

July/August 2019

Science & Technology

REVIEW



SUPPORTING A NEW
Carbon Future

Also in this issue:

- Modeling Debris and Shrapnel Risk**
- Big Data Boosts Scientific Research**
- Diamond Anvil Cells Apply Pressure**

About the Cover

The United Nations Intergovernmental Panel on Climate Change warns that the average global temperature could increase by more than 2°C this century if measures are not taken to reduce the amount of CO₂ in the atmosphere. As the article beginning on p. 4 describes, Lawrence Livermore researchers are working on new technologies and storage methods that support global-scale CO₂ (and methane) removal. The work is being done as part of the Laboratory Director's Engineering the Carbon Economy Initiative.



Cover design: Mary J. Gines

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.

The Laboratory is managed by Lawrence Livermore National Security, LLC (LLNS), for the National Nuclear Security Administration (NNSA), a semi-autonomous agency within the U.S. Department of Energy (DOE). LLNS is a limited liability company managed by Bechtel National, Inc.; the University of California; BWXT Government Group, Inc.; and AECOM Energy & Construction, Inc. Battelle Memorial Institute also participates in LLNS as a teaming subcontractor. Cutting-edge science is enhanced through the expertise of the University of California and its 10 campuses and LLNS's affiliation with the Texas A&M University system. More information about LLNS is available online at www.llnslc.com.

Please address any correspondence (including name and address changes) to S&TR, Mail Stop L-664, Lawrence Livermore National Laboratory, P.O. Box 808, Livermore, California 94551, or telephone (925) 423-3893. Our e-mail address is str-mail@llnl.gov. S&TR is available on the Web at str.llnl.gov.

© 2019. Lawrence Livermore National Security, LLC. All rights reserved. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344. To request permission to use any material contained in this document, please submit your request in writing to Public Affairs Office, Lawrence Livermore National Laboratory, Mail Stop L-3, P.O. Box 808, Livermore, California 94551, or to our e-mail address str-mail@llnl.gov.



Prepared by LLNL under contract
DE-AC52-07NA27344

This document was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor Lawrence Livermore National Security, LLC, nor any of their employees makes any warranty, expressed or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or Lawrence Livermore National Security, LLC. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or Lawrence Livermore National Security, LLC, and shall not be used for advertising or product endorsement purposes.

Contents

S&TR Staff

SCIENTIFIC EDITOR
Dawn A. Shaughnessy

MANAGING EDITOR
Ken Chinn

PUBLICATION EDITOR
Caryn Meissner

WRITERS
Holly Auten, Allan Chen,
Arnie Heller, Ben Kennedy,
and Ann Parker

ART DIRECTOR
Mary J. Gines

PROOFREADER
Deanna Willis

S&TR ONLINE
Lauren Casonhua, Rose Hansen,
and Pam Davis Williams

PRINT COORDINATOR
Diana Horne

S&TR, a Director's Office publication,
is produced by the Technical Information
Department under the direction of the
Office of Planning and Special Studies.

S&TR is available on the Web
at str.llnl.gov

Printed in the United States of America

Available from
National Technical Information Service
U.S. Department of Commerce
5285 Port Royal Road
Springfield, Virginia 22161

UCRL-TR-52000-19-7/8
Distribution Category UC-99
July/August 2019

Feature

- 3 Initiatives Help Propel the Laboratory Forward**
Commentary by William H. Goldstein
- 4 A New Carbon Economy Takes Shape**
Laboratory researchers are exploring revolutionary technologies and improved storage methods for reducing atmospheric waste gases.



Research Highlights

- 12 No Shots in the Dark**
At the National Ignition Facility, a specialized team assesses the risk of damage from target debris and shrapnel dispersal during high-energy laser shots.
- 16 Big Data Illuminates the Physical Sciences**
Livermore teams are applying innovative data analysis and interpretation techniques to advance fundamental science research.
- 20 The Pressure's On: Diamond Anvil Cells Reimagined**
A new design for diamond anvil cells puts the extreme squeeze on materials of interest to astrophysicists and stockpile scientists.



Departments

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

Advanced Biodetection with Microbiome Array

Veterinarians and agricultural inspectors who seek to detect and contain the spread of animal diseases can now turn to a newer, faster, and less expensive biological detection system. The device is the commercialized successor to Lawrence Livermore's earlier detection platform—the Lawrence Livermore Microbial Detection Array (LLMDA), which was licensed in 2016 to Thermo Fisher Scientific and went on sale later that year as Applied Biosystems™ AMA.

In a yearlong evaluation, published in the February 8, 2019, issue of the online scientific journal *PLOS ONE*, a team of researchers from Livermore, Kansas State University, and Thermo Fisher Scientific used AMA to test 14 veterinary samples and 30 environmental samples for pathogens and found that AMA performed at a resolution similar to the highly effective LLMDA, but with a much higher throughput. Livermore biologist Crystal Jaing, who leads the detection system effort, says, “AMA increases the throughput by 10- to 20-fold and decreases the cost by 5-fold.”

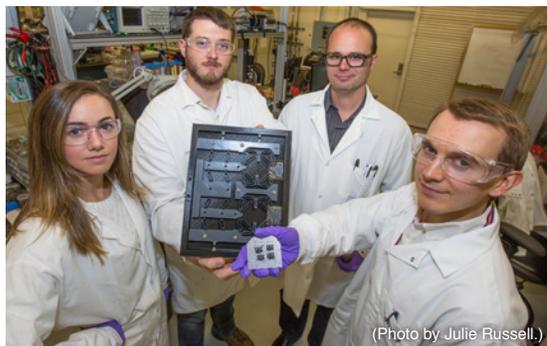
The AMA device is the most comprehensive and efficient microorganism detection platform built to date. It can analyze 96 samples in just 3 days (compared to 4 samples in a single day with LLMDA) and detect more than 12,000 microorganisms, including 6,901 bacteria; 4,770 viruses; and a combined total of 842 archaea, fungi, and protozoa. The new arrays can also analyze a variety of sample types and have applications in nutrigenomics, agrigenomics, and animal research and modeling.

Contact: Crystal Jaing (925) 424-6574 (jaing2@llnl.gov).

Printing the “Building Blocks” of Computers

Lawrence Livermore scientists and engineers with colleagues from the University of California at Los Angeles are using three-dimensional (3D) printing to create mechanical logic gates (see image at right)—the basic building blocks of computers that can perform any kind of mathematical calculation. The work is part of an effort to create materials that respond to changes in their surroundings, including in extreme environments such as high radiation, heat, or pressure, which would destroy electronic components. The research was reported online February 20, 2019, in the journal *Nature Communications*.

The mechanical logic gates incorporate flexure components that allow the system to bend and move, behaving similar to switches. The flexures are chained together and, when stimulated, trigger a cascade of configurations that can be used to perform mechanical logic calculations without external



(Photo by Julie Russell.)

power. Results are translated into movement, creating a domino effect throughout all the gates that physically changes the device's shape. Lead researcher Andy Pascall says, “If these logic gates were embedded into a material, it could respond to its environment in a controlled, precise way.”

Mechanical logic gates, while not as powerful as the physical ones used in typical computers, could prove useful in rovers sent to hostile environments, such as Venus, or in low-power computers intended to survive nuclear or electromagnetic pulse blasts. The gates also have potential uses in vaccine and food safety processes as well as industrial applications. “Using 3D printing, our design is not limited in scale,” says Pascall. “We can fabricate components down to several micrometers or up to as big as we need them to be, and they can be rapidly prototyped.”

Contact: Andy Pascall (925) 423-1926 (pascall1@llnl.gov).

Extreme Volcanism Played Role in Dinosaur Extinction

The catastrophic Chicxulub meteorite impact in Mexico has long been viewed as the sole cause of the mass extinction at the Cretaceous–Paleogene boundary—the geological moment when many creatures from the age of dinosaurs vanish from the fossil record. In research that appeared in the February 22, 2019, edition of *Science*, Lawrence Livermore scientist Kyle Samperton and colleagues present the most compelling evidence yet that massive volcanic eruptions in the Deccan Traps region of India also contributed to the fall of the dinosaurs approximately 66 million years ago.

Previously, the team analyzed ratios of uranium and lead isotopes in the mineral zircon to determine that Deccan flood basalt volcanoes began their main eruptions roughly 250,000 years before the extinction and were ongoing for the next 750,000 years, unleashing about 80 to 90 percent of the area's lava flows. The team's new findings suggest Deccan eruptions were highly nonlinear, having four major volcanic pulses. According to this eruptive age model, the largest volcanic pulse immediately precedes the mass extinction event with an approximate 90 percent probability.

Volcanoes spew both sulfur dioxide, which cools the atmosphere on short timescales, and carbon dioxide, which warms the atmosphere on long timescales. The pulsed eruptions likely resulted in extreme short-term cooling, followed by long-term warming. “Such dramatic shifts in atmospheric temperature can be catastrophic for delicately balanced ecosystems,” says Samperton. “Our finding confirms what researchers have long suspected regarding the pulsed tempo of flood basalt eruptions over Earth's history.”

Contact: Kyle Samperton (925) 422-9258 (samperton1@llnl.gov).



Initiatives Help Propel the Laboratory Forward

EVERY day the Laboratory is responsible to our sponsors for meeting numerous program deliverables and milestones. At the same time, our enduring national security mission requires us to anticipate future developments and threats by remaining at the cutting edge of science and technology. Director's Initiatives have proven to be a particularly effective mechanism for maintaining the Laboratory's technical vitality and expertise while ensuring it successfully carries out its national security mission.

Director's Initiatives are designed to advance science, technology, and engineering in emerging research areas that merit special attention. They enhance existing core competencies or spawn new ones, and may even promote entirely new research directions. Across the extraordinary breadth of the Laboratory's ongoing work, a small number of initiatives are designated based on the Laboratory's strategic intent, emerging trends in the external environment, and new scientific possibilities. Each initiative is unique in these three aspects. What is common among the initiatives is the purposefulness of management attention in these special topical areas.

Management attention notably includes designation of an initiative leader, who strategically approaches advances in science and technology, understands its national implications, and is fully aware of Lawrence Livermore's capabilities and ongoing work in the designated domain. These initiative leaders, all senior scientists, develop and provide a focused vision as well as guide and integrate the portfolio of work. Initiative leaders are also asked to consider the nature of needed investments in research, workforce development, and infrastructure. Initiative strategies and domain portfolios are regularly reviewed by the senior leadership team.

A particularly ambitious Director's Initiative—Engineering the Carbon Economy—is described in the feature article that begins on p. 4. This initiative is dedicated to helping create the science and technology required to mitigate global-scale climate change through carbon dioxide (CO₂) removal and recycling. I expect this endeavor to grow in size over the next few years as climate mitigation assumes greater national and global importance. The initiative recognizes the enormous undertaking necessary to move to a new and sustainable carbon future. In response, Livermore researchers are working with industry, academia, and other national resources.

Our research emphasis is aimed at manufacturing carbon-based products—fuels and chemicals—not from fossil carbon, but from CO₂ harvested from the atmosphere. For this effort, Livermore

researchers are developing electrochemical approaches based on advanced manufacturing. Scientists also recognize that the majority of the CO₂ removed from the atmosphere will ultimately be stored in the Earth, either through underground sequestration or through agricultural approaches. To that end, initiative researchers are working to return carbon to soil in long-lived forms to both improve the atmosphere and make land more productive.

In addition to Engineering the Carbon Economy, four other Director's Initiatives are strengthening Lawrence Livermore science and technology while looking ahead to emerging national security-related issues.

Accelerated Materials and Manufacturing: Laboratory missions require new specialized materials and components with previously unattainable properties. Through this initiative, we are developing breakthrough materials and manufacturing technologies to meet the needs of the National Nuclear Security Administration, which also have broad commercial applications.

Predictive Biology: This initiative combines the life sciences, precision experimental measurements, and high-performance computing to meet emerging challenges to human health and biosecurity. Such a predictive framework will enable a new data-driven, simulation-based approach to threat characterization, diagnosis, and intervention.

Space Science and Security: This initiative responds to other nations' efforts to develop counter-space capabilities in an increasingly complex global security environment. The program applies expertise in space science to respond to emerging threats, employs advanced modeling and simulation to evaluate mission concepts, and develops and deploys novel instruments for small satellite platforms.

Cognitive Simulation: This initiative focuses on integrating machine learning, high-performance simulation, and empirical data for national security applications. For example, the initiative combines large ensembles of simulations with experimental data to produce models with improved prediction performance of inertial confinement fusion experiments conducted at the National Ignition Facility.

By any measure, Director's Initiatives are producing large payoffs from relatively modest investments. They help keep Lawrence Livermore an exciting and challenging place to conduct research as well as serve the nation.

■ William H. Goldstein is director of Lawrence Livermore National Laboratory.

A New Carbon Economy Takes Shape

*A Laboratory Director's Initiative
responds to the unrelenting buildup of
greenhouse gases in the atmosphere
with new technologies and approaches
aimed at "negative emissions."*

A large, leafy green tree stands on the left side of the page, its branches extending towards the center. The background is a bright, hazy sky with a faint rainbow visible. The foreground is a lush green field of tall grass.

THE atmospheric concentration of carbon dioxide (CO₂) has surged in the last two centuries, from 280 parts per million during the preindustrial age in the early 1800s to more than 410 parts per million today. Climate scientists calculate that even with clean electrical power sources, such as the wind and Sun, and emission-free cars and trucks, the world will need the capabilities to remove 10 billion metric tons (10 gigatons) of atmospheric CO₂ per year beginning in 2050 to avoid a significant global temperature increase. For scale, 10 gigatons of CO₂ is the amount produced by approximately 2,500 coal-fired power plants in a single year.

Without such an enormous undertaking, the United Nations Intergovernmental Panel on Climate Change warns that the average global temperature could increase by more than 2°C this century. This warning was the basis of the Paris Agreement of 2016—an international accord aimed at strengthening the global response to climate change. “About 75 percent of the goal to keep global temperature below 2°C could be met by aggressive zero carbon–technologies,” says Roger Aines, chief scientist for Lawrence Livermore’s Energy Program. “However, humankind has no obvious option but to also remove large amounts of CO₂ from the atmosphere to meet the remaining 25 percent of the goal.”

Aines explains that global-scale atmospheric CO₂ removal (also called negative emissions) will be an unprecedented endeavor requiring enhanced scientific understanding, new technologies, collaborations, and companies dedicated to “cleaning” the atmosphere through CO₂ capture, sequestration, and conversion to useful products and fuels. The Lawrence Livermore Director’s Engineering the Carbon Economy Initiative, which is overseen by Aines, was conceived in 2018 to help support global-scale CO₂ and methane removal.

(Director's Initiatives focus on important emerging national needs.) The effort comprises several research areas that include manufacturing carbon-based products from CO₂, returning carbon to CO₂-depleted soil, sequestering CO₂ deep underground, and performing systems analysis to predict the costs and benefits of different carbon management approaches.

Supported by Laboratory Directed Research and Development (LDRD) funds, the Department of Energy (DOE), the ClimateWorks Foundation, and Cooperative Research and Development Agreements (CRADAs), this new carbon-reduction initiative involves approximately 50 researchers, including early career staff and postdocs. Numerous partnerships with universities, other national laboratories, California state agencies, and nongovernmental organizations have also been established. Researchers draw on Laboratory strengths in geoscience, atmospheric science, materials science, advanced manufacturing, and systems analysis and optimization.

The Engineering the Carbon Economy Initiative responds to the increasing threat presented by the buildup of greenhouse gases that trap heat within the planet and make it warmer. Aines explains that before the industrial age, the amount of CO₂ that plants and the ocean absorbed was in balance. "The extra 45 billion tons that we put into the air every year is affecting this stability. We have already put too much carbon dioxide into the atmosphere. Stopping these emissions is critically important, but it will take many years to build up the needed negative-emissions technology and infrastructure. The time is right for this research effort."

The new Director's Initiative is aligned with DOE's Rewiring

the Carbon Economy strategy, which aims to use waste CO₂ as a feedstock to produce chemicals, fuels, and other products and create a sustainable carbon-based economy. Low-cost renewable electricity is at the heart of this effort, and Aines points to the nation's Midwest region, where wind and solar farms are producing remarkably cheap electricity, as the likely place where CO₂ will be harvested and repurposed.

Capture and Convert

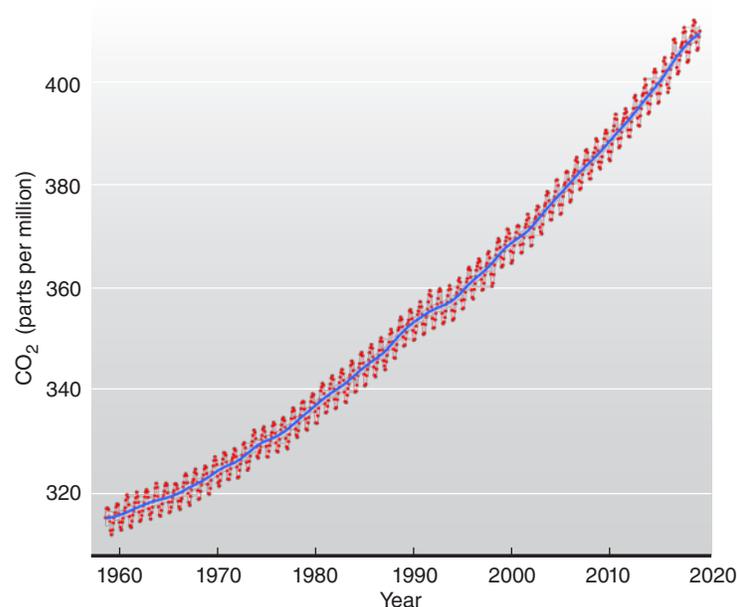
The Engineering the Carbon Economy Initiative builds upon the Laboratory's existing research to limit atmospheric carbon by capturing emissions. Environmental scientist Joshua Stolaroff notes that CO₂ is typically mixed with other greenhouse gases that together escape from factory smokestacks and power plants. The CO₂ must be at least 95 percent pure before it can be compressed and transported for use as a feedstock—a renewable, raw material that can be used as a fuel or converted

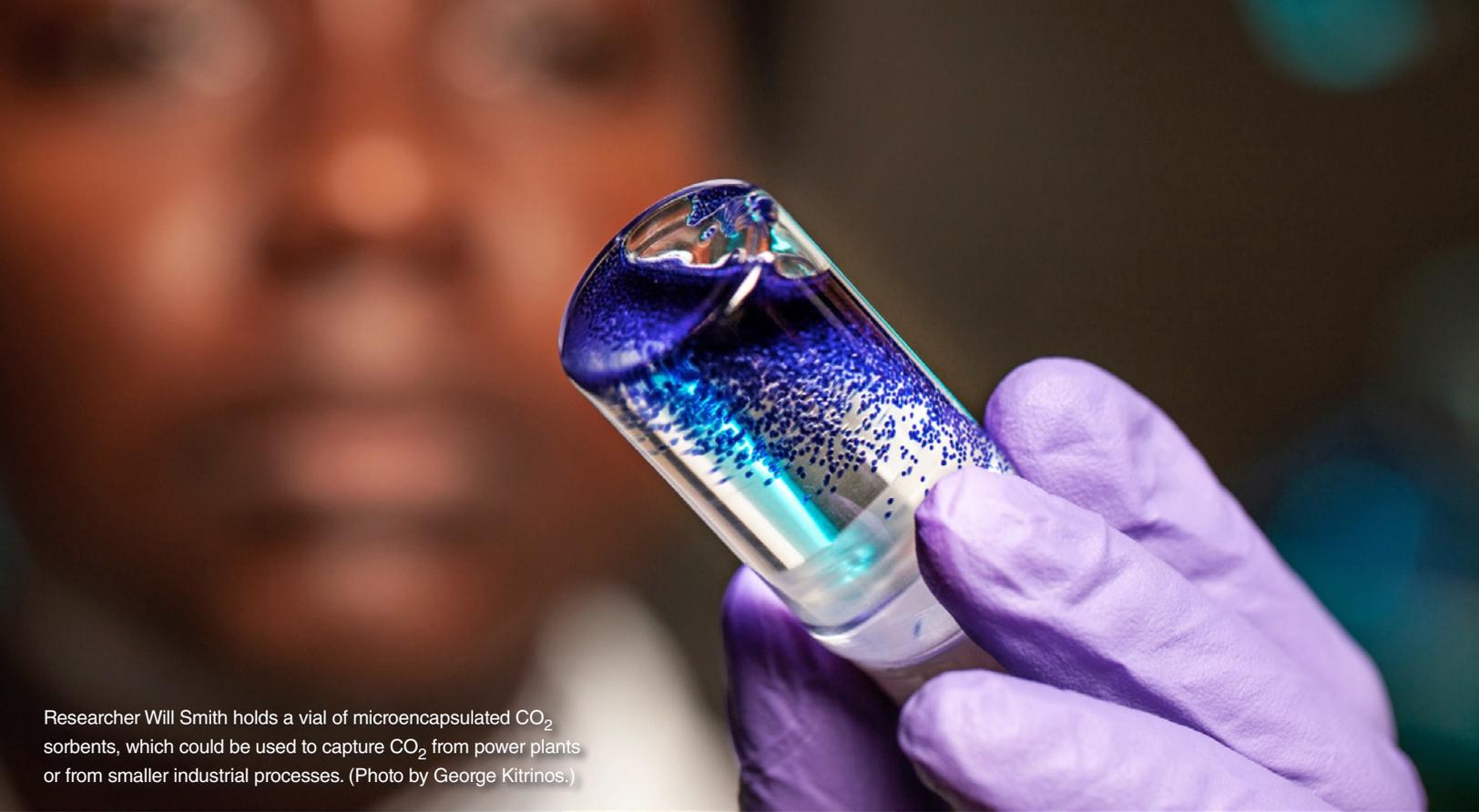
to one—or else stored underground. (*S&TR*, December 2015, pp. 13–16.)

DOE's Office of Fossil Energy supports Livermore's development of new carbon-capture approaches that use three-dimensional (3D) printing, also known as additive manufacturing, to make microengineered components that are cheap to produce. For example, Livermore researchers have developed microencapsulated CO₂ sorbents—reusable capsules measuring less than 1 millimeter in diameter. The capsules comprise a highly permeable polymer shell enclosing a fluid made up of sodium carbonate. Gaseous CO₂ diffuses through the shell and reacts with the sodium carbonate solution, forming crystallized sodium bicarbonate (baking soda). The capsules could be used to capture CO₂ from power plants or from smaller industrial systems. In addition, materials scientist Jennifer Knipe is leading a DOE-funded program to demonstrate how the Laboratory's capsule materials could be used for transporting CO₂ to algae. Knipe's team is showing that algae can live on CO₂ obtained directly from the materials as opposed to traditional bubbled CO₂. This discovery may prove useful for improving algal biomass production.

Similar significant sources of CO₂ include landfills, sewage plants, steel mills, and biogas facilities. In the case of biogas facilities, removing CO₂ would leave pure methane (natural gas) as a renewable fuel or to make specialty chemicals. Chemist Sarah Baker, Stolaroff, and others are working with Southern California Gas Company to build a pilot plant at a California biogas facility to capture CO₂ for later storage and produce a steady stream of methane. Capturing and then repurposing or storing CO₂ from a biological source would effectively remove it from the air—a prime example of a negative-emissions strategy.

The Keeling curve depicts the accumulation of CO₂ in the Earth's atmosphere based on continuous measurements taken at Hawaii's Mauna Loa Observatory from 1958 to the present.





Researcher Will Smith holds a vial of microencapsulated CO₂ sorbents, which could be used to capture CO₂ from power plants or from smaller industrial processes. (Photo by George Kitrinis.)

A Chemical Industry Transformation

In a separate project, Baker and materials engineer Eric Duoss are leading an LDRD Strategic Initiative (SI) to transform the way chemicals are made by creating 3D-manufactured reactors that catalyze the conversion of CO₂ into valuable feedstocks. Aines points to a recently completed \$18 billion petrochemical plant in Dubai that converts natural gas to various low molecular weight hydrocarbons such as ethylene (C₂H₄, the most abundant chemical feedstock). Such enormous plants use thermochemical reactors, which have high capital and operating costs. Aines says, “Chemical manufacturing today is a separations nightmare.”

Whereas temperature is the driving force in traditional reactor and separation technologies that use oil and gas as carbon sources, Livermore prototype reactors that harness CO₂ as the carbon source use electricity (ideally produced from renewables). The SI team of more than 15 researchers is developing these modular electrochemical reactors for converting CO₂ into industrial chemicals, lubricants, and polymers while radically improving efficiency and selectivity.

The reactors are designed to operate at ambient temperature and low pressure, thereby promising much lower capital and operating costs.

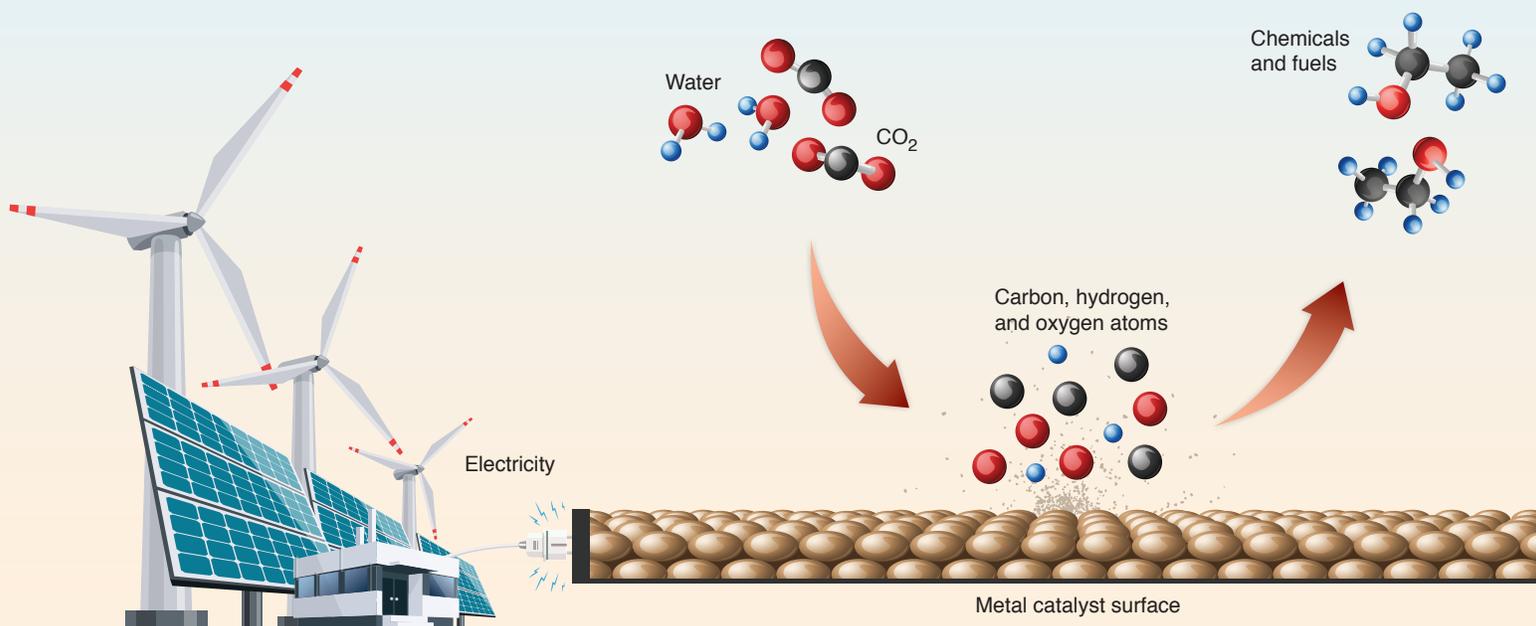
The team is working to control the local reaction environment (electric field, species concentration, ionic strength, pH, multiphase flow, and other factors) to an unprecedented degree. Similarly, the team is learning to control the 3D microstructure, from individual grains and crystal facets to the overall reactor system, of metal catalysts and other materials that are key to converting CO₂ to a host of organic compounds. Guided by multiscale models that span atomic to continuum levels in length and time, researchers are combining emerging computational design optimization methods with technoeconomic analyses to invent commercially viable reactors. “With these innovative designs in hand, we will use Livermore’s unique additive manufacturing approaches to implement the best catalysts onto our 3D reactor platforms. In doing so, we will achieve an unprecedented level of performance,” states Duoss.

Through application of these advanced manufacturing techniques, the researchers

aim to shorten development cycles from what are typically months (or years) in academic settings to weeks or even days for conceptualization, construction, and testing of electrochemical cells and reactors. Ultimately, the researchers envision their reactors mimicking biological structures, such as trees and lungs, that feature 3D and hierarchal flow paths to control and speed the transport of reactants and products. The researchers are collaborating with colleagues from Stanford University, the University of California (UC) at Santa Cruz, the University of Toronto, the California Institute of Technology, Carnegie Mellon University, the University of Massachusetts Amherst, and French multinational gas and oil company Total S.A.

Bacteria Do It Better

Commercial production of methane, along with agriculture and livestock activities and landfills, results in a large volume of methane lost to the atmosphere. In fact, methane emissions contribute about one-third of present net global warming. Conventional separation technologies, such as stirred tanks, are designed to convert methane to more valuable products



As depicted in this rendering, Livermore is developing a prototype electrochemical reactor that uses electricity (ideally produced from renewable sources) to convert CO₂ to valuable feedstocks. The team is learning to control the three-dimensional (3D) microstructure of metal catalysts and other materials that are key to this conversion process.

using high temperature and pressure, and they have a low conversion efficiency.

In an LDRD-supported endeavor, Baker and materials scientist Fang Qian are working to improve methane conversion by “printing” bacteria into the polymer walls of the 3D-printed reactors. The research team has partnered with the National Renewable Energy Laboratory, which provides Livermore with genetically modified microbes called methanotrophs that convert methane to organic acids, which can be used in other products.

Using live microbes instead of inorganic catalysts has advantages of mild reaction conditions, self-regeneration, low cost, and catalytic specificity. No added electricity or heat is needed, and the reactors continuously produce organic acids from methane at room temperature and pressure. This work is the first demonstration of 3D-printing live cells to create chemical reactors. In initial tests, the printed microbes were 20 times more productive than microbes in a stirred tank.

Returning Carbon to Soils

Soils are a huge natural sink for atmospheric CO₂, making carbon uptake by soils a promising method for removing gigatons of carbon from the air. Modern agricultural practices, such as routine machine tilling, have depleted soils’ natural CO₂ content, resulting in carbon oxidation and enormous losses of CO₂ from microbial respiration. “Loss of CO₂ from soil is on par with human-caused emissions,” says biogeochemist Jennifer Pett-Ridge. She and other researchers are exploring approaches for returning carbon to the soil in long-lived forms, which would reduce atmospheric CO₂ and make farmland more productive. The research team is using Livermore’s Center for Accelerator Mass Spectrometry and its NanoSIMS (nanometer-scale secondary ion mass spectrometer) to quantify carbon uptake in prairie soils and determine how soil microbes metabolize carbon compounds.

As part of this study, Livermore researchers Erin Nuccio, Pett-Ridge, and others are investigating key microbial

processes in soil, such as the decomposition of root residue and turnover of soil organic matter, to identify specific minerals that seem to absorb higher levels of carbon than other materials. In doing so, they are discovering that soil organic matter may be more vulnerable to climate change than previously thought. Plants store a large portion of the carbon from photosynthesis in their roots. Much of this carbon is secreted and then taken up by soil microorganisms. However, elevated CO₂ concentrations in the atmosphere can cause plants to oversupply root-associated microbes, causing excess decomposition activity, which frees organic compounds from protective associations with minerals, resulting in a net loss of soil carbon.

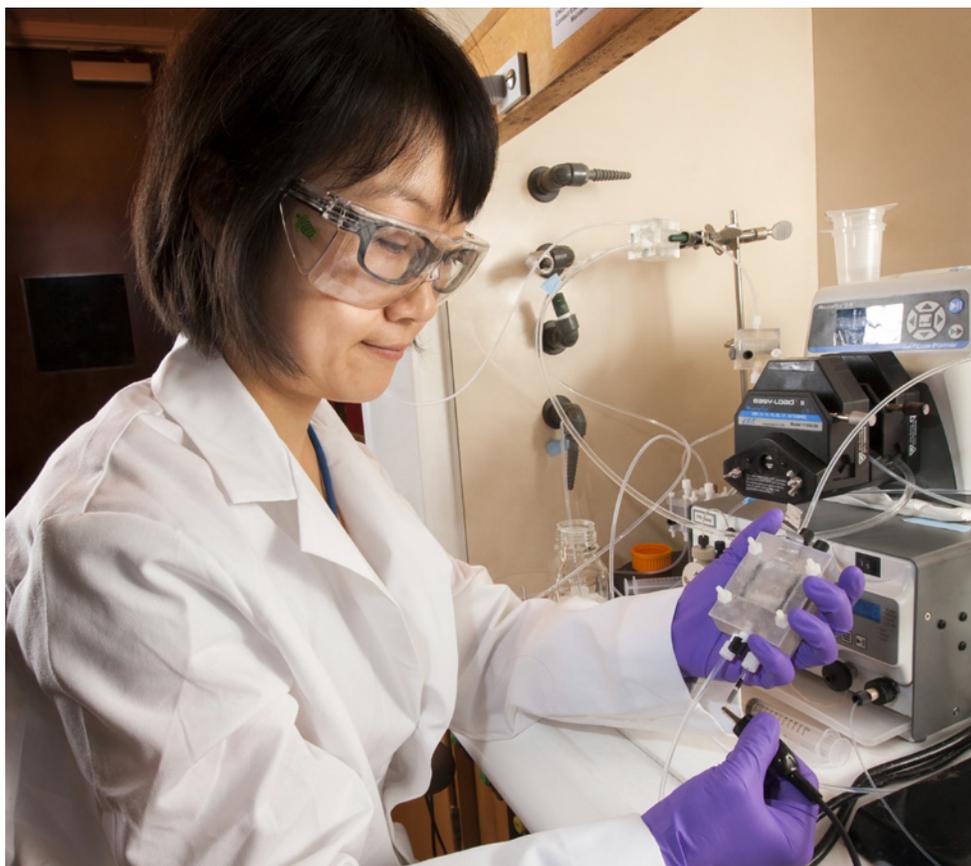
The researchers are also looking at the effects of deep-rooted plants on soil carbon stocks, especially perennial grasses found in the Midwest, which form roots that can extend down to 4 meters—deeper than the reach of a plow’s blades. The roots have a one- to two-year lifetime, and when they die, they are eaten by microbes. The steady

breakdown of the native prairie grass roots over tens of thousands of years has yielded the Midwest's black, rich soils. Tilling the soil disrupts the root networks, causing huge amounts of CO₂ to be liberated, in particular when native perennial grasses are replaced with shallowly rooted crops. Pett-Ridge says no-till agriculture, a relatively new movement, leaves the carbon-rich roots in place, and is one approach to slowing the relentless removal of soil carbon. Together with colleagues at UC Merced and UC Berkeley, Pett-Ridge, Nuccio, and postdoc Eric Slessarev have been quantifying the carbon contribution of switchgrass located at 12 sites in areas ranging from Texas to Wisconsin and from Oklahoma to Florida.

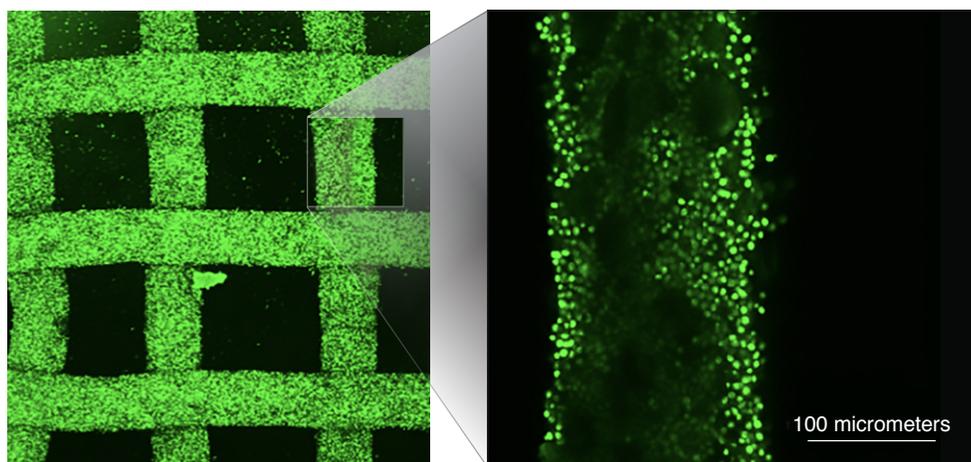
Taking Advantage of Biomass

An important part of the Engineering the Carbon Economy Initiative is performing systems analysis of how various industries contribute to CO₂ emissions. Livermore scientists are working with industry, academia, state, and federal partners to perform life-cycle and technoeconomic analyses to identify areas where carbon emissions can be drastically reduced. For example, both biomass-fired electricity and fermentation generate large amounts of CO₂ that could be stored underground or converted to useful products and fuels.

Biomass comprises waste from agricultural practices, food processing, animal manure, and even sewage treatment plants. Conventional pyrolysis, in which biomass materials are decomposed by heating them at high temperatures produced by natural gas and without oxygen, is a standard technique for turning biomass into other useful chemicals and fuels. Postdoc Wenqin Li and Laboratory scientist George Peridas are analyzing new technologies for making this process more efficient, collaborating with Iowa State University's Bioeconomy Institute to leverage autothermal pyrolysis for biomass conversion. Autothermal pyrolysis uses only air as the fluidizing gas, allowing for



Materials scientist Fang Qian checks the performance of a methane flow-through device for a 3D-printed reactor containing genetically modified microbes. The microbes, printed into the reactor's polymer walls, convert methane to organic acids.



In initial tests, "printed" microbes (green dots), shown here embedded within a reactor's polymer wall, were 20 times more productive than microbes used in a conventional stirred tank.

25 percent fewer capital costs and eliminating the heat transfer barriers of traditional methods.

In California, recent droughts and insect infestations have generated about 145 million dead and dying trees, which also pose a significant fire threat. Livermore researchers are studying how to best manage this enormous amount of biomass by applying expertise in systems design and technoeconomic and life-cycle analysis. “We’re working on understanding the economics of this process,” says Li. “Our goal is to mitigate CO₂ emissions by decomposing biomass in small, transportable units to produce valuable products.”

Livermore researchers are working with Sierra Pacific Industries, the state’s

largest private landowner, to erect a modular, pilot-scale autothermal pyrolysis plant that will take dry biomass materials, grind them, and dump them into a column operating at about 500°C at atmospheric pressure. The decomposed carbon constituents would be vaporized and then condensed to liquids that can be upgraded into transportation fuels and chemicals. Autothermal pyrolysis also produces solid biochar (charcoal), which can be used as a soil amendment and thereby sequester carbon underground.

Storing CO₂ Deep Underground

Livermore researchers have been instrumental in developing ways to sequester CO₂ deep underground (more than 1,000 meters), where the pressure turns it into a liquid. The researchers are particularly interested in engaging the U.S. oil industry to make underground CO₂ storage a reality in depleted oil fields. An attractive option is using the well-established infrastructure and expertise resident in oil and gas production companies in Central California. Aines points out that Livermore researchers provide the most advanced 3D fracture mechanics modeling for managing the risk of induced seismicity associated with underground CO₂ sequestration projects.

CO₂ sequestration is not a new concept, and

DOE-sponsored pilot studies for the past decade have demonstrated its utility by safely storing 16 million tons underground. Notably, since 1996, the Sleipner oil platform off Norway’s coast in the North Sea has been putting nearly 1 million metric tons of CO₂ underground per year, the first large-scale carbon removal plant in the world. Livermore researchers are working with an independent oil producer in California to determine if CO₂ storage under its oil fields is a safe and economical approach for the company.

Toward a New Carbon Economy

According to Aines, the United States is poised to become the world leader in negative emissions largely through CO₂ sequestration and production of carbon-based materials and fuels from atmospheric waste products. Development and demonstration of innovative technologies will be key to this new carbon economy, which could surpass today’s agriculture, oil and gas, or electrical power sectors in size. In many parts of the country, infrastructure exists for such a transformation. For example, California’s Central Valley has 100,000 trained oil workers, whose skills could be applied to putting large amounts of CO₂ under existing oil fields. “The technology, people, and jobs are comparable for both oil production and underground CO₂ sequestration. Today’s oil jobs could be converted to tomorrow’s carbon reduction jobs.”

New technologies for converting CO₂ into everyday materials and fuels will provide opportunities for commercial enterprises, especially where CO₂ and natural gas are readily available, and electricity is inexpensive. In the Texas to Iowa corridor, for example, CO₂ is an abundant feedstock, and new wind turbines and solar farms routinely sell power on the wholesale market for less than 2 cents a kilowatt hour, much cheaper than power from natural gas, coal, and nuclear power plants. Industries could use that electricity and CO₂ to



Using a Geoprobe 54LT coring device, researcher Eric Slessarev takes a 2.5-meter-long core sample to determine whether the deep rooting system of Texas switchgrass retains more soil carbon than annual crops. (Photo by Erin Nuccio.)

make chemical products in high yields without much of the expensive separation equipment required in today's refineries and chemical plants. Moreover, this new economy would improve national security through energy self-sufficiency, as well as promote climate and economic security.

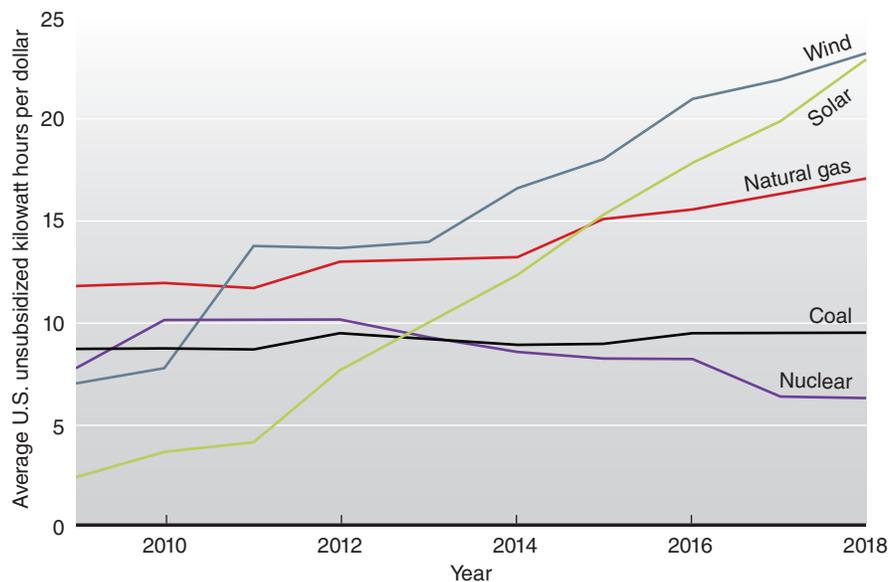
Aines reports that interest is high among U.S. businesses for the new Livermore technologies. In June 2018, Lawrence Livermore held a workshop for 20 companies, including ExxonMobil, 3M, and Nike, all interested in how their products can be produced with materials fabricated from CO₂. Aines says oil companies in particular are aware of shifting public attitudes about global warming and the industries responsible for generating large amounts of CO₂. The major oil and gas companies are looking at ways to supply the same products but with CO₂ and methane as the starting ingredients.

Partnerships Are Critical

French oil producer Total S.A. has two five-year CRADAs in operation with Livermore and Stanford University. One focuses on underground CO₂ sequestration and the other on reactors for conversion of CO₂ into useful products. Aines says, "Total S.A. wants to create its entire suite of products from CO₂ and methane."

Lawrence Livermore was a founding member of the New Carbon Economy Consortium, an alliance of universities, national laboratories, and nongovernmental organizations working to build a carbon-conscious world. The Laboratory was also a founding member of DOE's Joint Bioenergy Institute to accelerate research in biofuels. The institute combines the scientific expertise of four national laboratories, five academic institutions, and one industry partner.

Livermore researchers who are part of the Engineering the Carbon Economy Initiative have developed strong partnerships with California state



A new carbon-based economy would make use of electricity produced from renewable sources over more expensive natural gas, coal, and nuclear power plants. This graph shows the amount of electricity that would be generated per dollar invested in a new power plant, based on U.S. average costs for the full lifetime, using data from the investment firm Lazard.

agencies to create solutions to address climate change challenges. For example, the state's low carbon fuel standard attempts to combat the steady growth of transportation-related CO₂—half of California's yearly total. A 2018 executive order by former California Governor Jerry Brown declared a statewide goal to achieve carbon neutrality no later than 2045, and to achieve and maintain net negative emissions thereafter. In addition, a recent state law calls for renewable energy resources and zero-carbon resources to supply 100 percent of electricity retail sales to California end-use customers and 100 percent of electricity procured to serve state agencies by 2045. Another law requires statewide greenhouse gas emissions to be reduced to 40 percent below 1990 levels by 2030. Aines remarks that as the world's fifth-largest economy, California's actions cannot be ignored.

Meeting the former governor's executive order will require 100 to 150 metric tons of negative emissions per year. Aines asks the

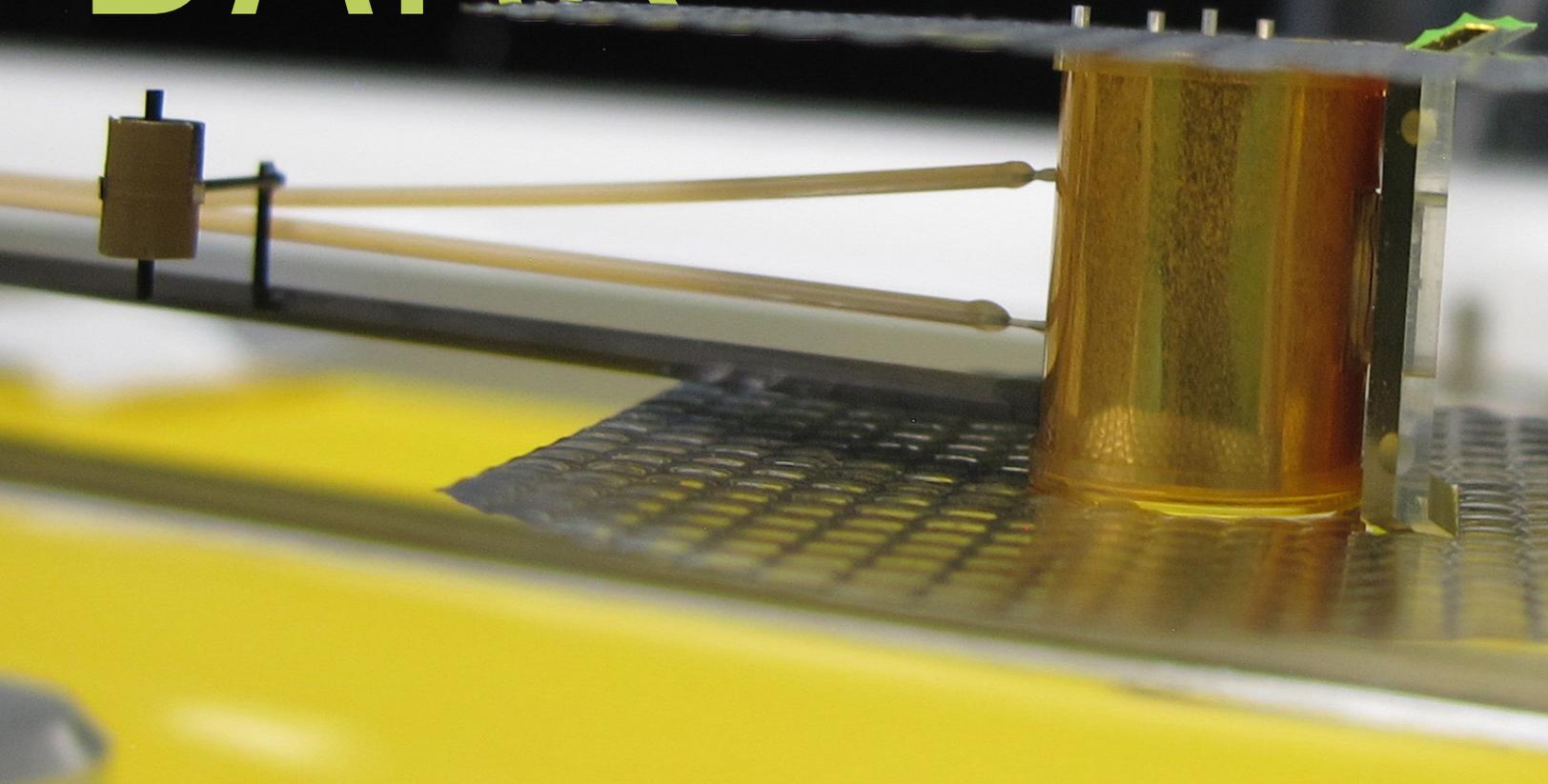
tough questions: "Can we really clean up the atmosphere? Can we create a negative-emissions infrastructure twice as big as today's oil industry?" His answer is equally direct. He states, "By engaging science, engineering, and most importantly, partnerships, we can help address one of the greatest challenges of this century. Lawrence Livermore is proud to be a part of finding the necessary solutions."

—Arnie Heller

Key Words: Bioeconomy Institute, carbon dioxide (CO₂), CO₂ sequestration, Cooperative Research and Development Agreement (CRADA), electrochemical reactor, Engineering the Carbon Economy Initiative, greenhouse gas, Intergovernmental Panel on Climate Change, Joint Bioenergy Institute, Laboratory Directed Research and Development (LDRD) Program, methane, microencapsulated CO₂ sorbent, National Renewable Energy Laboratory, negative emissions, pyrolysis, switchgrass, Total S.A.

For further information contact Roger Aines (925) 423-7184 (aines1@llnl.gov).

No Shots in the DARK

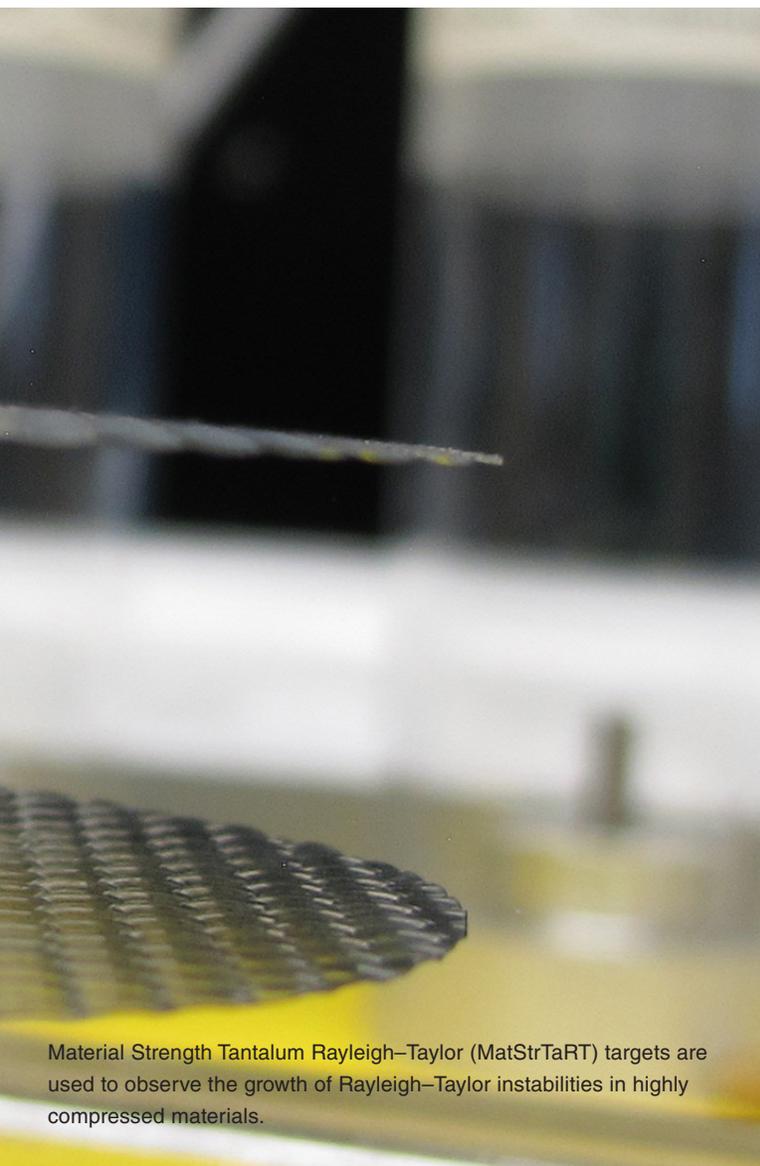


DURING experiments at the National Ignition Facility (NIF), 192 laser beams converge onto a tiny target at the center of the 10-meter-diameter, spherical target chamber in support of stockpile stewardship and fusion-ignition physics. Livermore scientists use the data from these experiments to certify the safety and security of the nation's nuclear stockpile and make progress toward achieving fusion ignition and energy gain. With NIF, researchers can also explore the physics of material conditions at the centers of gas giant planets and stars, as well as other extreme environments.

Researchers conduct approximately 400 shots a year at NIF. The facility relies on a small army of personnel to keep it operational 24 hours a day nearly year round. One of the many critical teams is the Debris and Shrapnel Working Group (DSWG). Its mission is to evaluate risks to NIF equipment from

target debris and shrapnel produced during experiments. Through computer modeling, risk assessment analysis, and experience, the team helps ensure that debris and shrapnel generated by laser shots does not damage optics, diagnostics, or other components that are expensive and difficult to replace.

DSWG is one of three groups within TaLIS (Target-Laser Interaction Sphere), an umbrella group led by Dean LaTray whose purpose is assessing the potential damage to NIF from the interaction of the laser with the target. A second group within TaLIS examines the danger posed by laser-plasma interactions, which can cause laser light to pass back through the beamlines, damaging mirrors and laser glass. A third group performs configuration reviews, examining the interface between laser light, targets, diagnostics, and the rest of the target chamber. "The service

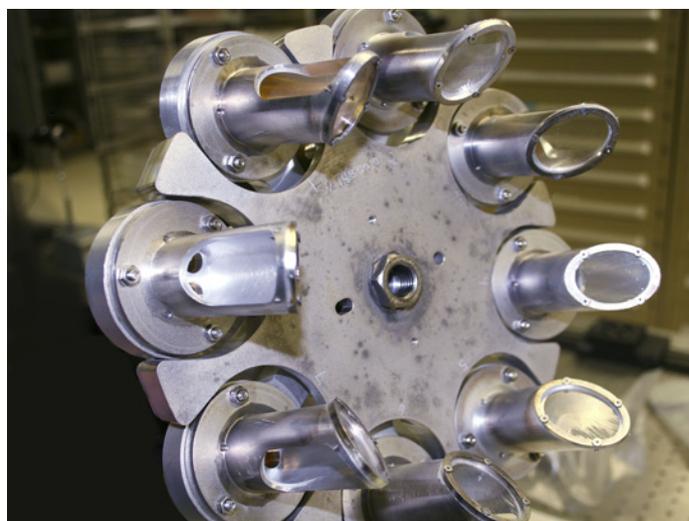
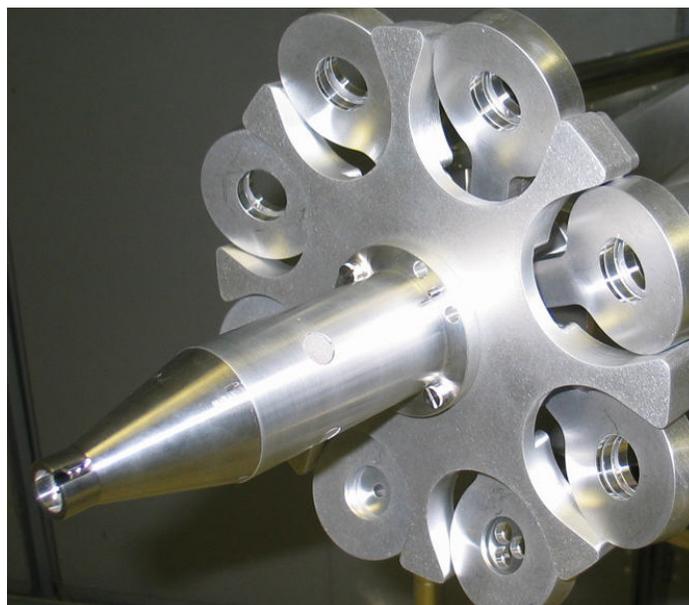


Material Strength Tantalum Rayleigh–Taylor (MatStrTaRT) targets are used to observe the growth of Rayleigh–Taylor instabilities in highly compressed materials.

TaLIS provides is unique because NIF is unique,” says LaTray. “We offer capabilities that no other facility can provide.”

Three Types of Risk

Debris and shrapnel risks stem from three sources: x-ray loads emitted from the target when hit by the laser, debris wind (vaporized material, low-density particles, or molten spray traveling at high velocity), and unvaporized target components. In the first case, laser energy heats up the target and the emitted x rays deposit energy onto diagnostics that cause materials on exposed surfaces to ablate—generating a damage-inducing pressure pulse. Debris wind poses a risk as a distributed, blast-like pressure wave. These two sources primarily threaten diagnostics in close proximity to the targets. Finally, when deposited laser energy is not sufficient to fully



(top) The original x-ray source application (XRSA) test cassette positions eight sample holders in the direct path of the x-ray source during experiments. Simulations done by the Debris and Shrapnel Working Group (DSWG) led to the re-engineered XRSA platform (bottom), which includes thin, tilted prefilters that absorb soft x-ray energy and are vaporized. (Image courtesy of Kevin Fournier.)

vaporize the target, chunks of molten or solid material driven at up to 10 kilometers per second can impact target chamber components, including optics and diagnostics.

To mitigate these risks, DSWG runs computer simulations of shots to model the deposition of the laser energy and the subsequent response of targets and diagnostics using several

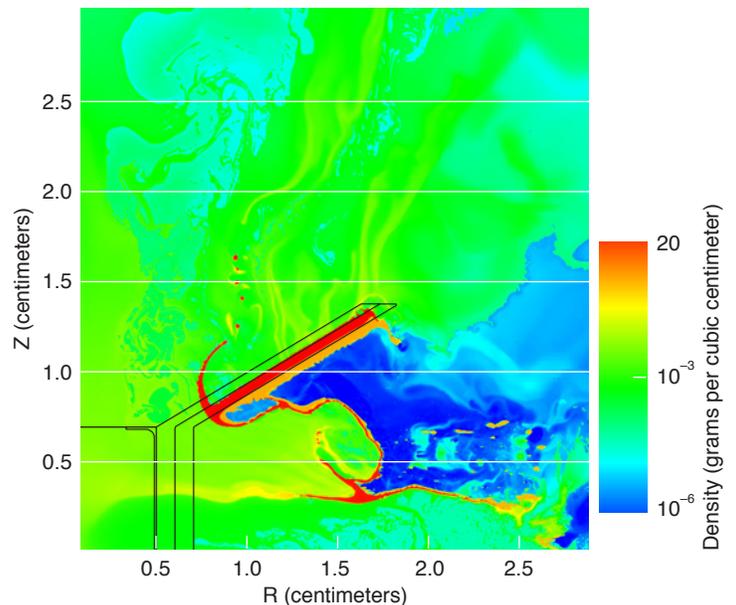
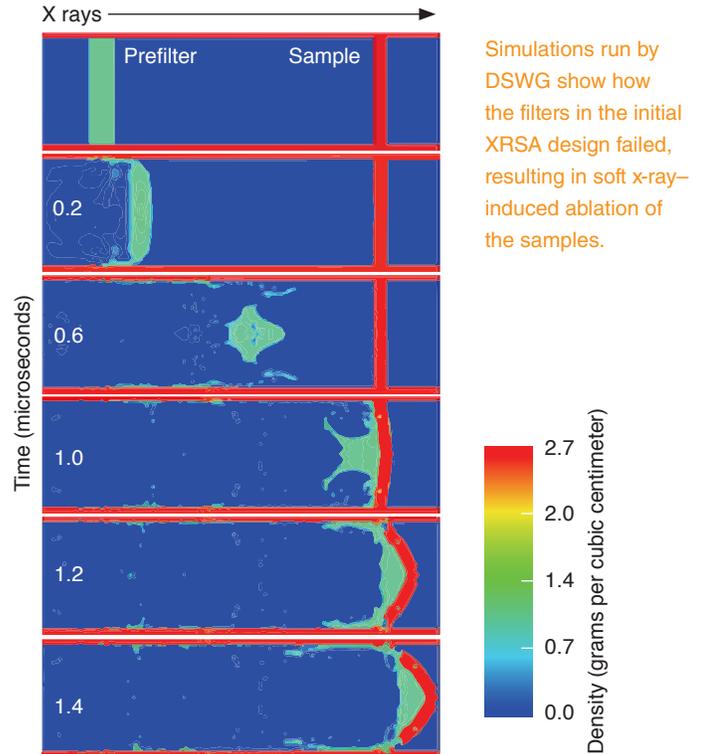
Livermore-developed programs, including ARES (for laser-matter interaction and radiation hydrodynamics) and ALE3D, Dyna3D, or LS-DYNA (for shrapnel impact and structural deformation). The models follow the evolution in time as far forward as possible to identify and characterize the risks. “We protect the facility and facilitate the science,” says DSWG leader Nathan Masters. “We ensure minimal risk to the facility. Our work is successful when nobody at NIF hears about us.”

Although experimental teams may only need data from the first 20 to 50 nanoseconds (ns) of a shot, Masters’s group tries to model the effects up to several microseconds and then extrapolate where the energy and debris are directed. Based on the simulation results and previous experience with similar experiments, Masters and the other members of his group, Rosita Cheung, Michelle Oliveira, Andrew Thurber, and Jae Chung, determine whether the damage risk is significant. If so, the group recommends changes to the experimental design that will reduce risk to acceptable levels. In the more than 10 years since the effort began, the team has analyzed hundreds of NIF experiments. “Through a combination of empirical and quantitative assessment,” says Dan Kalantar, target area senior scientist and advisor to the group, “we can say whether a configuration is safe based on our experience and our evaluation of risks.”

Tilting to Redirect Blowoff

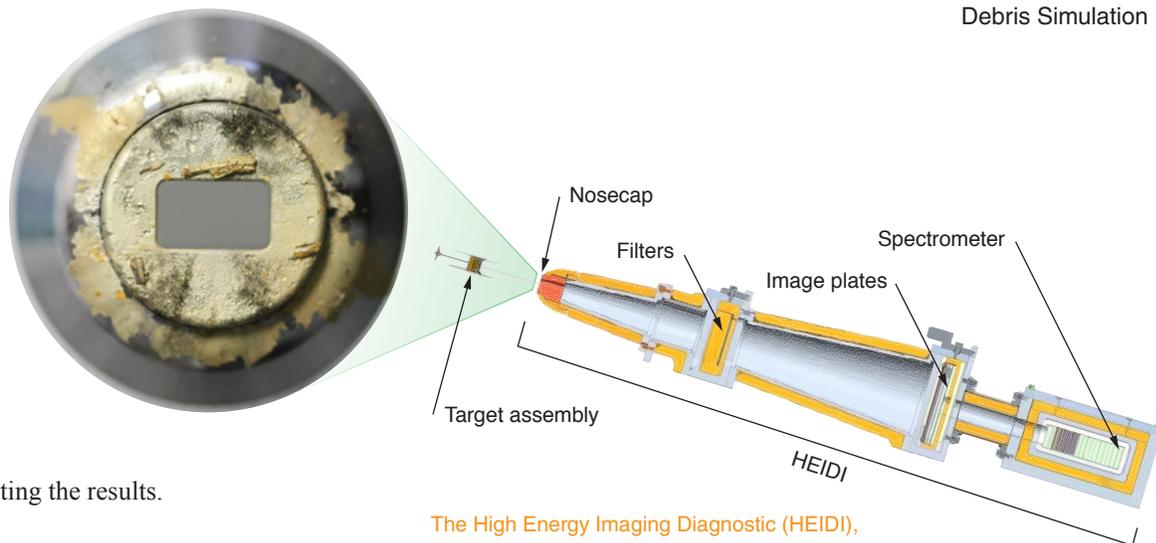
An early experiment to develop a platform for testing the effects of x rays on materials provides an example of DSWG’s utility. The x-ray source application (XRSA) test cassette was designed as a platform for mounting test samples needed in experiments that expose materials to x rays. Such experiments would allow researchers to study, for example, the effects of radiation damage on materials, or radiation-induced ablation. The original design of the cassette featured several sample holders (paddles) mounted in a circular pattern. The cassette was positioned by one of NIF’s diagnostic instrument manipulators, or DIMs, with the samples facing the x-ray source—a laser-driven target. Filters in front of the samples ensured that the appropriate x-ray spectrum was delivered to the samples for each experiment. However, with this initial XRSA design, the intense x-ray loads generated during the tests caused the filters to fail, resulting in sample damage. DSWG simulations of the experimental setup led to a redesign of the sample cassette. The re-engineered platform included a thin, tilted prefilter that could absorb soft x-ray energy and be vaporized. Debris from these sacrificial filters would then blow off away from the samples—effectively decoupling the potentially damaging portion of the x-ray load and ensuring survival of the remaining filters and samples. The change resulted in the platform performing without fail in 4 shots involving 60 samples. This design has been leveraged in other diagnostics to allow for thinner filters than otherwise possible.

However, frequently DSWG only has time to model the initial experimental setup and the modified experiment once,



A density plot from the ARES simulation at 5.6 microseconds shows low-density blow-off and displacement of the MatStrTaRT target and large gold shield (red), driven by x-ray ablation, from their initial position (black lines). The large shield’s velocity and mass could have resulted in significant damage to NIF optics.

generating a comparison by which to evaluate the risk. The change in conditions between the two simulations provides valuable information about how to reduce risk during the actual shot. Determining how closely the simulation will match reality requires DSWG's experience in interpreting the results.



The High Energy Imaging Diagnostic (HEIDI), which collects x rays generated by a backlighter foil on an x-ray-sensitive image plate, is used to obtain shot data. (inset) Craters and debris, including fragments of the gold shield, can be seen embedded on the HEIDI nosecap aperture after an MatStrTaRT experiment. (Original HEIDI rendering courtesy of Maryum Ahmed.)

Redesigning a Target

When a new shot's configurations and target design are similar to a previous experiment, additional simulations may not be necessary, and the experiment can be certified as meeting minimum risk expectancy. However, modifications to experimental setups, including targets, diagnostic participation or positioning, or different laser energies, require that DSWG take a closer look. "We'll recommend changes to shielding—we can propose thicker filtration, for instance, or modifications to the diagnostic itself," says Thurber. "If optics are at risk, we might ask the experimental team to change something in the experiment. Depending on the nature of the target, for example, we may ask them to turn off specific beams and close off the final optics assemblies from the chamber. Directional risks to the optics require a special solution."

The campaign, or series of experiments, called Material Strength Tantalum Rayleigh–Taylor (MatStrTaRT) offers a case in point. The purpose of the campaign was to observe the growth of Rayleigh–Taylor (RT) instabilities in highly compressed materials, providing data for evaluating material strengths under these conditions. During an MatStrTaRT experiment, a laser-driven hohlraum (a cylindrical container holding the target) produces x rays that partially ablate the sample assembly, compressing the sample and generating RT instabilities. The x-ray foil backlighter illuminates the growing instabilities, which are recorded on x-ray-sensitive image plates in the High Energy Imaging Diagnostic (HEIDI). A 1-millimeter-thick gold shield placed on the side of the target was designed to block x-ray emissions from the hohlraum that could overwhelm the image.

For the campaign, DSWG simulated the response of the thin-walled 13-millimeter-long target made of gold and epoxy—including the 1-millimeter-thick shield—to an 800-kilojoule laser pulse. The group's model, run with Livermore's ARES code, predicted that solid and molten debris from the gold shields would be driven by the target toward NIF's optics at velocities—about 2 kilometers per second—fast enough to cause significant damage. Working with the experimental team, DSWG devised a solution using smaller shields on the target in combination with a smaller rectangular aperture at the front of HEIDI. Simulations indicated that these new shields would melt

more completely, allowing little or no debris to be driven toward the optics. The group's efforts have been successful. Although MatStrTaRT targets still produce significant shrapnel, after the target modifications, little is directed toward the optics. Only a single disposable debris shield has been damaged in nearly 40 shots related to MatStrTaRT.

Intensifying Schedule Motivates Early Attention

With the high yearly shot rate at NIF and the increased complexity of experiments, DSWG and their TaLIS colleagues have more work than ever. "Shots used to be fairly routine," says Oliveira, who coordinates DSWG's activities. "Within the last two years, more changes have been made to shots, targets, and diagnostics than before, all of which affect the risk assessment. Shot complexity has definitely increased."

The changes have motivated the DSWG to recommend design alterations earlier in the process. Oliveira explains, "Now, we may work with engineering teams months in advance as they design new diagnostics to better protect the instruments from damage." Keeping damage from delaying NIF's work has made DSWG essential to its success—even if the group's own success means their NIF colleagues rarely hear about them.

—Allan Chen

Key Words: ablation, ALE3D, ARES, Debris and Shrapnel Working Group (DSWG), DYNA3D, High Energy Imaging Diagnostic (HEIDI), laser, LS-DYNA, Material Strength Tantalum Rayleigh–Taylor (MatStrTaRT) target, National Ignition Facility (NIF), Rayleigh–Taylor (RT) instability, x-ray source application (XRSA).

For further information contact Nathan Masters (925) 422-5236 (masters6@llnl.gov).

BIG DATA ILLUMINATES the Physical Sciences

LAURENCE Livermore's Physical and Life Sciences (PLS) Directorate is teeming with data. In research areas ranging from biomedicine and nuclear chemistry to high-energy-density physics and climate science, data from experiments and simulations accumulate quickly as ever more sophisticated tools are developed to collect it. Although manual data analysis may have been manageable in the past, this newfound abundance of information requires state-of-the-art, often automated techniques to achieve reliable interpretation.

Similar to their peers across the Laboratory, many PLS researchers are turning to data science to address Livermore's unique application-specific challenges. Data science includes many related disciplines such as artificial intelligence, big-data analytics, computer vision, machine learning (ML), predictive modeling,

statistical inference, and uncertainty quantification. (See *S&TR*, March 2019, pp. 4–11.) Fittingly, this rapidly growing field has become a focus for projects funded by the Laboratory Directed Research and Development (LDRD) Program. For fiscal year 2019, two PLS principal investigators—physicist Michael Schneider and materials scientist Yong Han—were awarded LDRD Strategic Initiative (SI) projects that apply data science to relevant PLS research. LDRD-SI projects are large in scope and address key science, technology, and engineering challenges related to Livermore's strategic planning.

For these initiatives, Schneider and Han have built multidisciplinary teams in which domain scientists work alongside data scientists, applying data analysis and interpretation techniques to inform scientific exploration. “Data is a tremendously

valuable commodity and just as important as physical inventory,” says Han, who recommends that for these types of projects, investigators devise a strategy to capture the right data, manage it, and formulate a legacy plan around it. Schneider adds, “Finding the expertise and resources to integrate data-driven approaches into the project from the beginning is an essential first step.”

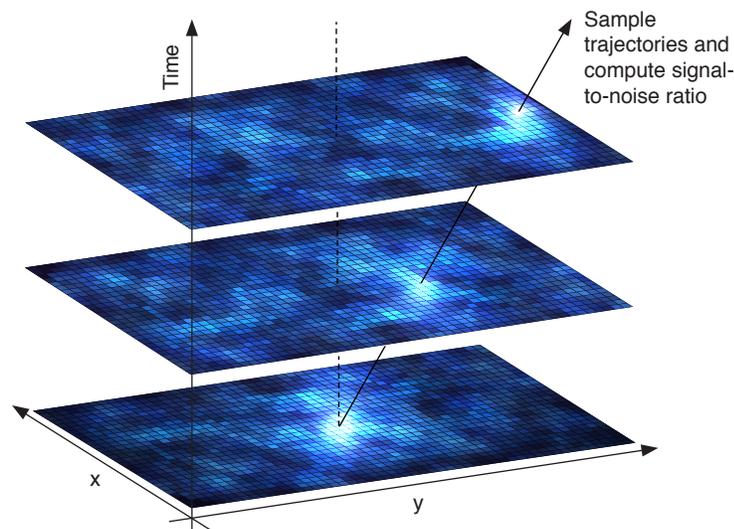
Mysteries of the Universe

Astrophysics is a growth area in the Laboratory’s advancement of basic science for national and global security needs. In this field, data science helps researchers catalog and interpret objects orbiting Earth and process huge volumes of data captured by ground- and space-based telescopes. Schneider says, “We are closing gaps in our understanding of how the universe works. Astrophysics data holds clues to resolving some of the most pressing unanswered questions.”

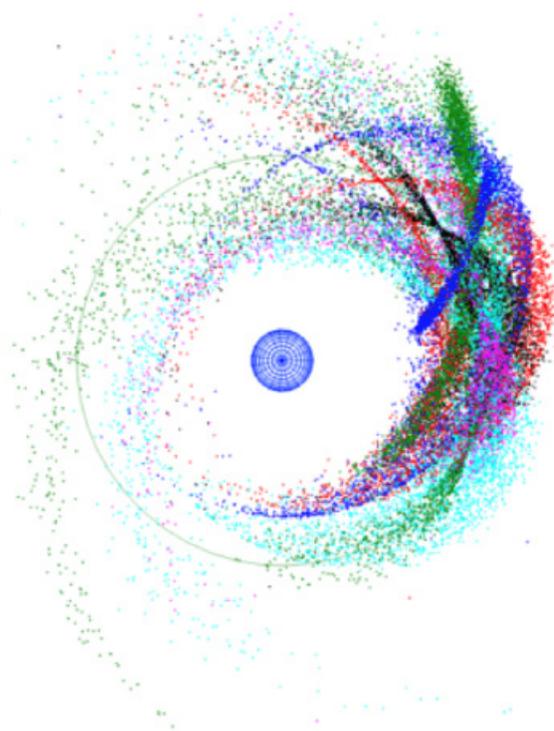
In an LDRD project that began in 2016, Schneider and colleagues studied the nature of dark energy—matter of unknown composition that does not emit or reflect electromagnetic radiation and is therefore difficult to observe directly. Specifically, the team developed image-analysis algorithms that make inferences from low signal-to-noise data. This process requires evaluating statistical versus systematic errors in the data set. Whereas statistical errors shrink as the data set grows, systematic errors are caused by variables that do not simply average out—for instance, atmospheric turbulence or imperfections in a camera lens. Gravitational lensing, wherein light from a distant object is bent, and thus distorted, by a massive object in the field of view, is a signal the team looks for in observations of galaxies and other light sources. Schneider’s team accounts for these errors with probability-based Bayesian models, simulations of noise, and data-processing software. “Measuring the average energy density of empty space in the universe is complicated because everything else gets in the way. We’re re-envisioning a data-processing pipeline to evaluate and correct those errors,” explains Schneider.

Similarly, another PLS-led LDRD project seeks to identify the gravitational lensing signatures of black holes. The research team, led by principal investigator Will Dawson, is processing 12 terabytes of imaging data—for more than 500 million stars—collected from telescope surveys. By combining observations and simulations of light curves, the team aims to make the first direct measurement of black hole mass spectra in the Milky Way galaxy. The ability to analyze such large volumes of data is also valuable for studies of other astrophysical phenomena, such as asteroid trajectories.

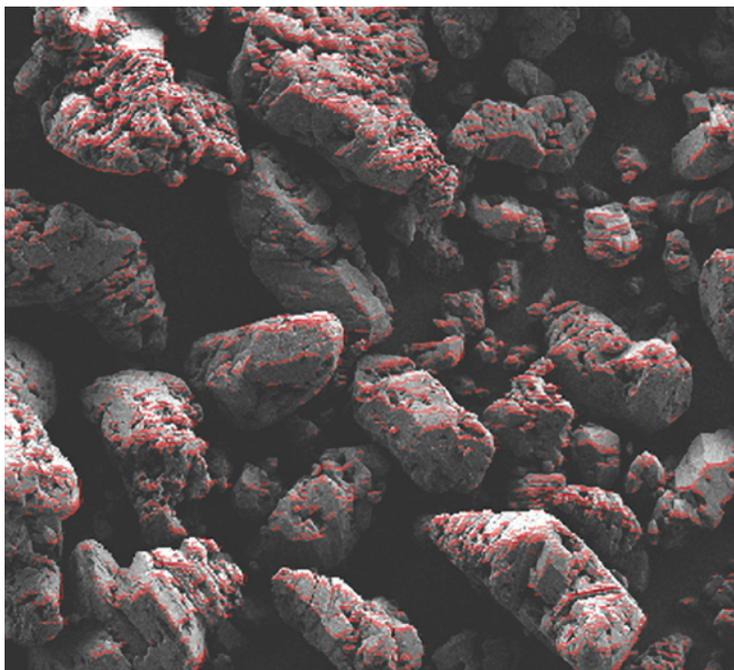
Schneider’s LDRD-SI project combines Bayesian statistical methods and deep neural networks (a subset of ML) to analyze debris, satellites, and other objects orbiting Earth. Unlike the dark energy and dark matter studies, these telescope-generated data sets are comparatively small. “We need a newer predictive physics model to achieve higher accuracy using the available



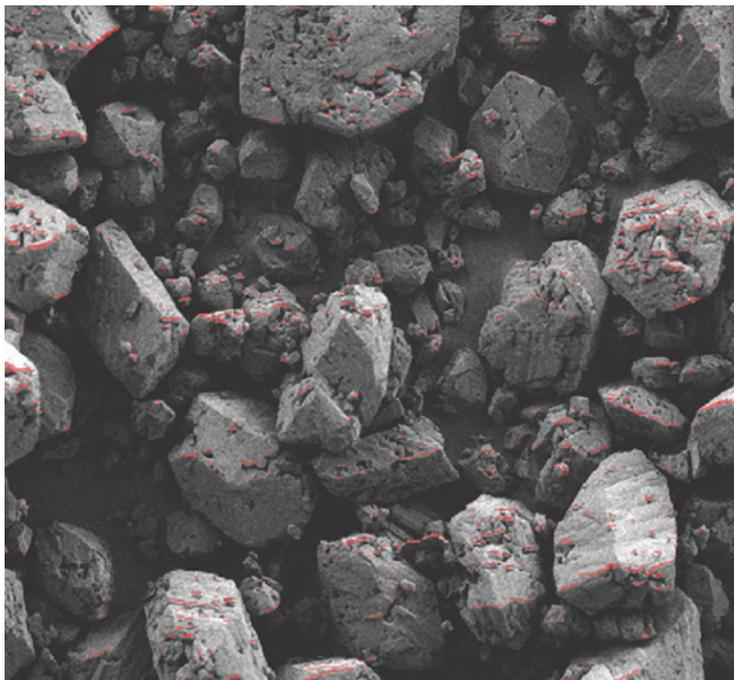
A Livermore-developed image-processing algorithm performs digital frame stacking to detect a moving asteroid in images captured by the Department of Energy–funded Dark Energy Camera, located at the Cerro Tololo Inter-American Observatory in Chile.



Data analytics algorithms generate probabilistic tracks of Earth-orbiting objects that are seen for only short time periods. The particle “clouds” shown here (represented by different colors) indicate the candidate positions for each object as projected into the future. (Blue circle represents Earth.)



Computer vision techniques are automated tasks that enable computers to analyze digital images and highlight specific regions of interest. In these scanning electron microscopy images, researchers are looking for ML-predicted features (shown in red) in high-performance (top) and low-performance (bottom) materials.



data,” notes Schneider, whose team has developed ML algorithms that predict orbital paths in this data-starved environment.

Looking ahead, similar techniques could enable collaborative autonomy within a constellation of satellites tasked with tracking orbiting objects. In this setup, each satellite exchanges data with the rest of the network until they reach consensus on an object’s location. This capability could help predict when space debris will hit a satellite or Earth. Schneider says, “We can make the most of big data using practical computing and by extracting interpretable features using data science techniques.”

Optimized Materials

Lawrence Livermore’s innovative materials include advanced metallic nanowires, high-performance alloys, freestanding polymer films, components that refresh the aging nuclear stockpile, and more. Regardless of the final product, feedstock materials (those raw materials directly used in the manufacture of other products) must be synthesized and optimized for system-level integration that will meet performance requirements with predictive behaviors.

Data science techniques are at the heart of projects focused on accelerating materials discovery, optimization, and deployment processes. Typically, the materials discovery process takes 10 to 15 years before application integration. “To improve the development cycle, we should leverage new tools, especially at the Laboratory where people across all disciplines are working on data analysis problems and solutions,” states Han, who leads several of Livermore’s data science-supported materials development projects.

One LDRD project was inspired by the growing volume of scientific literature. Materials scientists publish tens of thousands of papers every year that contain valuable information about the “recipes” they used to generate new materials. Han says, “Experimentalists must read a great deal of literature to stay informed in their fields while learning the new protocols and chemicals others have used in creating materials.” His team created a browser-based tool to extract targeted information from the published papers, thus automating a repetitive, formidable task. (See *S&TR*, July/August 2017, pp. 16–19.) The extraction pipeline begins with a supervised logistic regression algorithm that highlights recipe-like text sentences. Another algorithm combines a conditional random-field model with natural-language processing to extract chemical information—formulas, concentrations, relationships, reaction times, and morphology, among other variables. Visualizations render the data for further analysis by end users.

Another project, sponsored by Livermore’s Weapons and Complex Integration Principal Directorate and supported by the Weapon Simulation and Computing Program, goes beyond text descriptions of materials by analyzing images of high-explosive (HE) materials, whose physical properties often correlate with performance but are difficult to quantify. Han’s research team developed a feature extraction tool that determines



At the Data Science Institute's 2018 workshop, Livermore staff scientist Yong Han described a project that uses ML algorithms to extract targeted information from scientific papers emphasizing nanomaterials synthesis. Efficiently gathering data from the literature and rapidly analyzing complex relationships will accelerate the materials discovery, optimization, and deployment processes. (Photo by Ian Fabre.)

which features—among the hundreds revealed in a single scanning electron microscopy image—are meaningful. The tool uses open-source technologies that define engineered features, such as boundary detection, at a pixel level. The computer learns to weigh feature importance, then provides computed values that translate to mechanical performance prediction.

Han's LDRD-SI project further enhances the development of HE materials by combining multimodal data for feature extraction. With the help of data visualizations manipulated in a custom-built user interface, the team will correlate additional material properties with HE performance by identifying features in images and numerical values from varied sources. The team aims to advance the application of ML algorithms for small data sets while also implementing physics-based approaches. Robert Maxwell, leader of the Laboratory's Materials Science Division, states, "Our materials researchers generate terabytes of data on an hourly basis. Data science advances our ability to understand, develop, and deploy new materials. Tools that unite our multidisciplinary teams are the most powerful of all."

Building a Community

A collaborative data science community is a vital part of Livermore's investments in mission-driven research. The Laboratory's Data Science Institute (DSI) has quickly become a useful resource for researchers seeking expert analysis outside their scientific fields. DSI promotes multidisciplinary collaboration, enabling researchers to strengthen their work by applying data science expertise. Schneider, a member of DSI's governing council, states, "Our data science capabilities are as fundamental to Livermore's missions as our high-performance computing resources."

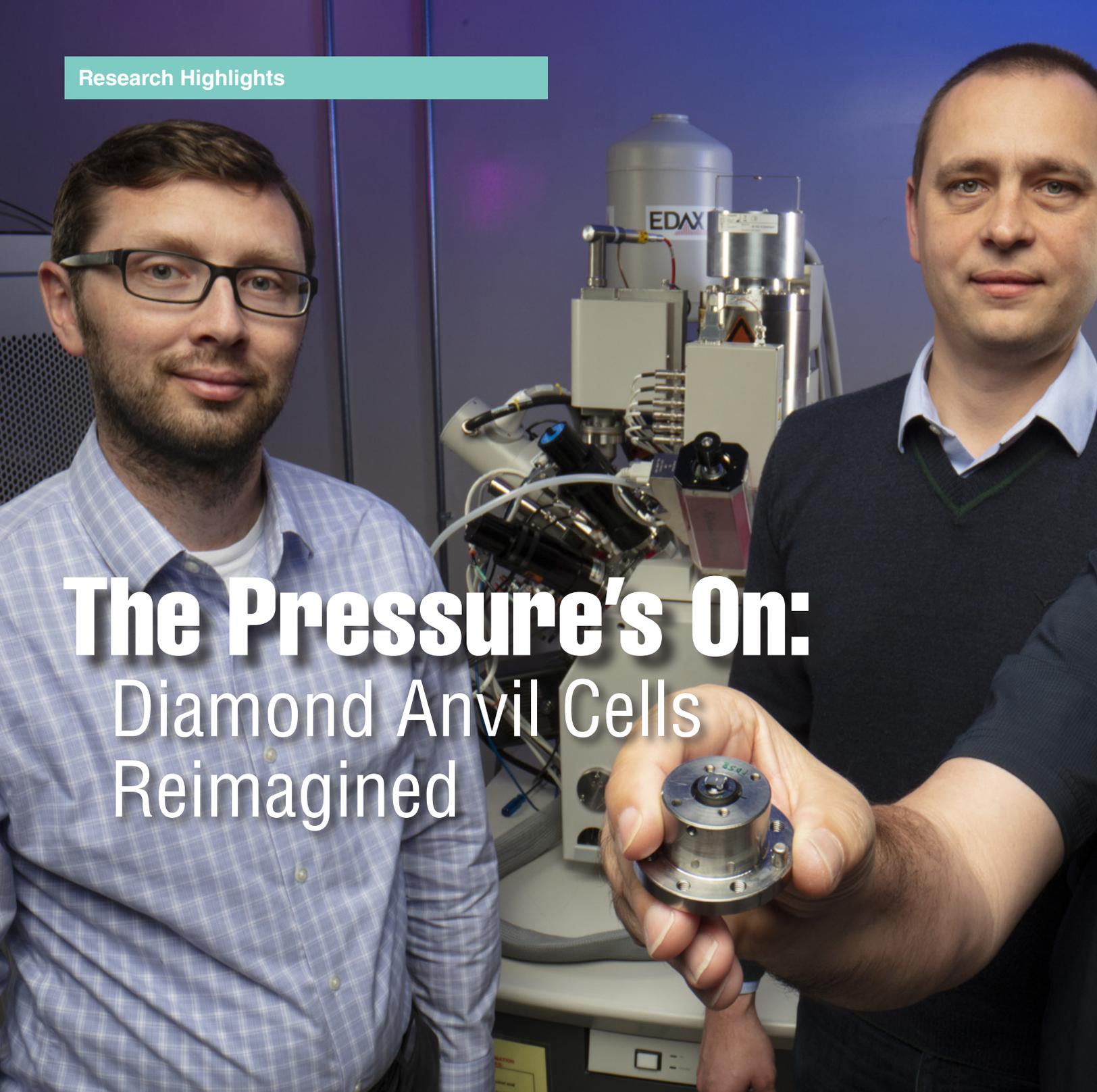
Scientists may not know how best to integrate data science techniques into their research, so DSI organizes on-site educational activities, such as reading groups and seminars. The DSI Consulting Service advises researchers on experimental design, data collection and sampling, and data-driven solutions for their projects. DSI's outreach extends beyond the Laboratory with technical workshops, invited speakers, and student internships. Such community-focused resources are increasingly valuable tools for 21st-century researchers.

With the help of PLS collaborators, the Laboratory's data science community is doing more than providing expertise on mission-driven projects. The field itself is expanding, with Livermore contributing to theoretical research in areas such as sample optimization and ML model interpretability. Schneider adds, "We have a responsibility to conduct quality science and produce reliable results, which requires innovation. The Laboratory has a leg up in advancing data science techniques because we have the sophisticated scientific expertise to understand and apply the underlying math."

—Holly Auten

Key Words: algorithm, astrophysics, big data, computer vision, dark energy, dark matter, data science, Data Science Institute (DSI), high explosive (HE), Laboratory Directed Research and Development (LDRD) Program, machine learning (ML), materials science, Physical and Life Sciences (PLS) Directorate, statistics.

For further information contact Michael Schneider (925) 422-4287 (schneider42@llnl.gov) or Yong Han (925) 423-9722 (han5@llnl.gov).



The Pressure's On: Diamond Anvil Cells Reimagined

WHEN it comes to subjecting materials to extreme pressures, scientists have several tools at their disposal, including gas guns, pulsed-power machines, and lasers. At Livermore's National Ignition Facility (NIF), for instance, intense, precisely timed and shaped laser pulses are used to shock samples hard and fast, driving materials to high temperatures and pressures.

(See *S&TR*, December 2016, pp. 4–11.) When scientists want to more slowly “squeeze” materials, they turn to diamonds to apply the pressure.

Unlike shock techniques, diamond anvil cells (DACs) act as small, mechanical presses that gradually produce ultrahigh pressure environments. Developed about 60 years ago,



Team members (from left to right) Earl O'Bannon, Zsolt Jenei, and Nick Teslich show a diamond anvil cell (DAC) component with the toroidal anvil used in the high-pressure experiments. (Photo by Randy Wong.)

conventional DACs routinely subject materials to pressures of approximately 300 gigapascals (GPa)—60 GPa less than the pressure found at the center of the Earth. (For comparison, the atmospheric pressure at sea level is about 1/10,000th of 1 GPa.)

Recently, a team of Lawrence Livermore experts led by physicist Zsolt Jenei developed a new diamond anvil design that

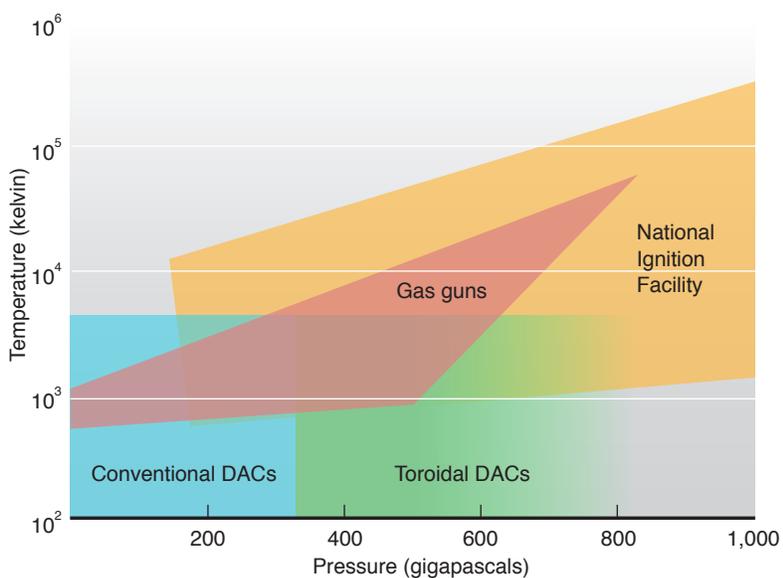
can reliably squeeze materials to pressures greater than 500 GPa. Such pressures are within a stone's throw of those in the cores of giant icy planets, such as Neptune. Experiments using this toroidal (donut-shaped) design are yielding data of interest to astrophysicists. The data also serve to refine the supercomputer codes that drive increasingly accurate simulations of stockpile weapons' performance.

Taking a New Approach

DAC anvils are created from opposing pairs of flawless, polished, single-crystal diamonds. The hardest known solid, a diamond can withstand ultrahigh pressures and is also transparent to diagnostic radiation, such as x rays and visible light. In experiments, a pair of flat diamond anvil tips (typically 30 micrometers wide), called culets, contains a microgram sample of a material held within a metal gasket. The cell increases the force on the back of the diamond anvils in small, controlled increments, pushing the culets together until they seal, and squeezing the sample into a smaller and smaller volume. Under such extreme pressures, the structure of a material as well as its electrical and magnetic properties can change, sometimes drastically. (See *S&TR*, December 2004, pp. 4–11.)

Livermore postdoctoral physicist Earl O'Bannon notes that the technique is powerful because it allows researchers to slowly increase the pressure on a material and take

Scientists use different experimental techniques to investigate how materials react to changes in pressure and temperature. The increased pressure range provided by DACs provides valuable data for planetary and stockpile scientists.

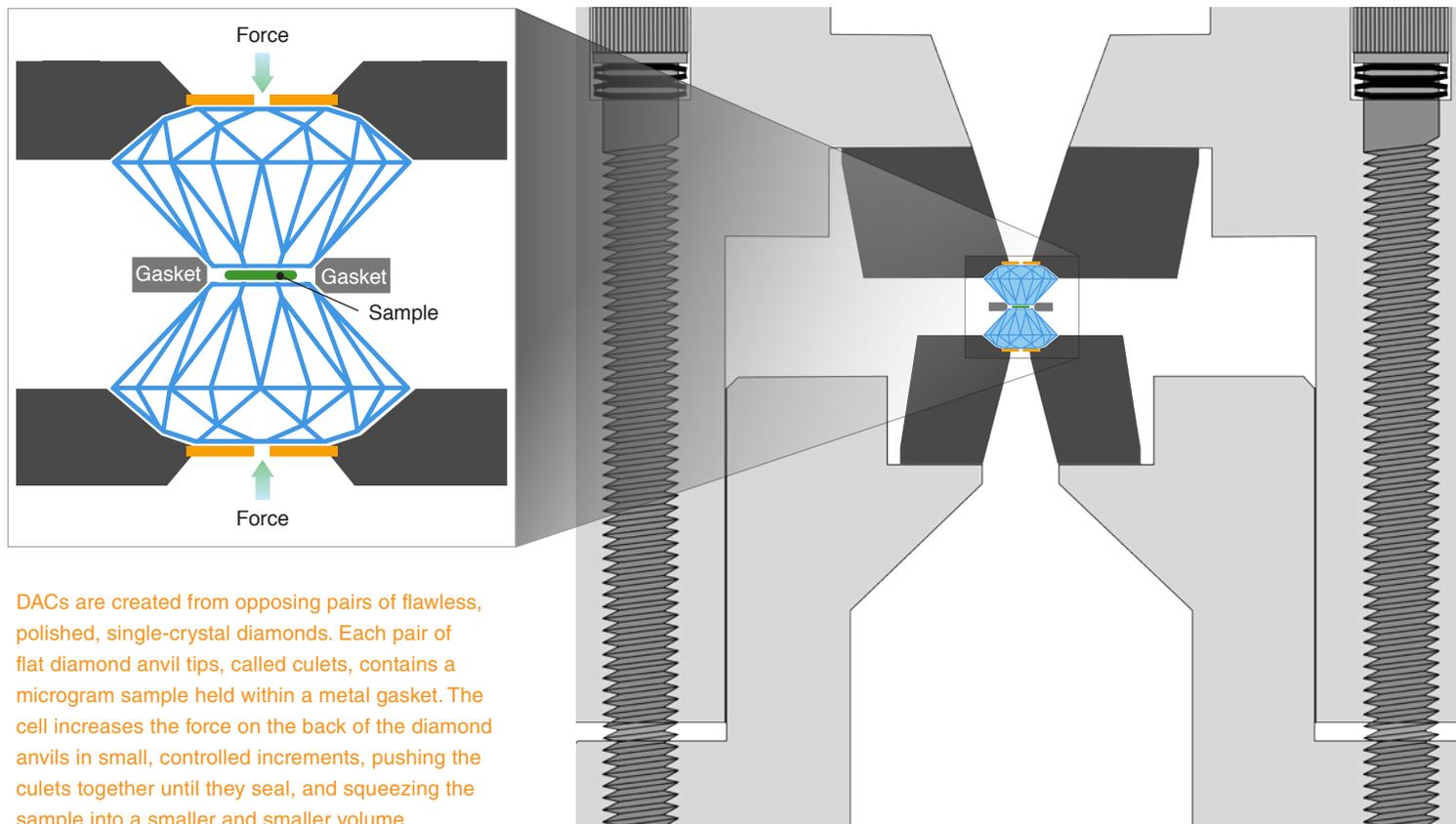


numerous measurements along the way. The resultant pressure–volume curves are used to define the equation of state (EOS) for the sample material. EOS data describe the relationship between the thermodynamic conditions of pressure, density, and temperature, and under what set of these conditions the material changes from one phase (solid, liquid, or gas) to another. This information is used to help refine computational models and validate calculations.

In 2016, Jenei was funded through the Laboratory Directed Research and Development (LDRD) Program to conduct a feasibility study to explore a new toroidal DAC design that could achieve higher pressures. The team succeeded in expanding the pressure range by modifying the shape of the diamond face to form a culet approximately 9 micrometers wide atop an elevated column. The column is surrounded by a circular torus (or depression), with a flat shoulder ringing the torus. The result resembles a tiny flat-topped tower surrounded by a circular moat. Jenei explains, “We arrived at this configuration after two years of work, reviewing and varying many design parameters, such as the diameter of the culet, the radius and depth of the torus, and the height of the flat shoulder outside the torus.”

One of the advantages of this design is that it overcomes the sample-containment problem that is encountered with small-culet conventional DACs. Jenei explains, “One of the goals of DAC design has been to make an ever-smaller culet. The smaller the culet, the higher the pressure one can obtain by applying the same amount of force. However, for traditional DAC designs, at pressures above 400 GPa with culets less than 20 micrometers in diameter, the gasket flows away, leading to sample-containment issues. Our design solves this problem. In a toroidal DAC, when the metal gasket starts to flow, the extruded material is trapped in the torus, keeping the central part of the gasket—and the sample—in place.”

To create a pair of toroidal diamond anvils, Jenei begins with two single-crystal diamonds. Using software he developed specifically for this task, Jenei generates a three-dimensional model of the final shape and dimensions for each gem. These models, which show the amount and shape of the material to be removed for each diamond, are translated into bitmaps. At Livermore’s focused ion-beam (FIB) facility, microbeam specialist Nick Teslich imports these bitmaps to use as patterns for FIB milling the toroidal surface for each diamond anvil. Once milled to specification, the diamond



DACs are created from opposing pairs of flawless, polished, single-crystal diamonds. Each pair of flat diamond anvil tips, called culets, contains a microgram sample held within a metal gasket. The cell increases the force on the back of the diamond anvils in small, controlled increments, pushing the culets together until they seal, and squeezing the sample into a smaller and smaller volume.

anvils are pressed into a thin metal foil to make a form for the gasket. Teslich's challenge is to then mill a hole or pore for holding the sample in the exact center of the gasket. Such pores generally measure about 4 micrometers in diameter and 4 to 10 micrometers in depth.

An added bonus for the development team is that toroidal DACs can be prepared and loaded using the same process as conventional DACs. O'Bannon says, "This versatility allows us to use the current infrastructure of a typical DAC laboratory for our design, which is a big plus."

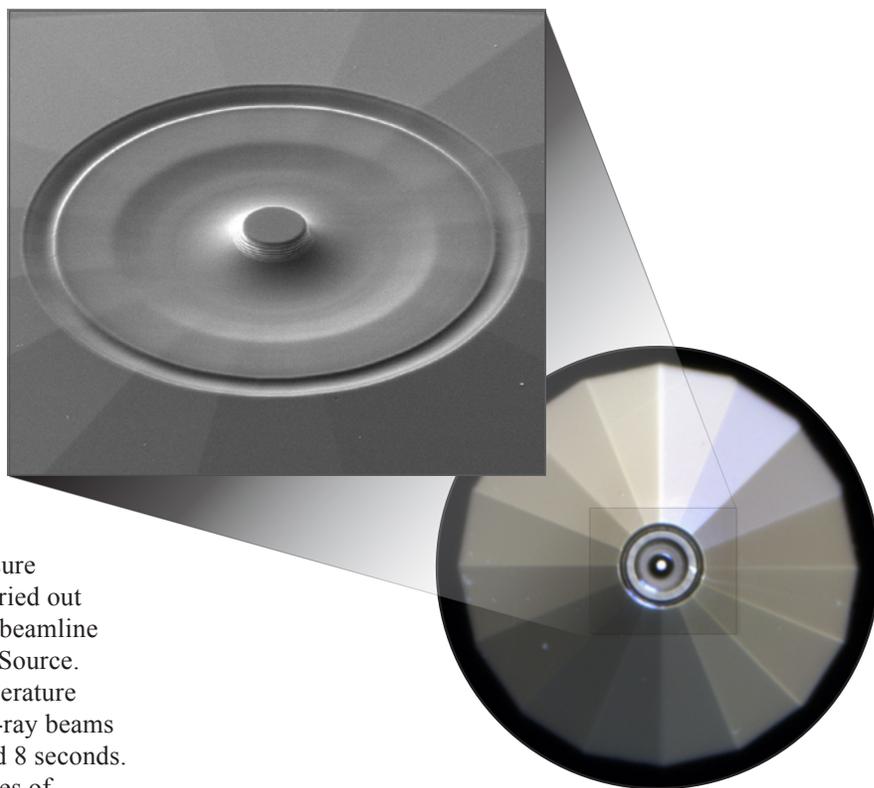
Taking DACs to the Experimental Table

With a working design in hand, the team moved on to the experimental stage, taking measurements of various metals under extreme pressure conditions at room temperature. Experiments are carried out using the High-Pressure Collaboration Access Team beamline at Argonne National Laboratory's Advanced Photon Source. X-ray diffraction patterns are collected at room temperature over the course of several experimental runs using x-ray beams of 30 kiloelectronvolts with exposures between 4 and 8 seconds. These diffraction patterns reveal the internal structures of crystalline samples, as well as phase-transition pressures, and ultimately, their EOS at constant temperatures.

One of the most important outcomes from this work has been the ability to generate the room-temperature compression curve for materials of interest. O'Bannon explains, "The curve is used as a base point for computer models. The data we gain from this technique can be used to validate and calibrate models to predict materials' properties at other temperatures and pressures." A future step for toroidal DAC experiments, notes Jenei, is to generate compression curves for materials using higher temperatures.

Early experiments on the metal rhenium, which served as both the gasket material and sample, resulted in a series of record-breaking results for single-crystal diamond anvils. Subsequently, the team has begun exploring the material behaviors of transition metals and other metals that are commonly used as pressure markers—gold, copper, and platinum, for example. In recent DAC experiments, they successfully compressed seven different metals beyond 400 GPa and routinely achieved pressures between 425 to 500 GPa. Their results show good agreement with previous data obtained from conventional DACs at lower pressures.

Looking to the future, William Evans, division leader for Physics in Livermore's Physical and Life Sciences Directorate, says, "As Dr. Jenei and his team continue to advance sample-loading techniques for this toroidal anvil



Unlike conventional DACs that have a flat diamond anvil tip, toroidal diamond anvils have a 9-micrometer wide culet atop an elevated column. (inset) A scanning electron microscopy image shows a closeup of the culet, torus (or depression), and outer shoulder.

approach, the study of material properties in the hundreds of gigapascals pressure regime is sure to identify new high-pressure phases and equations of state for materials. Such findings will have the potential to increase our understanding of planetary interiors and high-pressure science."

O'Bannon adds, "This new take on an established technique has opened the door to exploring molecular solids, such as water, and other planetary ices at pressures more than 500 GPa with x-ray and optical techniques. Reimagining DACs is a step in the right direction."

—Ann Parker

Key Words: culet, diamond anvil, diamond anvil cell (DAC), equation of state (EOS), high-pressure experiment, Laboratory Directed Research and Development (LDRD) Program, molecular solid, planetary ice, rhenium, toroidal DAC.

For further information contact Zsolt Jenei (925) 422-1497 (jenei1@llnl.gov).

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- or eight-digit number in the search box at the U.S. Patent and Trademark Office's website (<http://www.uspto.gov>).

Patents

Polymer-Carbon Composites for Temperature-Dependent Electrical Switching Applications

James Lewicki, Marcus Worsley

U.S. Patent 10,276,286 B2

April 30, 2019

Few-View Image Reconstruction

Kyle Champley

U.S. Patent 10,282,869 B2

May 7, 2019

Microporous Membrane for Stereolithography Resin Delivery

Joshua R. Deotte

U.S. Patent 10,286,600 B2

May 14, 2019

Polishing Slurry Preventing Agglomeration of Charged Colloids without Loss of Surface Activity

Rebecca Dylla-Spears, Michael Feit, Phillip E. Miller, William A. Steele,

Tayyab I. Suratwala, Lana L. Wong

U.S. Patent 10,287,457 B2

May 14, 2019

Awards

The **Geochemical Society** has recognized Lawrence Livermore geochemist **Thomas Kruijer** with the **F.W. Clarke Award**. The award honors a single outstanding contribution to geochemistry or cosmochemistry, published by an early career scientist as a single paper or a series of papers on a single topic. Kruijer was honored for his work on the hafnium–tungsten isotope chronometer, which has profound implications for the origin and evolution of the solar system. Kruijer determined when planetesimals (small bodies that formed before the larger planets in the solar system) solidified during the initial stages of planetary accretion, when Jupiter likely formed, as well as when and how the Moon formed following a giant impact on the proto-Earth.

Lawrence Livermore experimental plasma physicist **Tammy Ma** has been named **Woman of the Year** for the **16th Assembly District** by California State Assembly member Rebecca Bauer-Kahan. The annual Woman of the Year event, founded in 1987, is sponsored and organized by the California Legislative Women's Caucus as a way to highlight women who make important contributions to society.

Ma leads the X-Ray Analysis Group for Livermore's Inertial Confinement Fusion Program at the National Ignition Facility. She has authored or co-authored more than 150 peer-reviewed journal publications. She is also a member of the Fusion Energy Sciences Advisory Committee, advising the Department

of Energy's Office of Science on complex scientific and technological issues related to fusion energy and plasma research, and is one of 40 early career scientists worldwide appointed to a two-year term as a Young Scientist of the World Economic Forum.

The **Laser Institute of America** has recognized the Laboratory's **Jamie King**, a certified laser safety officer (CLSO), with the **R. James Rockwell Jr. Educational Achievement Award**. The award, presented biennially since 2005, honors outstanding contributions in laser safety education through efforts such as training and education courses, publications, software development, significant involvement in safety-related conferences, and educational website development.

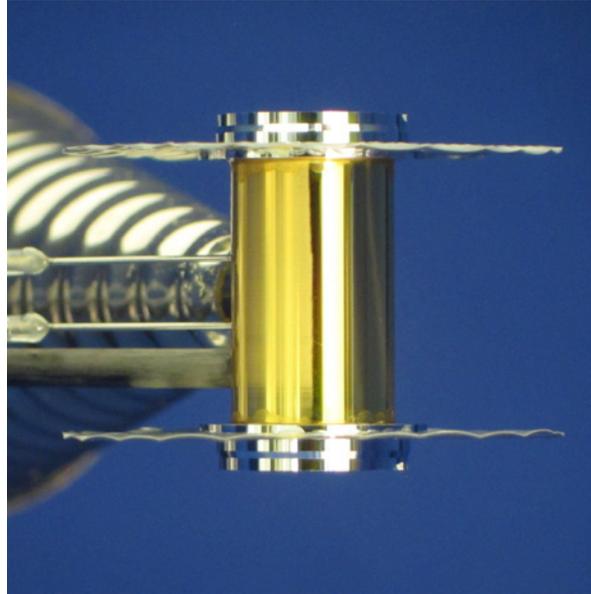
King has more than 25 years of experience in laser safety, and since 2011 has been the institutional LSO for the Laboratory. King serves as the chair for the Department of Energy's Laser Safety Task Group and has been involved in every technical planning committee for the department's LSO workshops since 2012. He was also co-chair for Technical Practical Applications Seminars for the International Laser Safety Conference in both 2017 and 2019, coordinating topics and speakers to deliver high-quality laser safety information and encouraging the next generation of laser safety professionals.

A New Carbon Economy Takes Shape

The atmospheric concentration of carbon dioxide (CO₂) has surged in the last two centuries, from 280 parts per million in the early 1800s to more than 410 parts per million today. The Lawrence Livermore Director's Engineering the Carbon Economy Initiative was conceived in 2018 to help support global-scale CO₂ (and methane) removal. The initiative comprises several research efforts such as manufacturing carbon-based products from CO₂, encouraging carbon storage within soil, sequestering CO₂ deep underground, and performing systems analysis to predict the costs and benefits of different carbon management approaches. Approximately 50 researchers are involved in the effort, including early career staff and postdocs. The initiative also includes numerous partnerships with universities, other national laboratories, California state agencies, and nongovernmental organizations. Researchers draw upon Laboratory strengths in geoscience, atmospheric science, materials science, advanced manufacturing, and systems analysis and optimization.

Contact: Roger Aines (925) 423-7184 (aines1@llnl.gov).

A "Gentler" Method Puts Pressure on Materials



Ramp compression experiments at the National Ignition Facility probe the equation of state of key materials made with unprecedented precision.

Also in September

- *Laboratory employees provide technical advice and leadership to government agencies through temporary off-site assignments.*
- *The Precision Oscillation and Spectrum Experiment investigates fundamental particle physics while offering new insights into nuclear reactor monitoring.*
- *By applying chemistry, nuclear physics, and accelerator expertise, Livermore researchers have contributed to the discovery, naming, and understanding of previously unknown elements.*

