occurring over a few microseconds, the team's time-resolved SAXS imaging of HNS experiments demonstrated particulate growth within 400 nanoseconds after detonation. The Livermore team also observed that, once formed, graphite particulates generated from HNS detonations do not continue to change shape or size at microsecond timescales.

Determining particles' morphology and resolving their formation at faster timescales would not have been possible without the ability to perform SAXS on the four-camera array at DCS. In more recent experiments using other HEs, Willey and colleagues have observed nanostructures that range from complex and twisted to relatively flat. They have also noticed formation of nanodiamond particles and nanostructures with spherical shell graphitic layers resembling tiny "nano-onions." According to Willey, the team's data uncover possibilities for improving HE models and detonator performance. He says, "We're opening a new chapter in detonation science."



Lawrence Livermore National Laboratory



#### Lighting the Fuse on New Experiments

Nanoscale characterization of HE processes has many applications. Commercially, nanodiamonds generated during HE detonations are used to seed synthetic diamond growth and are being explored for pharmaceutical purposes, fuel additives, and other uses. (See *S&TR*, March/April 2008, pp. 14–16.) In addition, the Laboratory's stockpile stewardship mission requires continual advancements to increase the safety, efficiency, and reliability of detonation technology. (See *S&TR*, July/August 2015, pp. 6–14.)

The team's tank setup has improved the fidelity and clarity of images showing flyers in motion during EFI detonation—data that will provide unprecedented feedback for new detonator designs. Future experiments will study changing detonation conditions to produce different pressure and temperature states for yielding supplementary postdetonation data on carbon condensates. Willey's team continues research with additional HEs, including DNTF (dinitrofurazanfuroxan), HMX (octogen), TATB (triaminotrinitrobenzene), and the Laboratory-developed molecule LLM-105.

Such breakthroughs in detonation experiments are inspiring new and early-career Laboratory scientists to pursue further advances in imaging and simulation capabilities. For example, researcher Will Shaw and colleagues are investigating another avenue related to EFIs by exploring in greater detail the initiation The Livermore Tomography Tools software generates three-dimensional renderings of flyers in motion during EFI imaging experiments. Only seven views of the detonation were needed to create this reconstruction, which is viewed along x (red), y (green), and z (blue) axes.

processes that occur when the flyer strikes the explosive. X-ray scattering expert Josh Hammons is coordinating construction of novel detector systems including camera configurations that capture two frames each to generate more images per detonation. Lawrence Fellow Mike Nielsen leads efforts to characterize the recovered detonation soot with transmission electron microscopy and related techniques. "Detonation is an interesting phenomenon," observes Willey. "With these technologies, we can conduct experiments that were not possible before."

*—Holly Auten* 

**Key Words**: Advanced Photon Source (APS), carbon condensate, detonation science, detonator, Dynamic Compression Sector (DCS), exploding foil initiator (EFI), high explosive (HE), High Explosives Applications Facility (HEAF), Livermore Tomography Tools (LTT), small-angle x-ray scattering (SAXS).

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# Computation BOOSTS Materials Discovery

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awrence Livermore National Laboratory

N the area of materials science, the hunt is on for revolutionary new materials to use in applications such as flexible electronic displays, higher capacity batteries, efficient catalysts, and lightweight vehicles. At Lawrence Livermore, such materials are needed for stockpile stewardship, inertial confinement fusion experiments, radiation detectors, and advanced sensors. Ironically, although materials themselves have become more sophisticated, their development process is still rooted in 19thcentury techniques. These techniques rely on the knowledge, experience, and intuition of scientists using a trial-and-error approach to synthesis and testing that is iterated until researchers achieve a material with the desired properties.

A group of Livermore materials and computation scientists and engineers have come together to create a more modern development approach that applies machine learning, highperformance computing, and big data analytics to accelerate materials discovery. Their effort is a perfect fit for Livermore, where interdisciplinary teams of researchers work together to solve difficult problems of national importance. The team, led by materials scientist T. Yong Han, is conducting a three-year project funded by the Laboratory Directed Research and Development Program to deploy advanced materials faster and at a fraction of the cost by integrating computational and experimental tools, digital data, and collaborative networks into the synthesis and optimization process.

Synthesizing a material involves many reaction parameters, including specific chemicals, chemical concentrations, temperatures, additives, reaction times, and solvents. Scaling up a high-quality material from the laboratory to more commercial applications is often hindered by the challenge of experimentally pinpointing the material's most critical reaction parameters to obtain the desired results. Han says, "If we can discover the most relevant critical reaction parameters from existing literature using computational and data-processing techniques and experimentally verify their veracity, we will have made a significant leap in the field of materials synthesis and materials informatics."

#### Following the Recipe

Materials scientists publish tens of thousands of papers every year that contain useful information about the "recipes" they used to generate new materials. Each recipe includes the list



A Livermore research team is developing a new structured knowledge base and application programming interfaces to analyze, query, discover, and optimize processes for quickly deploying novel advanced materials.

of ingredients, how the ingredients were synthesized, how much of each ingredient was needed, and the method used to create the final material. "The amount of data in this area of research is enormous and constantly growing," says Han. "We want to set up an ingest pipeline for large numbers of papers so that we can tease out relevant and important correlations in synthesis parameters, including chemicals and process conditions, to speed materials discovery, synthesis, and optimization."

The goal is to develop an extensive computational knowledge base that will enable researchers to query desired material properties. The knowledge base may not contain the exact recipes for a given material, but with the help of machine-learning algorithms and big data analytics, it may provide a way to narrow down the possibilities or even predict the synthesis pathways, significantly reducing the time needed to produce the desired materials. Livermore computer scientist Brian Gallagher, an expert in machine-learning algorithms, says, "One of the major challenges is re-creating the experimental procedure from the original write-up. The steps are not always described in order or even in the same portion of the article. Authors also leave out essential steps that may be viewed as 'understood' by trained scientists."

As part of the process, the team will use machine-learning algorithms running on Livermore computation clusters to identify the experimental procedure sections in scientific papers the section where most materials' recipes are located. The researchers will then "train" the machine-learning tool to look for typical recipe-related sentences, initially focusing on synthesis methods for silver nanowires. This material is key to developing technologies such as water-resistant flexible displays, wearable



Material "recipes" included in scientific literature describe how researchers develop a new material in a laboratory. (left) A commercial copper powder compared with (right) copper nanowires produced at Livermore show how recipes yield different results. Livermore's structured knowledge base will allow researchers to more quickly identify the common synthesis parameters needed to develop a material with desired properties.

electronics, optoelectronic circuits, more efficient solar cells, and nanomaterial-based sensors.

#### A Strategy Takes Shape

"One of the hardest parts of a project is gathering the data," says team member and computer scientist David Buttler, a specialist in information management systems and natural language processing. Obtaining access to a useful number of papers required negotiation and extensive Web searches. Thanks to an agreement with scientific publisher Elsevier, the team has assembled a collection of 70,000 papers on the synthesis of silver nanomaterials. The team's Kansas State University collaborators, led by Professor William Hsu, are developing an application engine to determine which papers are beneficial, a capability that will speed up Web crawling for relevant work beyond the Elsevier study. With the data gathering infrastructure in place, the team has begun developing and training machine-learning algorithms to analyze the papers.



Machine-learning algorithms can learn different materials properties—for example, thermodynamic constants and atomic information—and their correlations. This chart shows 145 material property correlations for 600 compounds. Positive (red) and negative (blue) correlations are indicated. The diagonal line represents a 1-to-1 correlation in the properties. With supervised machine-learning techniques, human operators provide the software with thousands of examples of words and images labeled by names, as well as rules about data relationships. In the case of Han's project, the team is training the machine-learning tool to search for the chemical ingredients and the relationships of the chemicals to one another—that is, the procedures the scientific teams used to synthesize their materials. This information will enable the software to differentiate procedures relevant to silver nanowires from those for other nanomaterials—for example, silver nanospheres or nanocubes.

The researchers are modifying two open-source chemistry codes, OSCAR (Open-Source Chemistry Analysis Routines), a chemical names recognition tool for natural language texts, and ChemicalTagger, used for data extraction from chemistry literature, to pull out the material recipes. Buttler says, "We're rewriting the identifier section of ChemicalTagger from scratch to improve its 70-percent accuracy rate. It must be able to



The team has a five-step approach for accelerating materials synthesis, optimization, and scale-up. Machine-learning algorithms first extract information from the scientific literature, providing information that can be used to develop process models. These process models are integrated into a structured knowledge base to analyze and discover optimized procedures and conditions for materials synthesis. Users can query the knowledge base for a particular material and then experimentally validate synthesis processes in the laboratory.

convert the text into something that is easier for the machinelearning algorithm to identify."

Perhaps several dozen papers on silver nanowire synthesis will have procedural elements in common to create a process model representation. The team will analyze and bin the papers into categories based on material types, resulting in a structured knowledge base of the procedures used to synthesize these materials. Users can then query the knowledge base for a material with the critical parameters they seek, fin d the recipes closest to possessing the material properties they want to develop, and then conduct experimental validation and scale-up in the laboratory. This workflow could help eliminate much of the trial-and-error process typical of materials research today. Ultimately, it may also enable predictions of synthesis pathways for new materials. Buttler says, "As far as we know, an automated process to identify and assemble the relevant text and convert it into steps that form a coherent recipe does not exist today."

#### Not Just for Nanowires

The team—which also includes materials scientists Jinkyu Han and Anna Hiszpanski, computer scientists Bhavya Kailkhura, Peggy Li, and Hyojin Kim, and engineer Erika Fong—is excited about the technology's capabilities. In its infancy, the machine-learning tool is designed specifically to help materials scientists working with nanomaterials, but the technology has broader applications. "The machine-learning pipeline is agnostic to the process—we are developing it for materials synthesis, but it could be used for any other process," says Han.

Machine-learning algorithms could help the pharmaceutical industry by screening papers describing natural products with medicinal properties. The technology could also assist the medical profession, increasing the speed at which life-saving modifications to medical procedures make their way into general practice. Han says, "If we are successful, the technology will help younger scientists gain knowledge more quickly from the experiences of many people—it will reduce the number of reallife experiments we need to conduct to obtain a result, and we will achieve desired results faster."

—Allan Chen

**Key Words**: algorithm, big data analytics, ChemicalTagger, informatics, machine learning, materials discovery, OSCAR (Open-source Chemistry Analysis Routines), silver nanowires, structured knowledge base, supervised learning.

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# SHOCKING GULISIONS of Cosmological Proportions

THE universe works in mysterious ways, but little by little, researchers from Lawrence Livermore and other institutions are uncovering the physics behind many of today's cosmological puzzles. One such conundrum involves the formation of radio relics (diffuse synchrotron radio sources) in merging galaxy clusters—events in which two of the universe's most massive bound objects, each containing thousands of galaxies, collide. These radio-emission sources are millions of light years across and filled with gas or plasmas superheated to 10 to 100 million kelvins. (For comparison, the Sun's core is about 15.7 million kelvins.)

Radio relics were initially thought to result from electrons being accelerated to relativistic speeds by shocks created when galaxy clusters collide. Observational evidence, including x-ray data, further suggested that the shocks were responsible for delivering these huge energy "kicks" to electrons. An international team, including Lawrence Livermore researcher Will Dawson, recently undertook a study to explore radio relics and the story behind their creation. What the researchers found was a one-two punch of truly cosmological proportions, involving particles being spewed from their orbits around supermassive black holes before being fast-tracked by the shocks created from the merging galaxy clusters.



#### The Relic–Cluster Connection

Although radio relics have been observed for years, they are not well understood. Dawson explains, "Galaxy clusters are not densely packed. Just as empty space exists between planets and stars in our own galaxy, mostly empty space is found between galaxies in the clusters. So, galaxy cluster collisions look more like two objects passing through each other." The empty space is filled with a diffuse intracluster medium of high-energy particles moving at a few thousand kilometers per second. Aside from the Big Bang, galaxy cluster collisions are the most energetic events in the universe, releasing up to about  $10^{57}$  joules on gigayear timescales—more than a trillion times the expected total energy output of the Sun over its 10-billionyear lifetime. Most of the energy released during cluster collisions is converted into thermal energy and turbulence in the medium, resulting in enormous shock waves that can be likened to a plasma "sonic boom."

Once these shock waves are formed, they propagate, compressing the magnetic fields and hot, x-ray-emitting gases. As the shocks travel forward, they encounter other particles, including electrons, which get trapped in the shocks' magnetic fields. Once captured by a field, electrons begin to spiral around, accelerating and emitting synchrotron radiation. A plausible rationale for the phenomenon was that the shock waves were causing nonrelativistic electrons to be "kicked" into relativistic regimes. However, the shocks alone were not enough to account for the observed accelerations. "We had many questions about this process," explains Dawson. "How could the shocks possibly accelerate initially nonrelativistic particles to relativistic speeds? Could the theory be wrong? Or, were we missing a key piece of the puzzle?"

One possible theory involved "fossil" relativistic electrons, whose lifetimes in the intracluster medium are relatively short, about 100 million years. After losing most of their energy, these electrons would be invisible to radio telescopes, no longer radiating within the observable band of radio frequencies. Fossil electrons could, in theory, be efficiently

A composite image shows the "Toothbrush Cluster" with a radio relic (green). The radio relic stretches over 6 million light years in its longest dimension. Visible light data captured with the Subaru telescope appears in white. Diffuse x-ray emissions observed using the Chandra X-Ray Observatory are shown in purple. The distribution of dark matter in the cluster, inferred by gravitational lensing, is shown in blue. (Image courtesy of NASA.) re-accelerated by shocks and eventually produce bright radio relics. One theory postulated that the fossil electrons may originate from active galactic nuclei (AGNs)—compact regions in the center of galaxies emitting radiation far higher than normal. Such radiation, which can come from any part of the electromagnetic spectrum, likely results from the accretion of matter by a supermassive black hole at the galaxy's center.

To determine whether the electrons accelerated by the cosmic shocks might have their beginnings in AGNs, the research team, which comprised scientists from 17 organizations, including Lawrence Livermore, the Harvard–Smithsonian Center for Astrophysics in Massachusetts, the University of California at Davis, Stanford University, and the National Centre for Radio Astrophysics in India, set out to find as many merging galaxy clusters as possible. Drawing from available radio-survey data from the Giant Metrewave Radio Telescope in India and the National Science Foundation's Karl G. Jansky Very Large Array,

the team began looking for evidence of shocks from merging galaxy clusters by their radio relic signature. "We started with radio data since it's less expensive to survey large fields of view compared to the previous methods relying on x-ray plus optical surveys," says Dawson. The team uncovered 27 cluster mergers with evidence of merger shocks, then zeroed in for more detail using optical data from the Hubble Space Telescope and the Keck and Subaru telescopes in Hawaii, as well as x-ray data from NASA's Chandra X-Ray Observatory. Using the multiwavelength data, the scientists discovered that several cluster galaxies contained AGNs with supermassive black holes. In particular, merging galaxy clusters Abell 3411 and Abell 3412 in the constellation Hydra (about 2 billion light years from Earth) had all the elements the team needed for the next step in their analysis. "This merger had everything we were looking for," says Dawson. "Evidence of the clusters merging, radio relics, and supermassive black holes with accompanying jets."

Combining radio (red), x-ray (blue), and optical (background field of galaxies) data, astronomers discovered what happens when a jet-like eruption of particles from a supermassive black hole is swept up in the collision of two galaxy clusters. The particles, initially ejected at relativistic speeds, slow down over millions of years before being re-accelerated by the shock waves of the merging galaxies. The comet-shaped x-ray-emitting cloud (top of image) indicates the hot gas of one cluster plowing through the hot gas of the other. (Image courtesy of NASA.)





The supermassive black holes feed off stars and gas, sucking in all materials, including photons, that come within their crushing gravitational fields. Accretion disks of gas form around the black holes, circling, heating up, and throwing off powerful x rays. Dawson explains, "Under certain conditions, a black hole can also produce a rotating and tightly wound magnetic 'funnel.' Although it may seem counterintuitive, the intense electromagnetic fields associated with these funnels can actually eject some of the particles from the accretion disks." These particles spew out in two intense, high-velocity gas jets, perpendicular to the accretion disk.

The ejected gas particles move at relativistic speeds. As they lose energy over cosmological stretches of time, their energies decrease to the point of no longer being detectable. When these particles—pre-excited and still very energetic—tangle with the shock waves created from merging galaxy clusters, they get a second boost and are re-accelerated to relativistic speeds, resulting in the swirling radio relic structures observed near the shock fronts.

#### Winning the Cosmological Lottery

Dawson and the team's research marks the first time that all of the puzzle pieces surrounding radio relics and merging galaxies were available and fit together. The research confirms and links the collision of two galaxy clusters, the ejection of relativistic Radio data of Abell 3411 illustrate areas (purple, dark blue) where particles are losing energy as they age after being ejected from the vicinity of the black hole. At the leading edge of the shock front (green, light blue), particles are re-accelerated, creating radio relics. (Image courtesy of Reinout van Weeren.)

particles spiraling around supermassive black holes in these clusters, the re-acceleration of particles from the shocks created by the collisions, and the formation of radio relics as a result of this process. The moment of discovery was serendipitous. "Consider," says Dawson, "the clusters were accelerating towards each other for more than 2 billion years, with the collision occurring about 1 billion years ago from the observed state. From our Earth-bound perspective, it has taken about 4 billion years for the light from the event to reach us. This event is comparable to seeing one single frame from a very long movie that was recorded cosmological eons ago. Luckily, here on Earth, we were in the right time and place to see it."

Many questions remain, among them, the origin of the largescale magnetic fields in the shocks and how particle acceleration processes operate in these dilute, cosmic plasmas. To gain further insights, Dawson and others are turning to Livermore's National Ignition Facility (NIF), which is no newcomer to this type of research. (See *S&TR*, December 2016, pp. 4–11.) As part of a NIF Discovery Science Program study, researchers are exploring the formation and structure of collisionless shocks produced by largescale, laser-driven plasmas. Ideally, data from these experiments will provide information about the role collisionless shocks play—if any—in generating and amplifying magnetic fields while accelerating particles.

Dawson stresses that the team's findings would not have been possible without astronomers with expertise in different areas joining forces to interpret data from diverse data sets radio, optical, and x ray. "By aligning the different expertise of individuals within our team, we were able to understand the importance of the complex events we were observing in the biggest particle accelerators of the universe."

-Ann Parker

**Key Words**: active galactic nuclei (AGN), cosmic ray, electron reacceleration, fossil relativistic electron, galaxy cluster, National Ignition Facility (NIF), radio relic, supermassive black hole.

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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).

S&TR July/August 2017

#### Patents

Emergency Sacrificial Sealing Method in Filters, Equipment, or Systems Erik P. Brown U.S. Patent 9,581,243 B2 February 28, 2017

Acceleration of Objects to High Velocity by Electromagnetic Forces Richard F. Post U.S. Patent 9,581,409 B2 February 28, 2017

#### Awards

The **Defense Advanced Research Projects Agency** (DARPA) named Lawrence Livermore engineer and physicist **Vincent Tang** as a **Program Manager of the Year** for 2016. The award recognizes Tang for leading a program involving multiple agencies to develop and deploy networked sensors for dynamic, real-time radiological and nuclear threat detection over large urban areas. Tang has created and led multiple efforts, including the SIGMA program, which is aimed at creating cost-effective, continuous, city-to-region-scale radiation monitoring networks to help prevent attacks involving radiological "dirty bombs" and other nuclear threats. Out of approximately 100 program managers at DARPA, Tang is 1 of 2 to win the award for 2016.

Lawrence Livermore researchers Jonathan Belof and Eric Duoss were named recipients of the 2016 Presidential Early Career Award for Scientists and Engineers (PECASE). This honor is the highest bestowed by the U.S. government on outstanding scientists and engineers who are early in their independent reseach careers. PECASE winners receive \$50,000 a year over five years to pursue research in their field.

Belof, a group leader in the Design Physics Division in the Weapons and Complex Integration Principal Directorate, won for his work in phase transition dynamics and nonequilibrium systems. He was also recognized for his efforts teaching science, technology, engineering, and math (STEM), mentoring underprivileged students, and participating in the Laboratory's High-Energy-Density Physics summer scholar program.

A member of Livermore's technical staff, Duoss was honored for his research in advanced materials and manufacturing combined with microarchitected design. He has dedicated himself to educating the younger generation of scientists and engineers about STEM pathways, volunteering in outreach programs, and conducting Laboratory tours for students and teachers.

The **National Academy of Engineering** (NAE) has bestowed its highest honor, election as a **Member**, to Lawrence Livermore senior scientist **Charlie Westbrook**. He was recognized for his Method for Chemical Amplification Based on Fluid Partitioning in an Immiscible Liquid Brian L. Anderson, Bill W. Colston, Christopher J. Elkin U.S. Patent RE46,322 E February 28, 2017 (Reissue date)

Transverse-Displacement Stabilizer for Passive Magnetic Bearing Systems Richard F. Post U.S. Patent 9,590,469 B2 March 7, 2017

"pioneering development, applications, and leadership in chemical kinetic modeling to advance combustion science and technology." Westbrook was part of a 105-person class inducted in October 2016. NAE members are peer-elected in recognition of their innovations in research, technology, education, or business. For more than 40 years, Westbrook has worked at the Laboratory, where he continues his research on chemical kinetic modeling with next-generation fuels.

Eight teams of Lawrence Livermore researchers and one individual were honored with **Defense Programs Awards of Excellence** from the **National Nuclear Security Administration** (NNSA). The awards honored work performed in 2015 that proved critical to ensuring the safety, security, and effectiveness of the nation's nuclear deterrent.

The 2015 L1 Reuse Milestone Team developed and strengthened capabilities for enabling reuse designs in the future stockpile. The Implosion Dynamics and Performance Team used breakthrough analytical methods and simulations of experimental data in support of the Stockpile Stewardship Program (SSP). Both teams also won the recognition of "Exceptional Achievements." The Planetary Defense team addressed a critical planetary defense challenge related to the threat posed by asteroids to the planet. The Advanced Radiographic Capability (ARC) Commissioning Team successfully commissioned ARC at the National Ignition Facility (NIF). The NIF Shot Rate Enhancement Team implemented shot rate improvement projects that enabled an 86 percent increase in experiments. The Commodity Technology System-1 (CTS-1) **Procurement Team** initiated the delivery of CTS-1 clusters that will support NNSA's life-extension programs. The 'FEusion' Library Productization Team created significant simulation capabilities that allow two distinct computational meshes to interact within one hydrodynamic simulation. The Radiochemical Threshold Detector Data and Uncertainty Assessment Team assessed and documented values and uncertainties for a complete suite of underground nuclear test threshold detector data. Finally, Frank Graziani led an effort to develop a working plan for addressing the "boost issue" in nuclear weapons performance.

#### **Advanced Laser Promises Exciting Applications**

In 2013, the European Union's Extreme Light Infrastructure (ELI) Beamlines facility contracted with Lawrence Livermore National Security (LLNS), LLC, which manages Lawrence Livermore for the National Nuclear Security Administration, to deliver a petawatt laser capable of firing 10 times per second, with each pulse delivering 30 joules of energy in less than 30 femtoseconds (30 quadrillionths of a second), for a peak power of 1 petawatt. An enterprising band of Lawrence Livermore physicists, engineers, materials scientists, and technicians, along with their visiting European colleagues, completed construction and final testing of the High-Repetition-Rate Advanced Petawatt Laser System (HAPLS) in 2016. The system was disassembled and then delivered in June 2017 to the ELI Beamlines facility in Dolní Břežany near Prague in the Czech Republic. The laser will integrated into the facility's laser beam transport and control systems. Both Livermore and ELI Beamlines personnel will oversee ramping of the laser to design specifications. ELI Beamlines plans to make HAPLS available by late 2018 to the international scientific user community. HAPLS is a major advancement over current petawatt lasers, which cannot fire more often than once per second. HAPLS's combination of extreme power and repetition rate will make possible new scientific discoveries. Its high-repetition pulses are of such intensity (up to  $10^{23}$  watts per square centimeter) that they can generate secondary sources, such as x rays and highenergy particles, to study fundamental properties of light-matter interactions. HAPLS follows by 20 years Livermore's historic development of the first petawatt laser.

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## The Game-Changing Telescope



Researchers move closer to unlocking mysteries throughout the universe with the Large Synoptic Survey Telescope.

#### Also in September

• Cosmochemistry is constraining the age of events in the solar system and revealing some surprises.

• A Livermore-designed array of thousands of tiny mirrors promises to advance a host of applications, including self-driving cars.

• The Laboratory's outreach programs provide opportunities for students, teachers, and the community.

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