Lawrence Livermore National Laboratory

September/October 2021

Science & Technology REVIEW

CLIMATE CHANGE COMES INTO FOCUS

Also in this issue:

About the Cover

The cover image shows a simulation run on the Department of Energy's (DOE's) state-of-the-science Energy Exascale Earth Systems Model (E3SM), which leverages DOE's advanced supercomputers for climate and earth science research. As the article beginning on p. 4 describes, the newly released version 2 will be used to simulate aspects of Earth's variability at weather-scale resolution and investigate decadal changes in climate that will critically impact the United States in coming years.

Cover design: Mark Gartland

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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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) 422-1651. Our e-mail address is str-mail@llnl.gov. *S&TR* is available online at str.llnl.gov.

National Nuclear Security Administration

Prepared by LLNL under contract
DE-AC52-07NA27344

S&TR Staff

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Holly Carlton

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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 online 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-52000-21-9/10
Distribution Category UC-99
September/October 2021

Science & Technology Review

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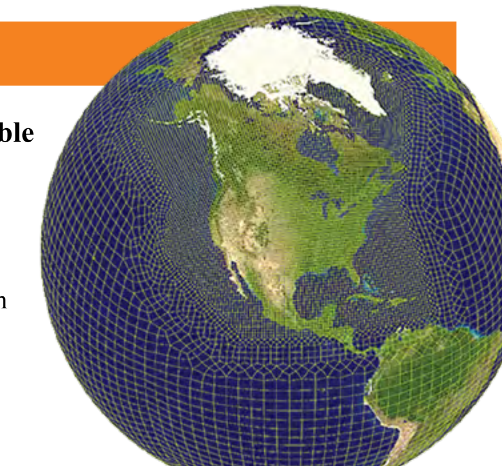
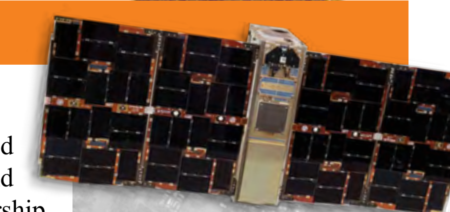


Research Highlights



Departments

Deflecting Asteroids with Neutron Energy

Lawrence Livermore National Laboratory and the Air Force Institute of Technology (AFIT) partnered to identify the best neutron energies for deflecting an asteroid. In research featured in the June 2021 issue of *Acta Astronautica*, the scientists compared the resulting asteroid deflection from two neutron energy sources, representative of fission and fusion neutrons, allowing for side-by-side comparisons and for the effect of the neutron energy on the resulting deflection to be quantified.

The two-phase study reviewed neutron energy deposition and asteroid deflective response. For the energy deposition phase, Los Alamos National Laboratory's Monte Carlo N-Particle radiation-transport code simulated a standoff detonation of neutrons, analyzing the thousands of cells within the asteroid and tracking each cell to generate energy deposition profiles or spatial distributions of energy throughout the asteroid. In the deflection phase, Livermore's 2D and 3D Arbitrary Lagrangian-Eulerian hydrodynamics code simulated the asteroid's response to the energy depositions. The results indicated which portions of the asteroid would remain solid and which would vaporize, causing blow-off debris and ultimately changing the asteroid's speed and direction. These findings provide insight into the ideal neutron energy spectrum needed for the necessary velocity change or deflection.

Research team members agree that two options exist for defeating an asteroid: disruption (imparting so much energy to the asteroid that it shatters into fragments moving at extreme speeds) or deflection. Livermore physicist and study co-author Joseph Wasem notes, "Deflection would be safer than disruption as long as sufficient warning time exists to launch a deflection response."

Contact: Joseph Wasem (925) 423-9232 (wasem2@llnl.gov).

Photocathode Enhances Hydrogen Production

As plants create energy from photosynthesis, a photocathode utilizes light and water for efficient hydrogen production. Lawrence Livermore and Lawrence Berkeley national laboratories collaborated with the University of Michigan following the university's discovery that silicon and gallium nitride (Si/GaN) photocathodes are capable of harnessing sunlight and water into carbon-free hydrogen. Their work, released in the April 5, 2021, issue of *Nature Materials,* found that a chemical reaction can transform gallium nitride into gallium oxynitride, resulting in self-improving capabilities of a Si/GaN photocathode—findings that could accelerate the production of hydrogen fuel cells.

University of Michigan professor Zetian Mi initiated the discovery when his Si/GaN photocathode achieved a record-breaking 3 percent solar-to-hydrogen efficiency. With Berkeley scientists, Mi conducted microscopy and spectroscopy experiments, revealing a 1-nanometer layer of gallium oxynitride had formed along the sidewall of the GaN grain, adding hydrogen evolution reaction sites. Livermore's Anh Pham and Tadashi Ogitsu performed density functional theory simulations, confirming the observations.

The self-improving ability of Si/GaN photocathodes marks a leap forward for solar-fuel production. Not only is the unusual property in Si/GaN more efficient and stable than semiconductor materials studied in the past, the technology is also relatively inexpensive. Livermore co-author Ogitsu says, "We hope our findings and approach will be used to further improve renewable hydrogen production technologies."

Contact: Tadashi Ogitsu (925) 422-8511 (ogitsu1@llnl.gov).

Pandemic Lowers U.S. Energy Consumption

An energy flow chart released by Lawrence Livermore National Laboratory shows that Americans used less energy in 2020—a change due, in part, to the COVID-19 pandemic. Shelter-in-place orders were the leading factor in the 14 percent decline in transportation and the 11 percent drop in commercial energy use. Continued deployment of renewables resulted in a 19 percent increase in solar energy and a 10 percent boost in wind energy, both of which can replace coal as a source of power.

"Solar and wind continue to show year-on-year growth, which is an impressive change for the energy system," says A.J. Simon, Livermore energy systems analyst. Although many more Americans worked from home in 2020, residential energy consumption rose only 2 percent due to a mild winter and higher efficiency homes. Energy consumption is measured in British Thermal Units (BTUs). One kilowatt-hour—comparable to the energy required to operate an LED lightbulb for one week—is equivalent to 3,412 BTUs. Overall, Americans used 92.9 quads (quadrillion BTUs) of energy in 2020, which is 7.2 quads or 7 percent less than energy consumption in 2019. The efficiency of the nation's cars, lightbulbs, and factories contribute to how much energy is rejected and how much fuel and electricity is being used productively. These numbers show positive changes in the way the country uses energy, and that less energy is being lost or rejected during use.

Contact: Hannah Goldstein (925) 422-9614 (goldstein12@llnl.gov).

Making Climate Change More Tangible

HEADLINES such as "Extreme Wildfire," "Bomb Cyclone," "Super Typhoon," and "Megadrought" make climate change tangible to billions of people who once viewed the phenomenon as a far-off, abstract concept. While these headlines are recent, the challenges of climate change and the national and international responses to it have been the subject of Lawrence Livermore National Laboratory research for nearly 40 years. The Department of Energy recognized early on that combining the big-science capabilities of high-performance computing with a strong foundation in physics and numerical modeling would inform what was then an emerging area of science. Our early contributions were foundational, and the Laboratory's work continues to have an outsized impact.

Much of this history, including the Laboratory's direct connections to Nobel Prize in Physics winners Syukuro Manabe and Klaus Hasselmann, is chronicled in this issue's feature article beginning on p. 4. While great attention is paid to Livermore's Program for Climate Model Diagnosis and Intercomparison (PCMDI), essential and continuing contributions to the Coupled Model Intercomparison Project (CMIP)—an earlier PCMDI-led international collaboration—can be recalled as well. Organized by Livermore's Jerry Potter and Bob Cess of Stony Brook University, the Feedback Analysis of GCMs and in Observations (FANGIO) climate model intercomparison was the first to quantify the large uncertainty in cloud–climate feedback in climate model results, spawning a new research area crucial to the development of accurate climate and Earth system models.

Continuing this legacy, Livermore's Steve Klein led a team of international experts, including the Laboratory's Mark Zelinka, that bounded the value of climate sensitivity per a process-based understanding of clouds and other climate feedbacks. Climate sensitivity, defined as the near-surface atmospheric warming projected from a doubling of the atmosphere's concentration of carbon dioxide, is crucially dependent on the correct evaluation of cloud–climate feedback. The team's results initiated a critical revaluation of the way clouds and aerosols are represented in climate models.

A common thread in the Laboratory's climate science research history is our role as an integrator, whether through building large multi-institutional collaborations or matching the big-science capabilities of a national laboratory with the expertise and creativity of its scientists. Today, we continue this role in our technical and intellectual leadership of the eight-laboratory Energy Exascale Earth System Model (E3SM)—just one tool in the chest as we seek solutions to the complex problems of resilience to climate changes happening now and mitigation against even more destructive changes in the decades to come.

Lawrence Livermore embraces these challenges head on, with Laboratory Director Kimberly Budil designating Climate Resilience as a Laboratory Mission Focus Area. The theme of the Laboratory as an integrator will become ever more important as we connect additional Livermore capabilities with external partners to address climate change—often described as the biggest threat to human civilization.

This issue of *S&TR* highlights two other examples of Livermore's culture of integrating individual creativity with the big-science capability of a national laboratory. The highlight starting on p. 12 describes how breakthroughs in materials and optics, both long-standing core competencies, support the small-satellite revolution. Like PCMDI's and the E3SM coalition's work in climate science, the Laboratory's strengths in data science and multi-institutional collaborations are key to advances in diagnosing brain injuries, as presented in the highlight starting on p. 16.

The final highlight beginning on p. 20 recognizes recent Distinguished Member of Technical Staff (DMTS) appointees, bringing the issue full circle as now-retired climate research scientists Ben Santer and Dean Williams were also DMTS members. Our culture of integration and excellence in science and our capabilities attract creative staff members with the opportunity to make a difference in our world in ways they could not in other institutions.

■ David Bader is director of the Laboratory's Climate Program.

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CLIMATE CHANGE COMES INTO FOCUS

Advanced computer models, simulations, and analysis capabilities help scientists zoom in on Earth system processes and improve climate research.

EVERY few months, a new prediction about Earth's changing climate makes headlines. The most prominent organization making them, the 195-nation Intergovernmental Panel on Climate Change (IPCC), has been instrumental in establishing the terms of future climate conditions. In 2018, IPCC issued the following statement: "Climate-related risks for natural and human systems are higher for global warming of 1.5°C than at present, but lower than at 2°C (high confidence)." This 1.5°C threshold became the bellwether for climate policy around much of the world.

In the latest IPCC report, published in August 2021, the organization updated its stance, projecting surface temperature to rise over the 21st century under all assessed emission scenarios. By 2100, IPCC expects surface temperature to exceed 1.5°C above the global pre-industrial mean, unless measures are taken to reduce carbon dioxide emissions and greenhouse gases (GHGs).

On one level, the report is a sobering look at the potential state of the planet over the next several decades. On another, it's a testament to the innovations made by Lawrence Livermore and others to improve the scientific tools used in climate research. The Laboratory's Program for Climate Model Diagnosis and Intercomparison (PCMDI) played an important role in producing all six IPCC reports and is continually expanding its efforts to help reduce uncertainty in climate predictions. Livermore's high-performance computing (HPC) capabilities are key to this work, helping scientists better understand Earth system processes and develop pattern-based analysis of climate change.

A Matter of National Interest

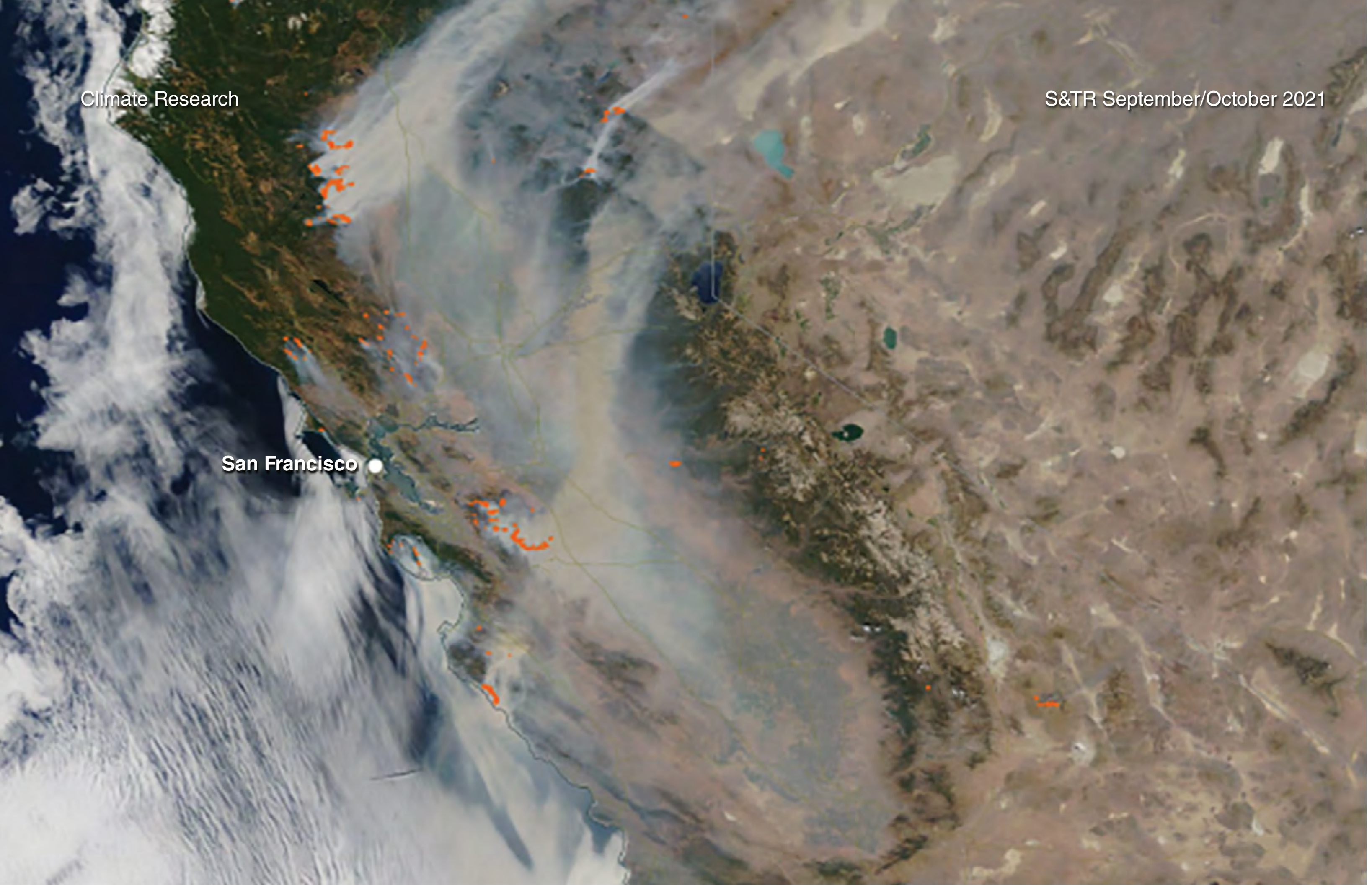
Earth is a wonderful, big, complicated planet. Its nearly 320-million-square kilometers of surface area is covered with oceans, mountains, cities, rainforests, deserts, and ice. Across the planet, temperatures; wind cycles; pressure systems; and varying amounts of sunlight, cloud cover, and precipitation; among other atmospheric conditions, create Earth's weather. An area's climate is defined by its prevailing weather conditions over long periods of time.

When predicting the weather, meteorologists typically use results of several weather models combined with their expertise to provide a forecast, usually for the week. "To create these forecasts, extensive data is collected up to the last day prior to the forecast," says Lawrence Livermore climate scientist Steve Klein. "The data is fed into the models using varying initial conditions, with the expectation that the meteorologist will then be able to 'predict the future'." This process is called deterministic forecasting, and after a few days or weeks, one would know if the forecast was correct. Forecasting climate is a much trickier undertaking, with greater potential impacts on energy production, resource consumption, and human settlement patterns. In fact, the Department of Energy (DOE) recently made researching climate risks associated with the national energy system a priority.

Livermore researchers apply HPC and expertise in fundamental sciences, such as meteorology, climatology,

Oak Ridge National Laboratory's Summit supercomputer was commissioned in 2018. Eight times more powerful than its predecessor Titan, Summit allows scientists to run more detailed processes and interactions within models. The Energy Exascale Earth System Model (E3SM) version 2 was validated on Summit. (Image courtesy of Oak Ridge Leadership Computing Facility.)

Lawrence Livermore National Laboratory



California wildfires have raged through the state over consecutive summers. In August 2020, catastrophic wildfires razed more than a million acres of land in just a little over a week. This satellite image shows the location of several fires (orange) and the resulting smoke emissions. (Image courtesy of NASA Earth Observatory.)

applied mathematics, and computational science, to the problem of understanding and predicting how Earth's systems evolve on timescales from a few years to several centuries. "We use 30-year statistical averages in climate research," says David Bader, director of the Laboratory's Climate Program. "However, the past 30 years are very different from the 30 years before that. We need new information that projects out 30 or 50 years to inform infrastructure design." DOE's Energy Exascale Earth Systems Model (E3SM) was born from the need to investigate climatological impacts and energy-relevant science using code optimized for the next-generation of DOE's advanced supercomputers. The first DOE exascale systems, Frontier and Aurora, are scheduled to come online in the year ahead.

Building a More Detailed Model

Earth system simulation involves solving approximations of physical, chemical, and biological governing equations on spatial grids at the finest resolutions possible. This resolution depends not only on the complexity of the model, but also on the peak performance of the supercomputer used to run the simulations. "E3SM was coded from the ground up with exascale computers in mind," says Bader. "We saw the need for a climate model that was well-suited for DOE's mission problems and would run well on the exascale computing architectures envisioned for the national laboratories."

The E3SM research team includes geophysical and computational scientists from multiple universities and DOE laboratories. In 2014, they began running the initial high-resolution E3SM model on Titan, at Oak Ridge National Laboratory's (ORNL's) Leadership Computing Facility, and Argonne National Laboratory's Mira. These leading-edge computing systems of the time were capable of trillions of calculations per second and boasted a higher-performing architecture that decreased time to solution, allowed for increased complexity of the models, and provided more realistic simulations. The development effort considered the availability of even more powerful supercomputers in the coming years. "The data structures in older climate codes and the way the information was laid out across the computer would not work with these more advanced machines," says Bader. "We did not start scientifically from scratch, but from a code perspective, we took a clean approach to building the model." The new climate model was compared and run side-by-side with its predecessors to certify its validity. Bader adds, "We needed to ensure that we hadn't made any errors." The data comparison and open-source code were also made available internationally to build support and promote further validation.

E3SM version 1 debuted in 2018. It simulates the fully coupled climate system at high-resolution and combines models of global atmosphere and land surface with ocean, sea ice, and river models. These components are important to DOE's primary research thrusts related to the energy sector: Earth's water cycle, biogeochemistry, and cryosphere (frozen water). With E3SM, researchers can simulate precipitation and surface water conditions in specific regions, examine how external and environmental factors can alter the chemical cycles of the planet, and investigate the vulnerability of the Antarctic Ice Sheet.

With further development and access to ORNL's Summit supercomputer, commissioned in 2018, a faster, more capable E3SM version 2 was delivered and released to the broader scientific community in September 2021. Summit's peak performance of 200,000 trillion calculations per second makes it eight times more powerful than Titan. "The increase in computing power allows us to add detail to processes and interactions that results in more accurate and useful simulations than the previous version," says Bader. Version 2 improves the representation of precipitation and clouds. "Specifically, how clouds change in a warmer climate is much more realistic," says Livermore atmospheric scientist Chris Golaz. In addition, E3SM version 2 offers scientists the ability to "telescope" to improve regional predictions. Golaz adds, "With E3SM version 2, we have two fully coupled configurations: a 100-kilometer globally uniform resolution and a regionally refined model resolution with 25 kilometers over North America and 100 kilometers elsewhere."

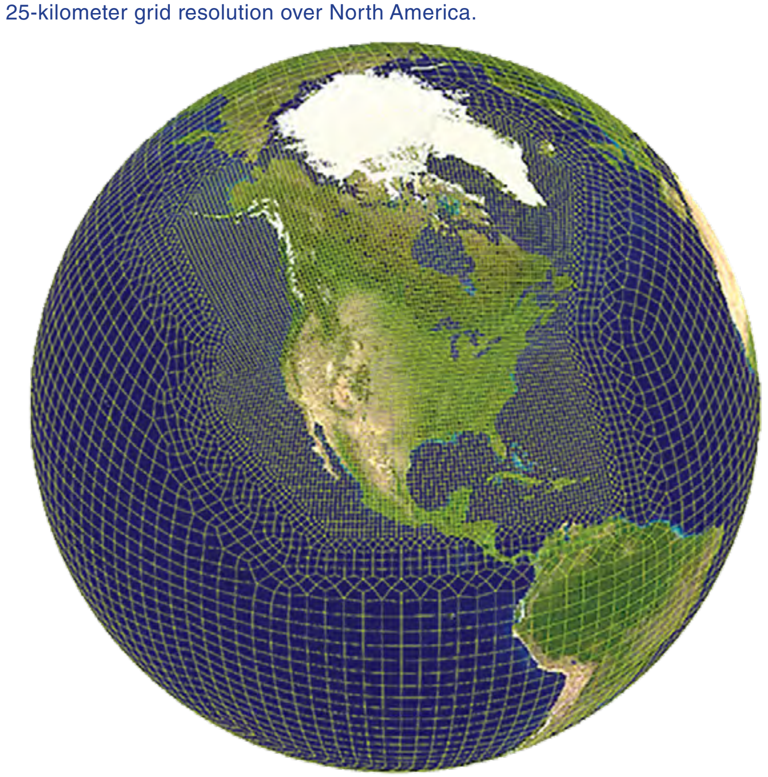
> "With E3SM version 2, we have two fully coupled configurations: a 100-kilometer globally uniform resolution and a regionally refined model resolution with 25 kilometers over North America."

For Klein, this feature will assist him in his work researching the behavior of clouds, which have a significant effect on the amount of sunlight that reaches the planet's surface. He says, "It doesn't make sense to spend computational time and energy simulating clouds on the other side of Earth while researching an especially sensitive region for energy production." With Livermore's climate research experience and computer-science competencies, more scientists like Bader and Klein will be enabled to study climate conditions, worldwide or at a near-neighborhood level. Bader says, "E3SM version 2 allows us to more realistically simulate the present, which gives us more confidence to simulate the future."

Climate Fingerprints

Over the last few years, California wildfires have become a devasting phenomenon. In the summertime, smoke from these seasonal wildfires drastically affects air quality in the inland valley and

E3SM version 2 offers two fully coupled configurations that improve grid-size resolution anywhere on the globe. The model shows a 100-kilometer globally uniform resolution and a 25-kilometer grid resolution over North America.

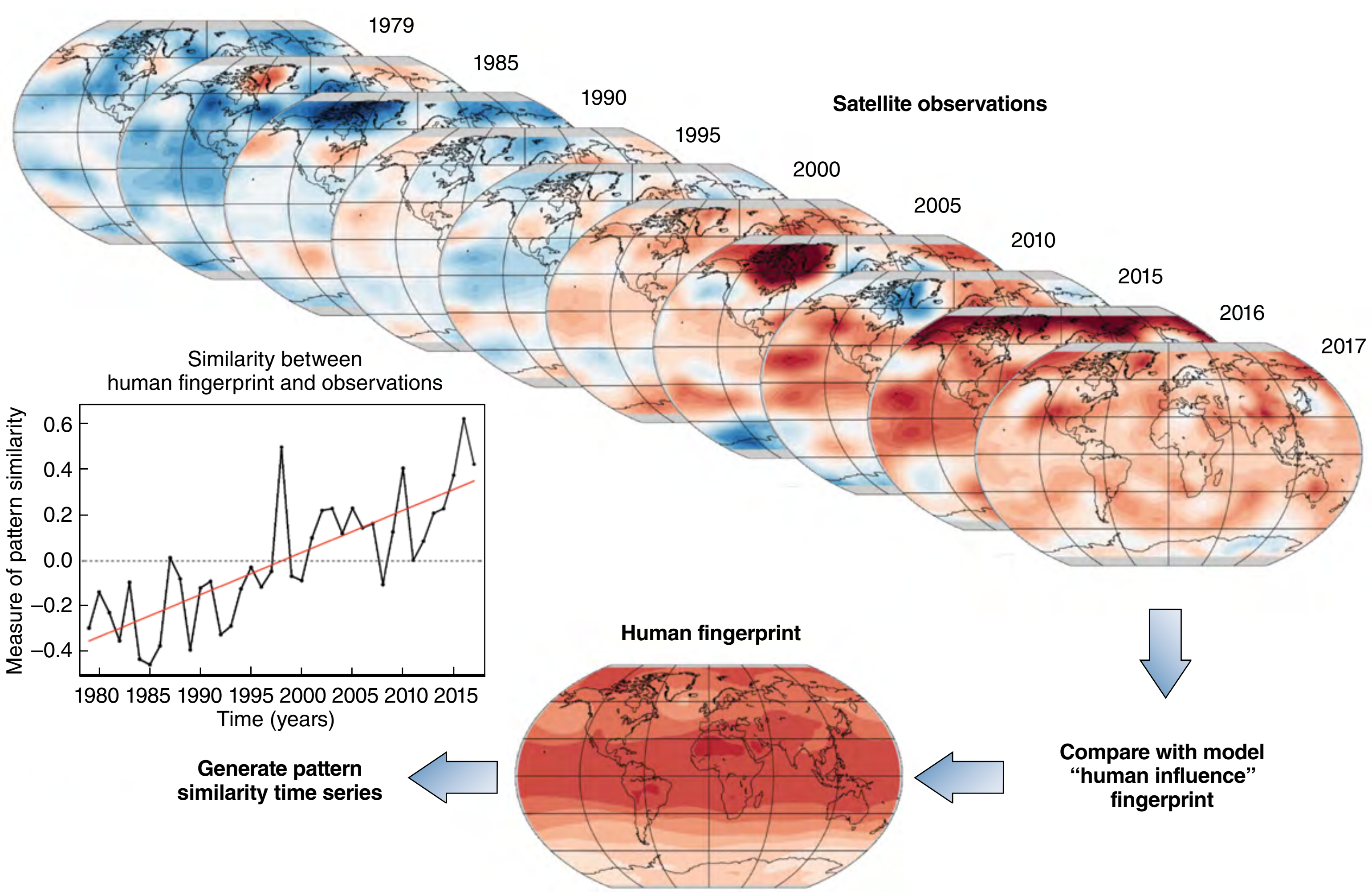


beyond, while the infernos themselves destroy homes and level the landscape. The 2012–2016 drought in California—the driest period in its recorded history—was only over for four years before exceedingly dry conditions returned in 2020. When droughts become regular and affect the water cycle on a large scale, a region becomes truly arid.

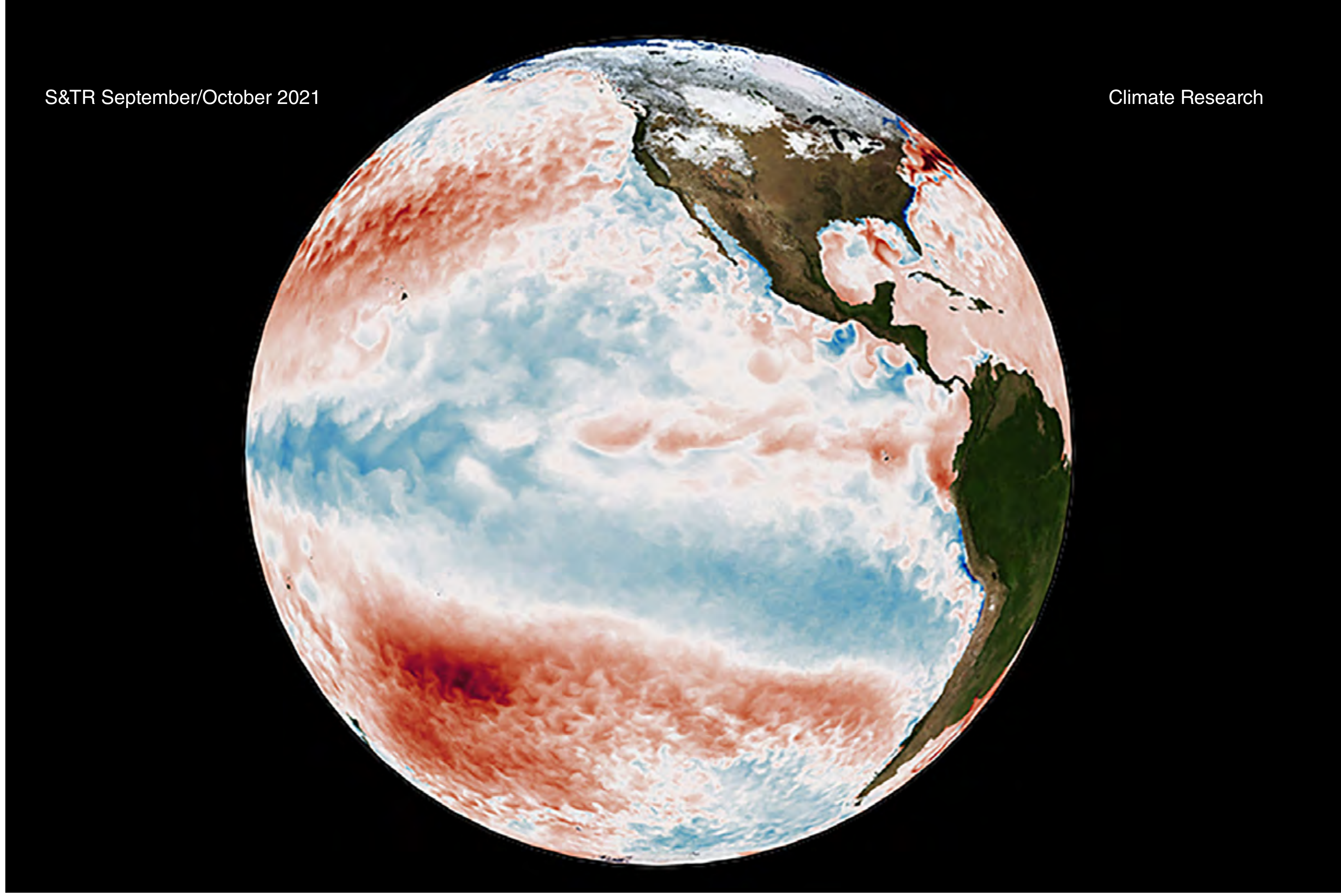
For Livermore climate scientist Céline Bonfils, long-term drought and regional aridity is of particular interest. Since 1980, California and the western United States have become drier. In contrast, during the same period, the Sahel region in Africa—the semi-arid transitional zone between the Sahara and savannas to the south—has recovered from its long dry spell. Scientists are using a technique called climate fingerprinting to better understand these changes and their cause and effect.

> “We can’t get the large-scale right if we don’t get the small-scale right, which is why we focus on improving model physics.”

“The main goal of fingerprinting research is to separate the relative roles of natural variation and human influences on global climate,” says Bonfils. “Earth’s climate is noisy in nature, but it is also impacted by several external factors that act at different paces and places, similar to how different musical instruments would contribute to a song, with their own rhythms, patterns, and notes.” In fact, for the last 30 years, now-retired Laboratory scientist Ben Santer and other Livermore climate scientists have developed and applied the fingerprint method originally conceptualized by Klaus Hasselmann, a co-recipient with Syukuro Manabe of the 2021 Nobel Prize in Physics.



In climate fingerprinting, scientists search for a pattern of climate change (a “fingerprint”) resulting from human activities as predicted by computer models. Statistical methods are then used to measure whether observations are becoming progressively more aligned with the model-based human fingerprint over time and away from noise patterns. The process attempts to separate the relative roles of natural and human influences on global climate. Shown above are satellite observations and the human fingerprint predicted for the tropospheric temperature field. (Image provided by Ben Santer.)

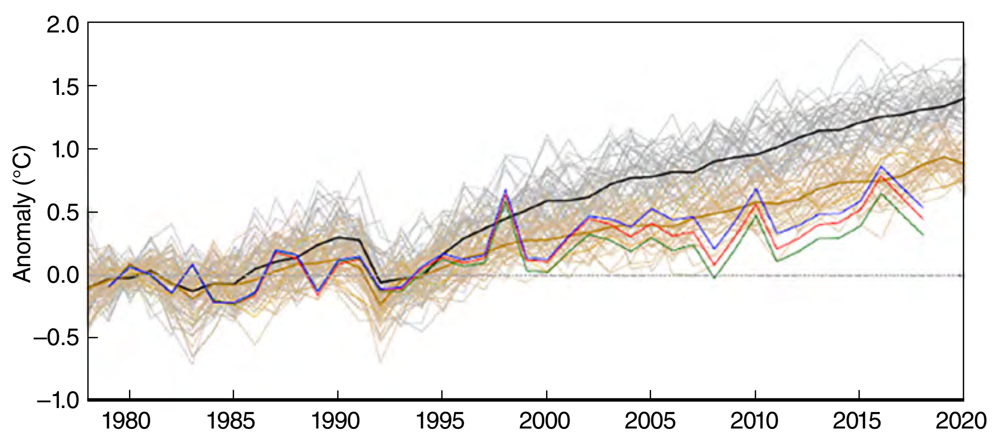


A composite image shows sea surface temperature anomalies indicative of a La Niña event (courtesy of the National Oceanic and Atmospheric Administration’s Coral Reef Watch) blended with a NASA Blue Marble image. (Blue Marble is a NASA-generated image of Earth created from high-resolution satellite images.)

Bonfils led a multi-institution research team that identified two primary mechanisms, or fingerprints, affecting temperature, precipitation, and aridity levels on a continental scale. “One can think of this work like tuning a radio and capturing two different songs playing simultaneously out of the noisy background.” The first “song,” louder and clearer than the other, mainly characterized the large-scale warming and drying effect of GHGs from burning fossil fuels. The second tune, more subtle than the first, mainly represents the cooling effect of past particulate emissions from Europe and North America, leading to different rates of warming between the two hemispheres. Together, these two mechanisms help explain the changes in aridity in many parts of the world.

To detect these two human-related climate fingerprints, Bonfils and colleagues examined the simultaneous changes in temperature, precipitation, and the climate moisture index. The index measures aridity based on precipitation and atmospheric evaporative demand, factors that also affect water usage such as irrigation and hydropower. The team analyzed multiple, distinct global climate models simulating the historical climate in response to recent volcanic eruptions and the evolution in GHG and aerosol emissions. From these simulations, they extracted the climate fingerprints of human activities and measured whether the observations are becoming increasingly similar with the fingerprints through time.

In Bonfils’ case, she and her team used the World Climate Research Programme’s Coupled Model Intercomparison Project Phase 5 (CMIP5) framework to estimate Earth’s climate without human influence—providing an indication of what the



Shown here are trajectories from a large initial-condition ensemble study looking at annual-mean atmospheric temperature in the mid- to upper troposphere. Researchers ran 50 simulations using the Canadian Earth System Model version 2 (CanESM2, light grey) and 40 simulations using the U.S. Community Earth System Model version 1 (CESM1, light brown). Trajectories and their averages (CanESM2, black line; CESM1, dark brown line) were compared to satellite data from several sources (red, blue, and green lines). Temperature changes are expressed as departures from the model and satellite annual averages from 1979 to 1981.

planet would do naturally. By contrasting those simulated results with historical climate observations and simulations incorporating the human component, the researchers determined that GHGs and particulates were the most likely contributing factors. "In this study, we switched from the traditional fingerprinting technique based on linear-trend statistics to a new regression-based fingerprinting technique," says Bonfils. "Doing so, we were able to better account for the complex temporal behaviors of forcings of the climate system, such as the slowly evolving increase in atmospheric GHGs, the complex temporal evolution of aerosol emissions, and the episodic occurrence of volcanic eruptions, and to better distinguish their individual responses."

The Laboratory climate scientists also found a possible connection between a drying California and the wetter Sahel. Before 1980, particulate pollution—think Victorian-era London, England—increased from U.S. and European industries, cooling the Northern Hemisphere, and pushing the tropical rain belt to the south in search of warmer climes. This shift meant more precipitation on the American West, and less in the Sahel, until regulations began to reduce particulate pollution. Without as many particulates shielding sunlight, the land-rich Northern Hemisphere began to warm faster than its ocean-dominated Southern counterpart (with help from GHGs), allowing the rain belt to come back north again. As a result, this mechanism has helped wildfires continue to rage each summer in unprecedentedly dry California, while record flooding in 2020 devastated large areas of Sahel countries such as Niger and Burkina Faso.

Hiding Behind a Volcano

Climate fingerprinting was an essential component of another research study led by Santer. With colleagues from PCMDI, the Canadian Centre for Climate Modelling and Analysis, and the Massachusetts Institute of Technology, Santer set out to determine at what point human-related fingerprint patterns became detectable within certain layers of the atmosphere.

The team used two large ensembles, one based on the Canadian Earth System Model version 2 (CanESM2) and the other on the U.S. Community Earth System Model version 1 (CESM1). The CanESM2 large ensemble had 50 simulations, while the CESM1 included 40 simulations. Each simulation started with slightly different spatial distributions of initial weather conditions, for example, a Monday rainstorm or a Thursday wind event in a particular location. Weather, by nature, is complex and chaotic, thus small differences in initial conditions—temperatures, winds, and humidity in places—generate different future weather patterns for the whole system that, over time, represents a plausible climate trajectory. When plotted, each set of ensemble paths forms an envelope of climate trajectories. Researchers examined the evolution of the envelopes and compared these envelopes and their averages to actual data gathered from several satellite sources.

Results from the study showed that stratospheric cooling (approximately 14 to 29 kilometers above the Earth's surface), which is primarily due to increases in ozone-depleting substances, was first detectable between 1994 and 1996. Detecting GHG-driven warming in the troposphere (from the surface of the Earth to approximately 18 kilometers up), however, did not occur until between 1997 and 2003—thanks to a volcano. The 1991 eruption of Mt. Pinatubo in the Philippines warmed the lower stratosphere while cooling the troposphere, temporarily hiding human influences on atmospheric temperature.

The two ensembles generated by the models differed in how consistent the fingerprint detection times were when compared to the satellite data, yet the results are encouraging. "This was the first time that the large initial-condition ensemble method was used to look at the detection time for human fingerprints on the global climate," says Santer. Although more research is needed to better understand climate response to natural variability and human-related causes, the technique is showing its worth as a tool for separating the two. "It enables us to differentiate more clearly between human-caused signals and noise, or natural internal variability in climate, and helps us better understand how and when human activities first began to affect climate."

Variations Are Key

In early 2021, Livermore scientists untangled a long-standing mystery: most climate models simulated more warming in the tropical troposphere than was observed in satellite data. Previous research studying the differences between satellite observations and model simulations suggested that climate models are overly sensitive to GHG changes. In contrast, Lawrence Livermore researchers found that natural climate variations, such as episodic warming and cooling from El Niño and La Niña events, respectively, can largely explain the discrepancy.

Analyzing more than 400 simulations from the newest generation of climate models, the team found that 13 percent of simulations are in accord with satellite observations. Climate models with both small and large sensitivities to GHG changes had individual simulations in accord with the satellite observations. This finding suggested that additional factors must be at play.

Natural climate variations turned out to be an important consideration. "While models are intended to represent the average climate, its forced changes, and realistic natural variations, they can only simulate the observed timing of natural climate events—and their effect on the long-term warming trend—by chance," says Livermore scientist Stephen Po-Chedley. The research team demonstrated that the pattern of surface temperature change and the accompanying

> "We now have a much clearer picture of the past, present, and future climate, which is essential for understanding where we are headed, what can be done, and how we can prepare."

rate of tropical tropospheric temperature change is strongly modulated by natural climate variations. Model simulations with greater-than-average tropical tropospheric warming tend to have an El Niño-like pattern of surface warming. The real world, in contrast, has had a La Niña-like pattern of surface warming over the years of interest. Simulations with this pattern exhibit reduced tropical tropospheric warming and are more likely to agree with satellite observations. These results demonstrate that climate models can simulate warming of the tropical troposphere that is consistent with observations, and that natural variability has likely reduced tropospheric warming over the satellite era. "In reconciling modeled and observed warming rates, we showed that climate sensitivity is not the sole determinant of atmospheric warming," says Po-Chedley. "Natural variability is an important piece in the puzzle."

Looking Forward

Earth's physical, biological, and chemical systems are complex and interconnected. Understanding and predicting how climate affects those systems, and additionally, what drives climate change is a monumental task, requiring the tenacity and expertise of climate scientists around the world. "Climate modeling is a nonlinear problem. We can't get the large-scale right if we don't get the small-scale right, which is why we focus on improving model physics," says Bader.

Despite the obstacles, Lawrence Livermore, in partnership with its sister laboratories and other collaborators, continues to advance the tools and methodologies needed to accurately predict future climate conditions. With powerful computers and an ongoing refinement process, scientists build and improve sophisticated climate models such as E3SM to zoom in on elements of climate-vulnerable U.S. infrastructure. These models also enable enhanced techniques, such as climate fingerprinting, to clarify both natural and human-related influences affecting Earth's atmosphere.

By comparing and validating research and data over more than three decades of study and using state-of-the-art tools of this era, the Laboratory is bringing into focus the evolution of climate change and its potential effects. In the 2021 IPCC report, Valérie Masson-Delmotte, the IPCC Working Group 1 co-chair, summarized the importance of this work, stating, "We now have a much clearer picture of the past, present, and future climate, which is essential for understanding where we are headed, what can be done, and how we can prepare."

—Ben Kennedy
(with additional reporting by Ann Parker and Anne Stark)

Key Words: Canadian Earth System Model version 2 (CanESM2), climate change, climate fingerprinting, Community Earth System Model version 1 (CESM1), Energy Exascale Earth System Model (E3SM), ensemble modeling, exascale computing, greenhouse gas (GHG), Intergovernmental Panel on Climate Change (IPCC), Program for Climate Model Diagnosis and Intercomparison (PCMDI), stratosphere, troposphere.

For further information contact David Bader (925) 422-4843 (bader2@llnl.gov) or Céline Bonfils (925) 423-9923 (bonfils2@llnl.gov).

S&TR September/October 2021

EYES HIGH IN THE SKIES

WHAT'S smaller than a breadbox, orbits hundreds of kilometers above Earth's surface, and can take photographs that show cars on the road one minute, then provide images of galaxies millions of light-years away the next? The monolithic telescope, or MonoTele—a space telescope developed at Lawrence Livermore National Laboratory—can, with more images on the way. In 2021, a small satellite bearing an imaging payload featuring two MonoTeles hitched a rideshare on a SpaceX Starlink launch at NASA's Kennedy Space Center in Florida.

The MonoTele is fabricated from a single, monolithic fused silica slab, optically shaped and with reflective coatings at both ends. One MonoTele has a high-resolution narrow field of view for Earth observation, the other has a high-sensitivity medium field of view for space domain awareness and astronomy applications. The compact optical imaging payload, called GEOStare2, is incorporated into a satellite about the size of a large shoebox: the Tyvak-0130 nanosatellite, designed and developed by Tyvak Nano-Satellite Systems, Inc. The GEOStare Space Vehicle 2 (SV2) payload-plus-satellite system, now orbiting at almost 550 kilometers above Earth's surface, can take both monochrome and color images.

GEOStare SV2 is the most recent achievement of a four-year, $6 million Cooperative Research and Development Agreement (CRADA) between Lawrence Livermore and Tyvak, a Terran Orbital company. The collaboration seeks to develop compact, robust, high-performance telescopes for nanosatellites, transitioning the Laboratory's MonoTele technology to space demonstration and eventual commercial use for applications such as space domain awareness and intelligence surveillance and reconnaissance applications. Alex Pertica, deputy program leader for the Laboratory's Space Science and Security Program is principal investigator for the CRADA. The effort

From left: Lawrence Livermore National Laboratory optical engineer Brian Bauman; mechanical designer Darrell Carter; and Alex Pertica, deputy program leader for the Laboratory's Space Science and Security Program, display small monolithic telescopes (MonoTeles) ranging in approximate size from 2.5 to 36 centimeters.

The GEOStare SV2 consists of the GEOStare2 optical imaging payload integrated into the Tyvak-0130 nanosatellite. The payload (center metal rectangle) holds two compact Livermore-developed monolithic telescopes, along with sensors, cameras, and electronics. The nearly 36-centimeter-tall, 120-centimeter-long GEOStare SV2 is the latest development of a collaboration between Lawrence Livermore and Tyvak Nano-Satellite Systems, Inc., to demonstrate the feasibility of using these small systems for space domain awareness (monitoring and tracking space debris), astronomical observation, and ground imaging. (Photo by Tyvak Nano-Satellite Systems, Inc.)

Lawrence Livermore National Laboratory

GEOStare2 peers outward, into the universe, when not focused on Earth or tracking space debris. This composite false-color image of the Andromeda galaxy, 2.5 million light years away, was created by stacking five wide-field-of-view images for an exposure of eight seconds. During these exposures, two satellites, represented as two aligned streaks in the image, moved through the field of view.

is headed by Livermore astrophysicist Wim de Vries, who leads a multidisciplinary team of engineers, physicists, and astrophysicists. In addition to designing the imaging payload and working closely with Tyvak to integrate the payload and nanosatellite, the Livermore team is responsible for analyzing the images captured in orbit. De Vries notes that in its first six months of operation, GEOStare2 has taken more than 29,000 images of Earth and space, with more pouring in every day. "The satellite and its imaging system never sleep," he adds.

Birth of the MonoTele

The story of "the little telescope that could do a whole lot" started long before the current CRADA. MonoTele inventor, optical engineer Brian Bauman, explains, "Like many good ideas, the monolithic telescope was born from a failed experiment." In 2010, Bauman and a team were building a small conventional telescope that could be used in nanosatellites for Space-Based Telescopes for the Actionable Refinement of Ephemeris (STARE), a multi-institutional project to monitor space debris. (See *S&TR*, April/May 2012, pp. 4–10.) Once the telescope was aligned, it was given a "shake test," submitting it to the kinds of forces experienced in a space launch. The team checked the telescope afterwards, only to find that the telescope had been shaken out of alignment, yielding blurry, out-of-focus images.

Bauman says, "I realized it was going to be very difficult to hold the primary and secondary mirrors in alignment as long as these two pieces of optical glass required fasteners to hold them in place." He eventually came up with the notion of having a solid telescope created from one piece of glass instead of two. One inspiration for his breakthrough included the Livermore-inspired design of the Vera C. Rubin Observatory, previously known as the Large Synoptic Survey Telescope, a game-changing telescope in which the primary and tertiary mirrors are designed as a single piece of glass. (See *S&TR,* September 2017, pp. 4–11.)

That's not to say that bringing the MonoTele into being was easy. "Initially, I didn't think a monolithic telescope could be fabricated from a single glass slab to the exacting, micrometer-level tolerances required to form the mirror surfaces," Bauman notes. "So, we assembled the telescope from four glass pieces that we glued together. But that didn't work terribly well and was difficult to align." Eventually, thanks to a vendor's improved, proprietary manufacturing processes, a monolithic telescope was formed from a single glass slab. Bauman's invention resulted in a telescope that is shorter and more robust against shaking and vibration. Other MonoTele advantages include no need to focus, easier alignment between the telescope and the cameras that record the images, and insensitivity to temperature swings. All big pluses, considering the environment of space.

Bauman says, "The fabrication was only possible because, at this time, there existed glass with extremely high homogeneity and low absorption, modern manufacturing techniques, and modern testing techniques. "If we'd tried to fabricate the MonoTele 10 years earlier, I doubt we could have."

And it wasn't just the fabrication of the MonoTele that presented challenges. "Space is hard," de Vries notes. If hardware breaks or malfunctions, one cannot just "go and fix it." So, the hardware must be ultra-hardy and reliable. An orbiting satellite faces extreme temperature swings—from 80°C in the Sun to –80°C in shadow. "The MonoTele is well suited for this environment," says Bauman. Additionally, the one-piece design eliminates much of the difficult mechanical engineering required by conventional telescopes.

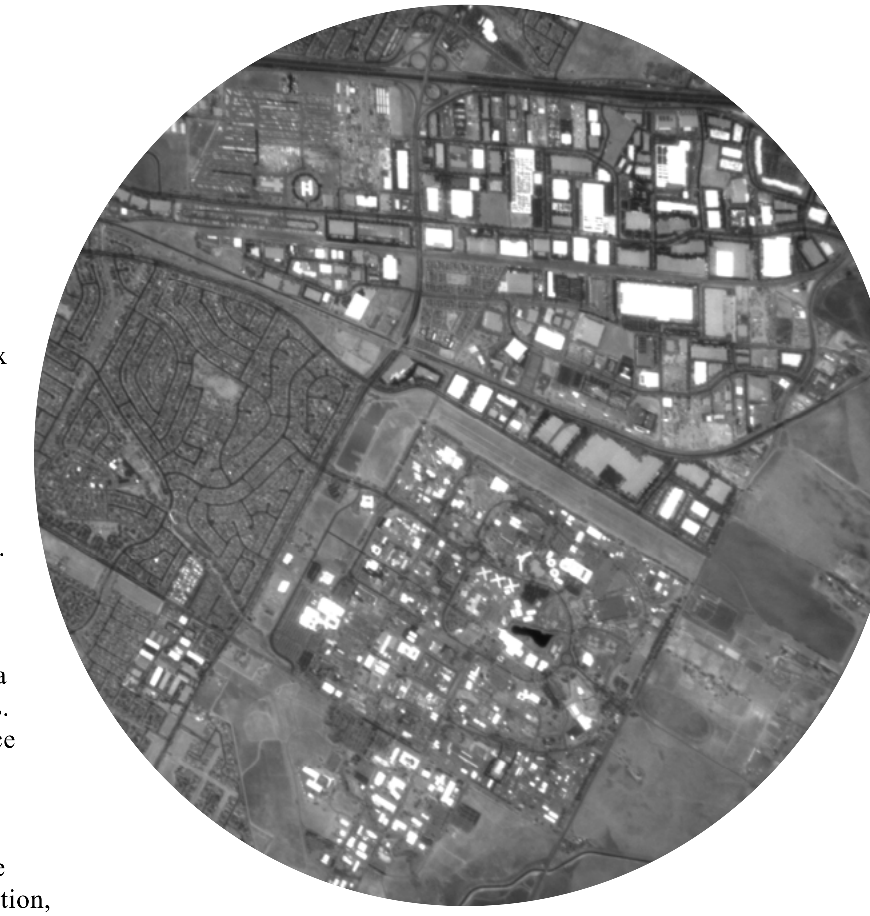
GEOStare-ing into the Future

GeoStare SV2 is the third time Lawrence Livermore has flown its telescopes with Tyvak's satellite technology, a partnership that has yielded much in just a handful of years. The MonoTele got its first chance to shine when a Lawrence Livermore team led by de Vries partnered with Tyvak and the U.S. Air Force to develop GEOStare1, which launched in 2018 with a single MonoTele about 7.5 centimeters in diameter. The flight tested the performance of the telescope design for collecting remote sensing data for Earth observation, astronomy, and space debris tracking applications. "The test produced beautiful data and validated all our ideas," says de Vries. (See *S&TR*, April 2019, pp. 4–11.)

In 2020, a tiny 2.5-centimeter "mini-monolith"—about the size of a large earring—was incorporated into Tyvak's Cerberus satellite. This tiny MonoTele took on the role of "star tracker," measuring the positions of stars to determine the orientation of the spacecraft. De Vries says, "Tyvak is very flexible and open to taking risks. When their Cerberus satellite had some room, we asked if we could fly our new design for a mini-monolith, and they didn't hesitate. They make things happen. It's a great situation for advancing technologies quickly."

Tyvak President Boris Becker adds, "Terran Orbital values our long-standing partnership with Lawrence Livermore and is honored to have the opportunity to work with Alex Pertica, Wim de Vries, and the talented professionals of their team. Together, we have developed and deployed a leading-edge capability in small satellite imaging. GEOStare2 has produced thousands of images of Earth in support of the Laboratory's mission, from a satellite that could fit inside a backpack."

The Livermore–Tyvak team is busy developing systems for the next CRADA mission, GEOStare3. De Vries notes that the imaging payload will be larger than that for GEOStare2, with four telescopes instead of two. One MonoTele will be optimized for the ultraviolet portion of the spectrum, a second for visible, a third for the shortwave infrared, and a fourth will be coupled to a prism to function as a point-source spectrometer, with all the telescopes focused on the same spot. The team is looking to launch the system sometime in 2022.



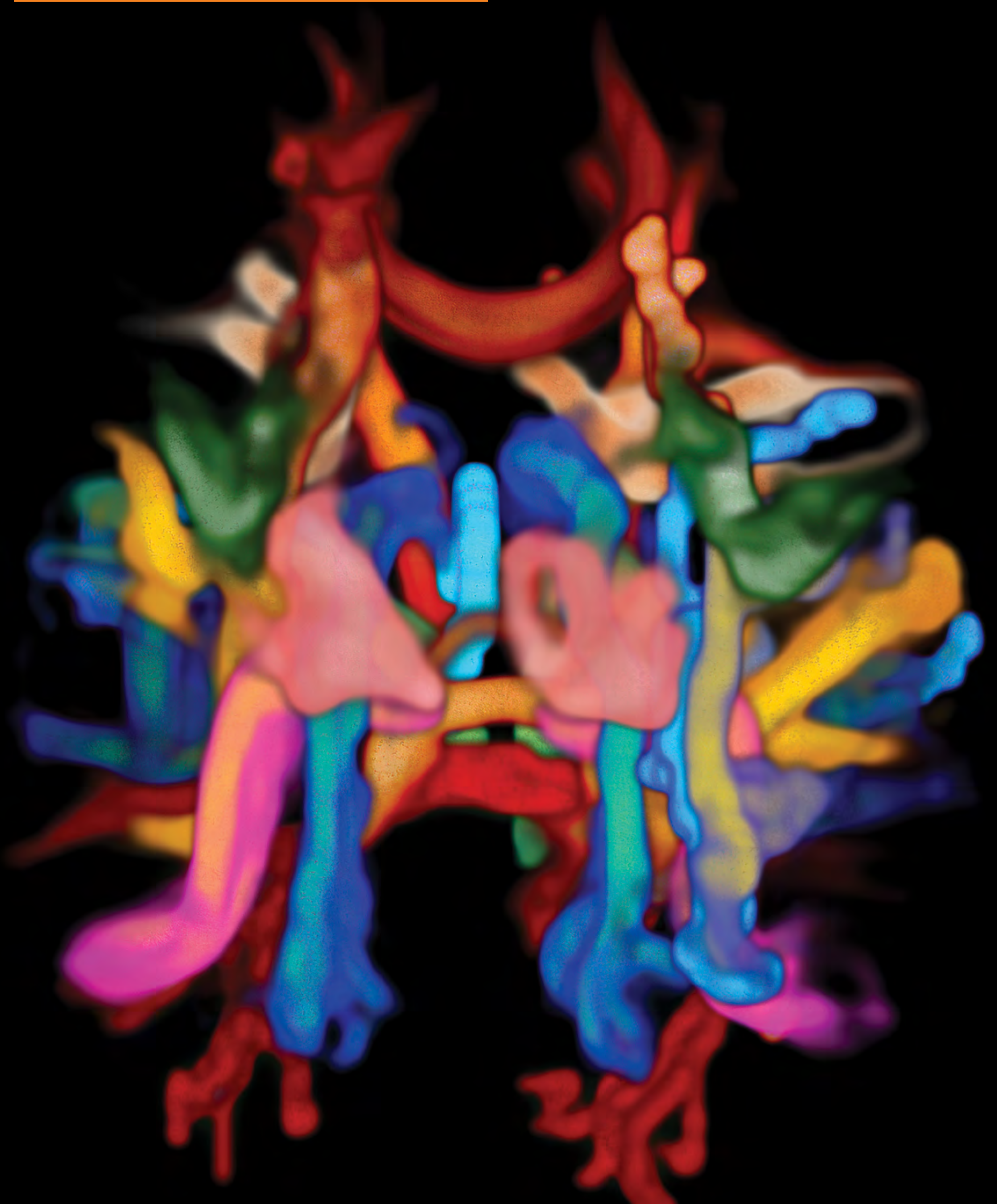
GEOStare2's narrow-field-of-view telescope captured this image of Lawrence Livermore National Laboratory from an altitude of about 600 kilometers.

De Vries says, "We are excited for what the future holds. What is special about these small satellites and their tiny telescopes is how very capable they are. It allows us to put a long focal length, which in a classical telescope would be about a meter long, into something the size of a milk carton. And the images we have so far from GEOStare2 are fantastic, very impressive. We look forward to what we obtain from GEOStare3." Pertica notes that eventually the goal is to have GEOStare systems that will be able to complement high-end, exquisite satellite systems by adding capacity and increasing how often data can be collected from a given location. He adds, "It's really rewarding to put technology in space and demonstrate these new capabilities, capabilities that weren't possible before nanosatellites and these incredibly compact, high-performance imaging systems."

—Ann Parker

Key Words: astronomy, Cooperative Research and Development Agreement (CRADA), GEOStare, Large Synoptic Survey Telescope, monolithic telescope (MonoTele), nanosatellite, optical payload, Vera C. Rubin Observatory, Space-Based Telescopes for Actionable Refinement of Ephemeris (STARE), space debris, space domain awareness, Tyvak Nano-Satellite Systems, Inc.

For further information contact Alex Pertica (925) 423-3354 (pertica1@llnl.gov).



ACCELERATING THE PATH TO PRECISION MEDICINE

ACCORDING to the U.S. Centers for Disease Control and Prevention, traumatic brain injury (TBI) affects millions of Americans each year, resulting in hundreds of thousands of emergency room visits and hospitalizations every year and as many as 150 deaths daily. Despite the ubiquity of TBI, targeted treatment, and, in many cases, a prognosis, for many patients, remains elusive. Clinically categorized as “mild, moderate, or severe,” the majority of TBIs, including concussions, fall into the mild category. However, people with mild TBI can later experience debilitating symptoms. Clinicians struggle to explain why someone experiences certain symptoms, but not others, and if they will ever go away. “Outcomes can range from a complete recovery after a devastating injury to debilitating depression or memory loss because of what, at first, seemed like an inconsequential incident,” says Shankar Sundaram, director of Lawrence Livermore’s Bioengineering Center and principal investigator of the Laboratory’s TBI research efforts.

With 100 billion neurons and 10,000 connections at the end of each neuron, the brain’s complexity confounds researchers. Yet, data analysis of the complex networks of neurons is mathematically well suited for applying Lawrence Livermore National Laboratory’s high-performance computing (HPC), machine learning, and data science expertise. In March 2018, Lawrence Livermore joined the Transforming Research and Clinical Knowledge in Traumatic Brain Injury (TRACK-TBI) consortium. The national, multiyear, multidisciplinary effort, led by the University of California at San Francisco (UCSF) in collaboration with Lawrence Berkeley and Argonne national laboratories and other leading research organizations and universities, combines neuroimaging, blood-based biomarkers, clinical, and outcome data for thousands of TBI patients and advances supercomputing and machine learning with the aim of developing precision medicine diagnoses and treatments for TBI patients. So far, the results have accelerated, democratized, and simplified the data-processing workflow of TBI patient data and revealed the multifaceted nature of TBI. “Working with the TBI data set has presented us with one of the most complicated computing challenges we’ve ever faced,” says Sundaram. “We have been pushed, but I can say we’ve met the first set of challenges with success.”

Diffusion magnetic resonance imaging (dMRI) measures the directional diffusion of water molecules in tissue, enabling the mapping of the underlying white matter structure of a living human brain. (Images courtesy of Tianhao Lanya Cai, University of California at San Francisco.)

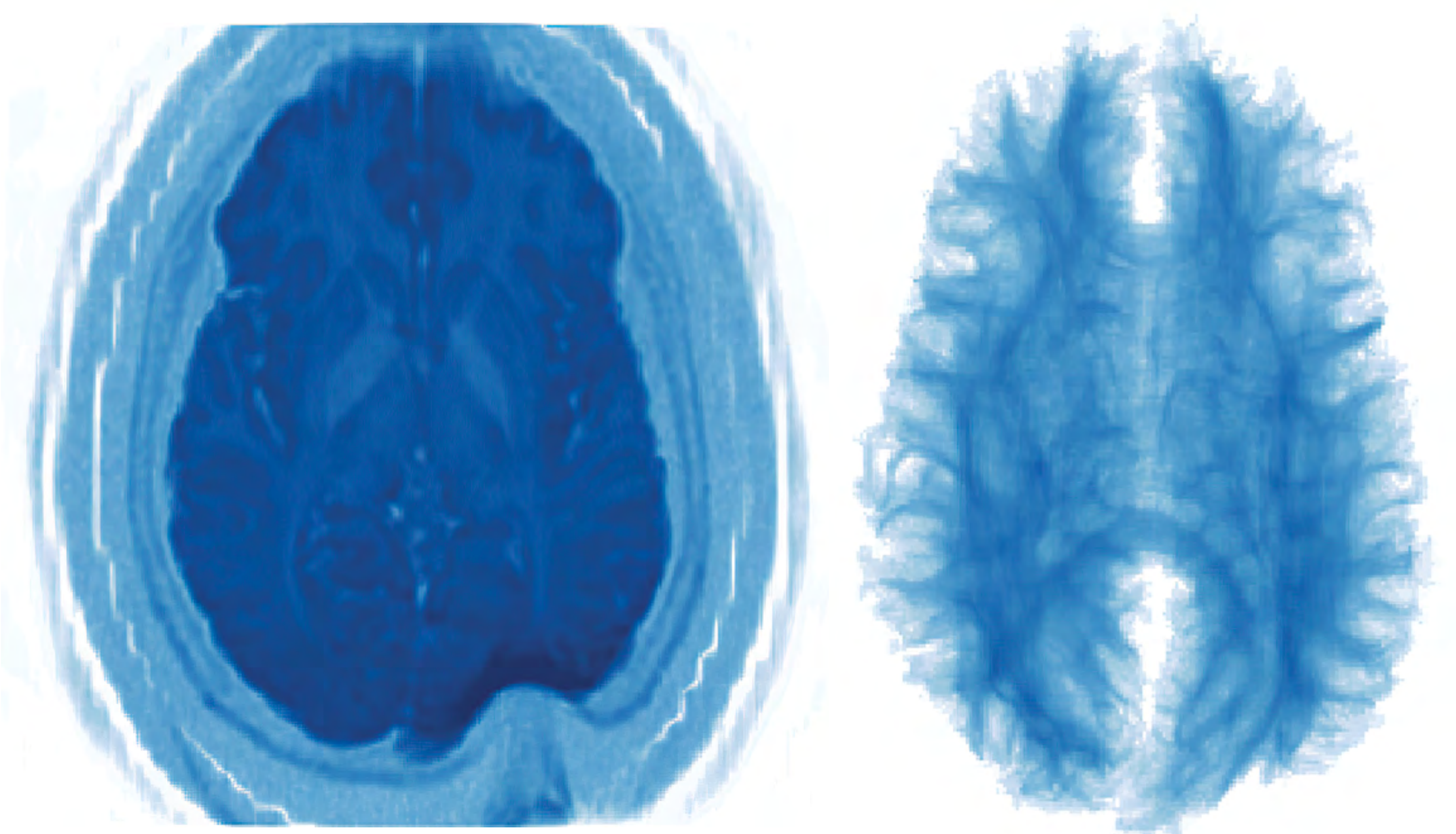
Connectome Container

One of the first obstacles the Livermore team tackled was building a suitable data infrastructure to transfer, store, and provide access to huge quantities of complex, intricate multimodal patient data at high speeds to clinicians and TBI researchers. In the past, processing data from magnetic resonance imaging (MRI) of a single brain would take 24 hours before it could be read by a radiologist. Large-scale diffusion of MRI tractography—the visually stunning 3D-modeling technique depicting the brain’s nerve tracts—renders connectomes, comprehensive maps of neural connections or disruptions in the brain. Connectomes present researchers with significant computational hurdles such as orchestrating multiple software packages with multiple dependencies and high computational costs. The prospect of sorting through and ingesting anonymized data from 3,000 TBI patients demanded the creation of a fast, streamlined system that could share data across laboratories participating in the TRACK-TBI consortium.

To solve this bottleneck and speed up data processing, Livermore software developer Joseph Moon and Peer-Timo Bremer, research scientist in the Laboratory's Center for Applied Scientific Computing, developed the Massively Parallel, Portable, and Reproducible Tractography (MaPPeRTrac) workflow for HPC. MaPPeRTrac incorporates novel technologies to simplify and accelerate neuroimaging research. "One of the biggest obstacles to applying the latest data science techniques—graph analysis, statistical methods, and machine learning—is the complexity of neuroscience software," says Moon. "Dozens of tools, all designed by different teams around the world, must be connected to generate biophysically meaningful data." MaPPeRTrac is a containerized parallel-compute infrastructure, which means it can be executed anywhere on top of any computing system without having to use multiple software packages or a supercomputer.

MaPPeRTrac fully automates the tractography workflow from management of raw MRI data to edge-density visualization of a connectome with the aim of providing clinicians in diverse hospital settings off-the-shelf access to clinically actionable data. The MaPPeRTrac container enables high-performance, parallel, parametrized, and portable generation of connectomes that is fast, efficient, well-tested, robust, and easy-to-use for the research community.

To lower the barrier to entry for users, Bremer's team has also made MaPPeRTrac available on the open-source GitHub cloud so that any researcher—not only computer scientists—can generate connectomes using state-of-the-art software



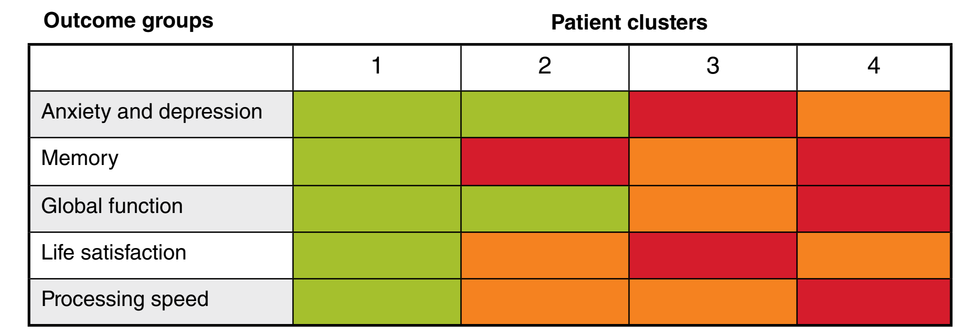
These images show (left) an MRI scan of a patient with traumatic brain injury and (right) a visualization of the simulated neural streamlines composing a brain's connectome edge density. The latter was generated with the Laboratory's Massively Parallel, Portable, and Reproducible Tractography workflow.

libraries and HPC. "Users don't have to be at a Department of Energy national lab with a high-performance computer to use MaPPeRTrac," says Geoff Manley, director of the TRACK-TBI consortium at UCSF. "MaPPeRTrac democratizes the quality of TBI care clinicians can provide. Clinicians at a rural hospital, for example, can potentially access the fastest MRI analysis and predictive models. The team at Lawrence Livermore has vastly accelerated our data pipeline. Our collaboration and outcomes have been truly remarkable."

Messy Data Challenge

The other major challenge was developing new algorithms that can process multimodal data—images, clinical assessments, biomarkers, and other data points—and produce reliable, interpretable diagnostics and prognostics even when some of the data is missing or uncertain. "An important aspect of applying machine learning in healthcare is managing missing data," says Alan Kaplan, a Livermore research scientist working on the TBI project. "Many algorithms cannot utilize arbitrary 'missing-ness' patterns or require ad hoc preprocessing on 'messy' data. A research subject with incomplete data would typically be dropped from an algorithm's analysis. But we all know that in real-world situations, life is messy, someone forgets to ask a question or leaves an answer blank. We had to figure out how to ensure that we don't lose a subject if there are gaps in the data."

The Livermore team created a statistical model, not just to impute but to account for "missing-ness" as well as random or deliberate omissions, considering if groupings or even sub-groupings might emerge despite gaps in the data. So far, the sub-groupings the algorithm has identified can predict outcomes using biomarkers, stratify patients into similar groups, stratify variables into similar groups, simulate patient data, and rank dependence of biomarkers on patient outcomes. The model allows for movement toward the idea of enhanced specificity among subgroups of TBI patients. "We now know that 'mild, moderate, or severe' is inadequate in terms of categorizing TBI," says Kaplan. "The model we've developed incorporates data that portrays TBI's truly multifaceted nature. The initial findings indicate a 20 percent improvement over baseline predictions. If validated, our work could help clinicians make more accurate prognoses and aid in decision making for early clinical management and determining targeted treatment interventions."



The algorithm developed by Livermore data scientists can predict traumatic brain injury outcomes using biomarkers and rank dependence of these biomarkers from absence/low burden of specific symptoms (green) to some evidence/medium burden (orange), and presence/high burden (red), demonstrating the ability to provide enhanced clinical specificity beyond mild, moderate, or severe traumatic brain injuries.

Precision Medicine Goal

Having developed MaPPeRTrac to synthesize and process MRI connectome data as well as a machine-learning model to identify and organize swaths of TBI patient data despite missing data points, the Livermore team, working with TRACK-TBI, has a proof-of-concept. The team hopes to scale up the project by collaborating with other institutions including the National Collegiate Athletic Association, Veterans Affairs, and the Department of Defense to leverage their data sets of TBI patients and further engage the TBI research community. "This research isn't about telling people there's a cure, per se," says Bremer. "But so often people experience overwhelming symptoms due to TBI, and clinicians have no way of predicting what the short- and long-term consequences may be. We're hoping that our research can offer clinicians and their patients some insight into the cause of symptoms and the trajectory for treatment."

"What's really exciting about this work is that it could be used down the road to improve patient outcomes and have positive real-world impacts," says Kaplan. Sundaram adds, "The tools are ready. With additional support, we will apply them to larger aggregated data sets to assess our predictive analytics and validate those biomarkers."

—Genevieve Sexton

Key Words: brain tractography, connectome, high-performance computing (HPC), Massively Parallel, Portable, and Reproducible Tractography (MaPPeRTrac), magnetic resonance imaging (MRI), Transforming Research and Clinical Knowledge in Traumatic Brain Injury (TRACK-TBI), traumatic brain injury.

For further information contact Shankar Sundaram (925) 423-6468 (sundaram1@llnl.gov).

SHINING A LIGHT ON TECHNICAL EXCELLENCE

Physicist Hye-Sook Park holds a target assembly from the National Ignition Facility (NIF). Her work at NIF includes studying solid-state dynamic material properties and high-speed plasma flow interactions. (Photo by Garry McLeod.)

CLIMBING the management ladder is not the only upward route on a career path, a fact long recognized by Lawrence Livermore National Laboratory. Ten years ago, the Laboratory established the Distinguished Member of Technical Staff (DMTS) program to provide a career path for advancement for those who choose to remain working in their technical fields rather than step out, full time, onto the managerial track. Livermore Director Kimberly Budil explains, “Our Lab was created to bring innovative science and technology to bear to tackle the most significant challenges facing the nation and the world. To do this well requires a high level of technical excellence, so it is critically important that we develop exceptional leaders in our science and technology ranks. The DMTS program was created to recognize these exceptional leaders from across the Lab and to shine a light on their extensive expertise and many contributions.”

Appointment to the DMTS level is the highest technical staff level achievable at the Laboratory. Those who are nominated to DMTS have a history of high-level achievement in important Laboratory programs or distinguished scientific achievements. They are often recognized authorities in their fields responsible for important discoveries with lasting impacts. Laboratory leaders nominate candidates at the request of the director, who decides when to open nominations. The last DMTS staff were named in 2019. A sample of DMTS members, from the early years of the program to the most recent induction, demonstrates that the word “outstanding” truly applies.

Hye-Sook Park

In 2017, physicist Hye-Sook Park was 30 years into her Livermore career and leading multiple projects at the National Ignition Facility (NIF). Among her projects was a successful campaign to develop a new “high foot” shape for NIF’s laser pulse that was more forgiving of fusion fuel capsule imperfections, the first plutonium strength experiment, and an astrophysical collisionless shock campaign. She remembers, “All of my projects were delivering incredible results, and I was in the middle of an exciting time.” Adding to the excitement that year was the notification that she received the DMTS award. “When I heard, I gave two thumbs up and shouted, ‘Yes! I did it!’ I truly appreciated that the Laboratory and my nominator recognized my enthusiasm for science and my hard work, even though I did not follow a managerial track.”

Challenging, cutting-edge science is what Park thrives on—from her early projects working on the Clementine lunar mapping satellite mission and chasing after optical counterparts of galactic gamma-ray bursts that last only tens of seconds, to studying the density evolution of metal ejecta from high explosives. “I wouldn’t be where I am now without my mentor’s and colleagues’ help,” she says. “Everything is a

team effort.” Park notes that she became a DMTS without an Ivy League degree and as a foreign-born woman. She offers the following advice to young scientists: “Find a good mentor and work hard.”

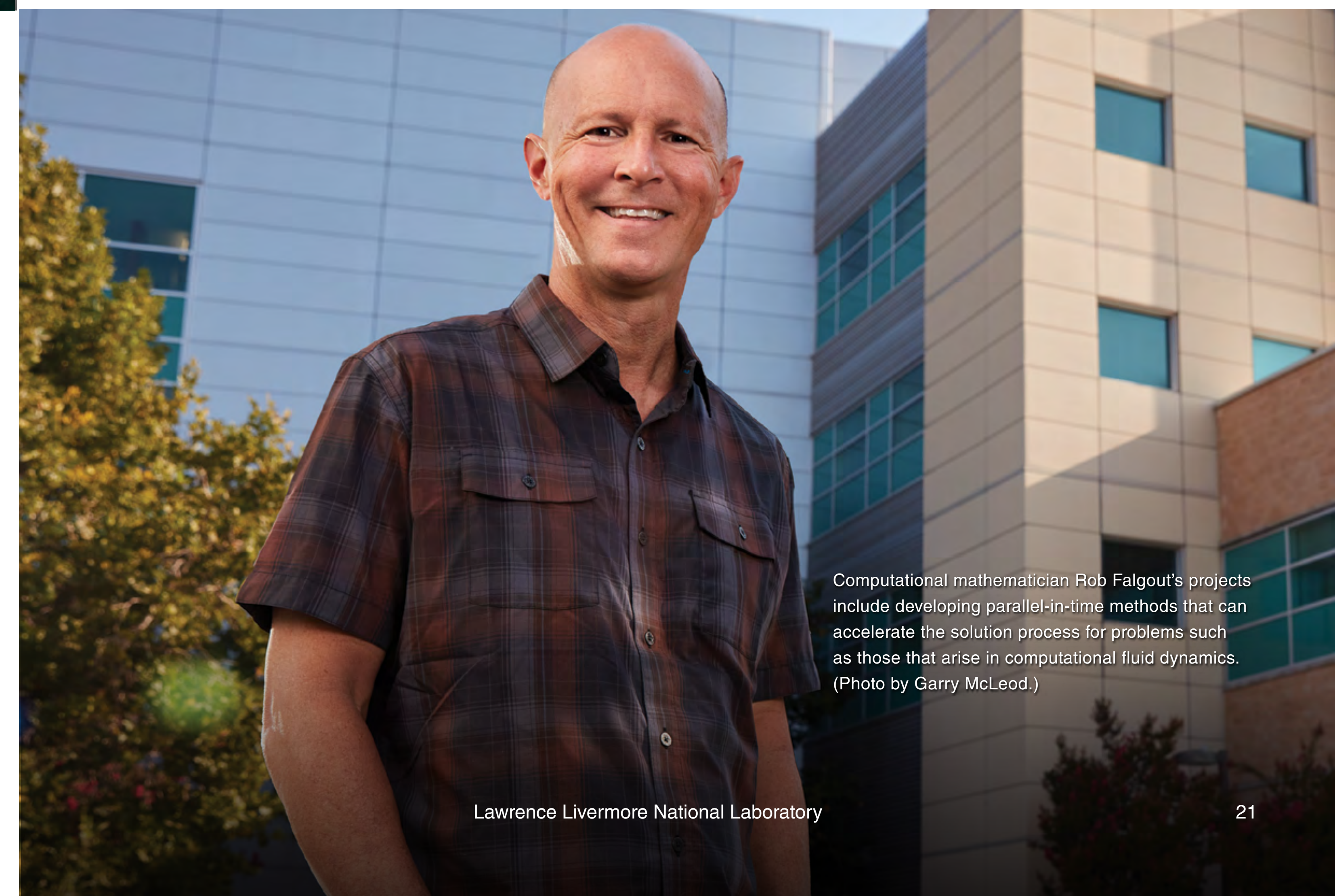
Rob Falgout

Computational mathematician Rob Falgout professes he was completely surprised when he learned he received the DMTS award. “I knew my name had been thrown into the hat,” he says, “but figured my chances were slim.” When he was awarded the designation in 2018, Falgout had been at the Laboratory for nearly 27 years. One of his earliest projects involved development of the ParFlow groundwater flow code, used today to do continental-scale watershed modeling. Other, more recent efforts include *hypre*, a popular parallel multigrid code, and research on multigrid methods for linear systems of equations. “An area that has occupied me over the past 10 years is the development of parallel-in-time solvers,” he adds. “This research has led me to work on solving nonlinear problems, not just linear ones, and getting involved in new application areas.”

Recently, he has been developing parallel-in-time methods for hyperbolic and chaotic problems such as those that arise in computational fluid dynamics. Falgout appreciates that, through DMTS, the Laboratory supports a technical track that is on par with the one for management. He says, “I have the highest regard for people who prefer doing management work. Management is so important, but the role just doesn’t fit my personality. I believe I’m more effective leading smaller research teams and staying active in the technical work.”

Frank Graziani

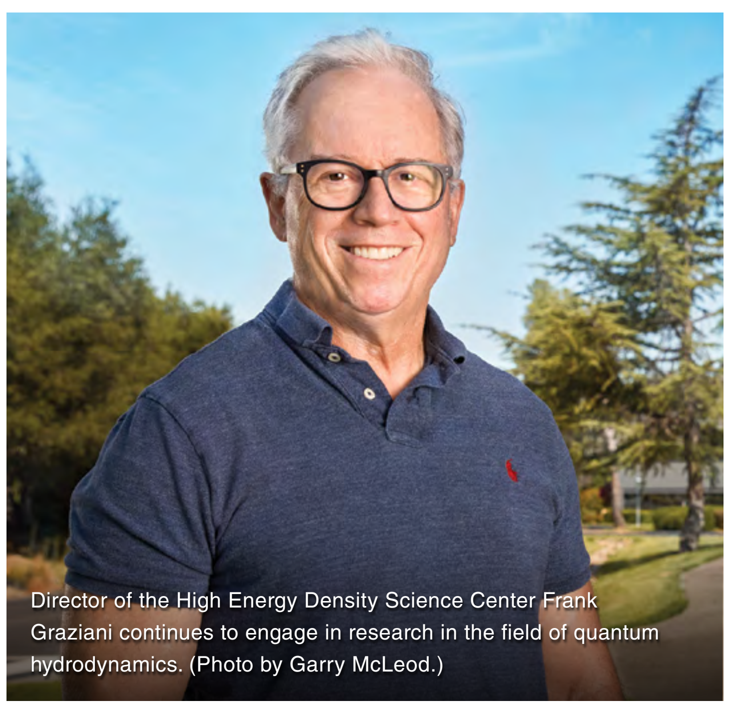
In 2017, when physicist Frank Graziani achieved DMTS status, he was juggling roles as computational physics associate division leader and lead for the National Boost Initiative—a multidisciplinary, multinational laboratory effort aimed at answering scientific questions underlying nuclear weapons operation—all while conducting research in high-energy-density science (HEDS). He recalls feeling honored at being accepted into the program. “Two of my mentors, George Zimmerman and Robert Tipton, had previously been selected



Computational mathematician Rob Falgout’s projects include developing parallel-in-time methods that can accelerate the solution process for problems such as those that arise in computational fluid dynamics. (Photo by Garry McLeod.)

for DMTS, as well as several colleagues such as Juliana Hsu and John Castor. Being considered in the same category as these excellent scientists was humbling.” Graziani notes that everyone he has worked with in his 32-year career has made him a better scientist. “The support and encouragement by management to pursue simultaneous paths in research and technical leadership was of great help to me. In many ways, my education began when I came to Lawrence Livermore. At 65 years of age, I am still learning.”

Graziani joined the Laboratory in 1989 as a code physicist before engaging in research in boost science and computational approaches in HEDS, becoming a verification and validation manager, among other roles. Today, he is the director of the High Energy Density Science Center. He also conducts research in quantum hydrodynamics—a hydrodynamic description of the quantum many-body problem useful for warm dense matter studies—and is developing quantum computing algorithms for solving many-body quantum systems and solving radiation diffusion problems. “Throughout my career here, I have worked hard to balance research and technical leadership so I could do both simultaneously,” he says. “There is no other place in the world, other than a national laboratory, that I could have this type of career. The DMTS program is a wonderful way to reward an individual for a lifetime of technical contributions to Livermore’s mission areas.”



Director of the High Energy Density Science Center Frank Graziani continues to engage in research in the field of quantum hydrodynamics. (Photo by Garry McLeod.)

Natalia Zaitseva’s research on the growth mechanisms and physics properties of single crystals grown from low-temperature solutions has revolutionized the fields of crystal growth and radiation technology. (Photo by Garry McLeod.)

Natalia Zaitseva

Reflecting on receiving the DMTS award in 2015, Natalia Zaitseva says she was honored by the recognition, adding, “Any accomplishment I’ve been a part of became possible only because of the hard work and devotion of the people I’ve been privileged to work with.” Her research, which focuses on the growth mechanisms and physics properties of single crystals grown from low-temperature solutions, has revolutionized the fields of crystal growth and radiation technology.

Her early work at the Laboratory included developing methods for rapid growth of super-large crystals for the NIF laser system. More recent research on developing new organic scintillation materials for radiation detection led to the development of the first plastic scintillators that differentiate between neutrons and gamma rays as well as a novel method for quickly growing organic single crystals, which was subsequently transferred to industry.

Zaitseva continues to develop new materials resulting in crystals with unique properties, including crystals that are the basis of solid-state organic scintillators that can be used for neutron spectroscopy and differentiation between fast and thermal neutrons. “I am glad for the DMTS recognition, but it hasn’t changed how I work or the work that I do,” she says. “The Laboratory provides an excellent research environment for scientists. I feel privileged to work with an outstanding team and great colleagues and appreciate the opportunity to continue doing the work I love.”

Larry Fried

In 2019, Larry Fried was hard at work with the Cheetah thermochemical simulation code team when he was notified of his appointment to DMTS. “Since the nomination process considers your contributions across your entire career,” he says, “being elevated to DMTS is a great affirmation that a researcher has provided value to the Laboratory in an area of expertise.”

An internationally recognized leader in high-explosive science and high-pressure chemistry, Fried started at the Laboratory in 1992 as a postdoctoral researcher. By 2019, he was splitting his time between project management and technical work, including overhauling Cheetah, an advanced model based on the fundamental chemistry of detonation. “Cheetah was originally developed in the mid-1990s to run on central processing unit-based (CPU-based) computer systems. By 2019, we were working on ways to make it run on next-generation, graphics processing unit-based computing platforms, such as (Livermore’s) Sierra,” he says. A recent breakthrough now allows Cheetah to run on a Sierra node 15 times faster than on CPU-based nodes.

Fried is also part of a team that is investigating new techniques for predicting the chemical reactions of explosives and other organic materials. “Technical work is what I enjoy most,” says Fried. “Besides working with codes, I also talk with experimentalists and people who do molecular simulations. The DMTS program shows that the Laboratory has two demonstrable career ladders—one managerial and a second that is technical—with DMTS being the apex of the technical ladder. Receiving the DMTS recognition encouraged me to continue focusing much of my energy in the technical direction, doing the work I love to do.”

An internationally recognized leader in high-explosive science and high-pressure chemistry, Larry Fried works closely with experimentalists and molecular simulations experts at Lawrence Livermore’s High Explosives Applications Facility (HEAF). (Photo by Garry McLeod.)

Extraordinary Accomplishments

Regarding DMTS staff, Patricia Falcone, the deputy director for Science and Technology, notes, “Laboratory scientists and engineers who are recognized as DMTS are truly distinguished. Each one has delivered extraordinary accomplishments in science and engineering in support of the Laboratory’s missions. Each one is widely recognized within their scientific disciplines and the academic and sponsor community. Each one is a Laboratory role model for discovery and innovation. I know I benefitted in my career from opportunities to work with the most distinguished technical people in my research community; I hope all our staff take advantage of opportunities to work with these outstanding people.”

—Ann Parker

Key Words: algorithm, Cheetah, Clementine, collisonless shock, computational fluid dynamics, computational physics, detonation, Distinguished Member of Technical Staff (DMTS) program, gamma-ray bursts, high-energy-density science (HEDS), High Energy Density Science Center, high explosive, high-foot pulse, high-pressure chemistry, high-pressure material properties, *hypre*, lunar map, molecular dynamics, molecular simulations, multigrid, National Ignition Facility, quantum hydrodynamics, parallel-in-time solvers, ParFlow, science and technology, Sierra supercomputer, thermochemical simulation code.

For further information contact Terry Land (925) 423-5836 (land1@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 (uspto.gov).

Patents

In Situ Monitoring of Direct Ink Write Process Using Electromagnetic Resonant Coupling
Manyalibo Matthews, Eric Duoss
10,981,375 B2
April 20, 2021

Adsorption Cooling System Using Metal Organic Frameworks
Theodore F. Baumann, Joe H. Satcher, Jr., Joseph C. Farmer, Todd Bandhauer
10,994,258 B2
May 4, 2021

Controlling AM Spatter and Conduction
Saad Khairallah, Gabe Guss, Wayne King, Sonny Ly, Manyalibo Matthews, Alexander Rubenchik
10,994,337 B2
May 4, 2021

High Performance, Rapid Thermal/UV Curing Epoxy Resin for Additive Manufacturing of Short and Continuous Carbon Fiber Epoxy Composites
James Lewicki
10,994,472 B2
May 4, 2021

Multi-fluid Renewable Geo-Energy Systems and Methods
Thomas Buscheck
10,995,972 B2
May 4, 2021

Self-Powered and Reversible Light-Directed Electrophoretic Deposition Device for Use in Smart Windows and Photodetector Displays
Jeronimo Mora, Brian Giera, Jessica Dudoff, Elaine Lee
10,642,123 B2
May 5, 2021

Adsorption Cooling System Using Carbon Aerogel
Theodore F. Baumann, Joe H. Satcher, Jr., Joseph C. Farmer, Todd Bandhauer
11,000,823 B2
May 11, 2021

Multifaceted Radiation Detection and Classification System
Simon E. Labov, Karl E. Nelson, Brandon S. Seilhan
11,009,622 B2
May 19, 2021

Three Dimensional Vertically Structured Electronic Devices
Adam Conway, Sara Elizabeth Harrison, Rebecca Nikolic, Qinghui Shao, Lars Voss
11,018,253 B2
May 25, 2021

Neutron Generation Using Pyroelectric Crystals
Vincent Tang, Glenn A. Meyer, Steven Falabella, Gary Guethlein, Brian Rusnak, Stephen Sampayan, Christopher M. Spadaccini, Li-Fang Wang, John Harris, Jeff Morse
11,019,717 B2
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System and Method for Controlling Oxidation of Metals during Freeform Casting
Andrew Pascall, Joshua Kuntz, Scott McCall
11,020,797 B2
June 1, 2021

Three Dimensional Vertically Structured Electronic Devices
Adam Conway, Sara Elizabeth Harrison, Rebecca Nikolic, Qinghui Shao, Lars Voss
11,024,734 B2
June 1, 2021

Integrated Optics for High Energy Laser Applications
Christopher Walton, S. Mark Ammons, Brian Bauman, Robert Bickel, Wim de Vries, Alexander Pertica, Michael Pivovaroff, Vincent Riot
11,025,025 B2
June 1, 2021

Additive Manufacturing for Multi-Component Parts for Customizable Energetic Systems
Kyle Sullivan, Alexander Gash, Robert Reeves, John Vericella
11,027,482 B2
June 8, 2021

Awards

Chris Cross, acting Strategic Partnership program leader for the Laboratory's Weapons and Complex Integration Principal Directorate, received the **Department of the Army's Meritorious Civilian Service Award** for his time on the Army Science Board (ASB). While serving on the ASB, an all-volunteer Department of Defense science board, Cross contributed to intelligence, technical, warfighting, and investment strategies for replacing the M1A2 Abrams tank on the battlefield of 2040. The Meritorious Civilian Service Award is the second-highest award granted by the Secretary of the Army or a major Army commander to civilian personnel.

The Krell Institute awarded Lawrence Livermore computational scientist **Jeff Hittinger** its **2021 James Corones Award in Leadership, Community Building, and Communication**. Hittinger, director of the Laboratory's Center for Applied Scientific Computing, was recognized for initiatives plotting a course to exascale computing for the Department of Energy (DOE) as well as service to the DOE Computational Science Graduate Fellowship community, mentorship, and scientific outreach. The nonprofit Krell Institute manages graduate fellowships for DOE and the National Nuclear Security Administration, organizes scientific meetings, and develops computational science websites and magazines.

Abstract

Climate Change Comes into Focus

Researchers at Lawrence Livermore apply high-performance computing and expertise in fundamental sciences such as meteorology, climatology, applied mathematics, and computational science to the problem of understanding and predicting how the Earth's systems evolve on time scales from a few years to several centuries. However, they face challenges in reducing uncertainty in climate predictions and leveraging high-performance computing to better understand Earth system processes. Livermore's participation in the Energy Exascale Earth System Model (E3SM), a multilaboratory, international program, aims to reduce uncertainty in predicting future change by linking Earth system and energy models into a single system to assess how changes in energy use affect ecosystems, water availability, and other factors. Climate fingerprinting applies computer simulations to identity patterns of climate change and account for naturally occurring processes to improve the reliability of future climate predictions.

Contact: David Bader (925) 422-4843 (bader2@llnl.gov) or Céline Bonfils (925) 423-9923 (bonfils2@llnl.gov).

U.S. Government Printing Office: 2021/570-075-20017

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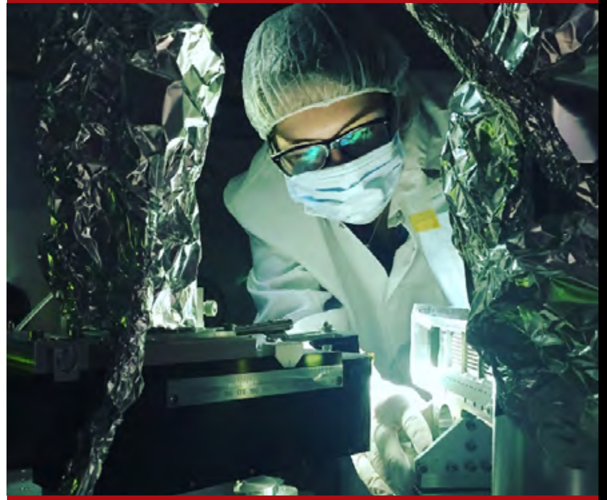

Around the world, multidisciplinary teams of Lawrence Livermore scientists are utilizing world-class, light-source facilities to uncover how materials react and change under extreme conditions.

Also in this issue…

- *A more fully integrated Lawrence Livermore–Kansas City National Security Campus partnership features a newly constructed Polymer Production Enclave to accelerate additive manufacturing development and production.*
- *Expanded hydrodynamic testing and Livermore-developed technologies are providing experimental preparations and data in support of upcoming subcritical tests.*
- *An update on Early and Mid-Career Recognition Award recipients demonstrates the many ways Laboratory scientists deliver on their exceptional promise.*

Coming Next Issue

Science & Technology Review
Lawrence Livermore National Laboratory
P.O. Box 808, L-664
Livermore, California 94551

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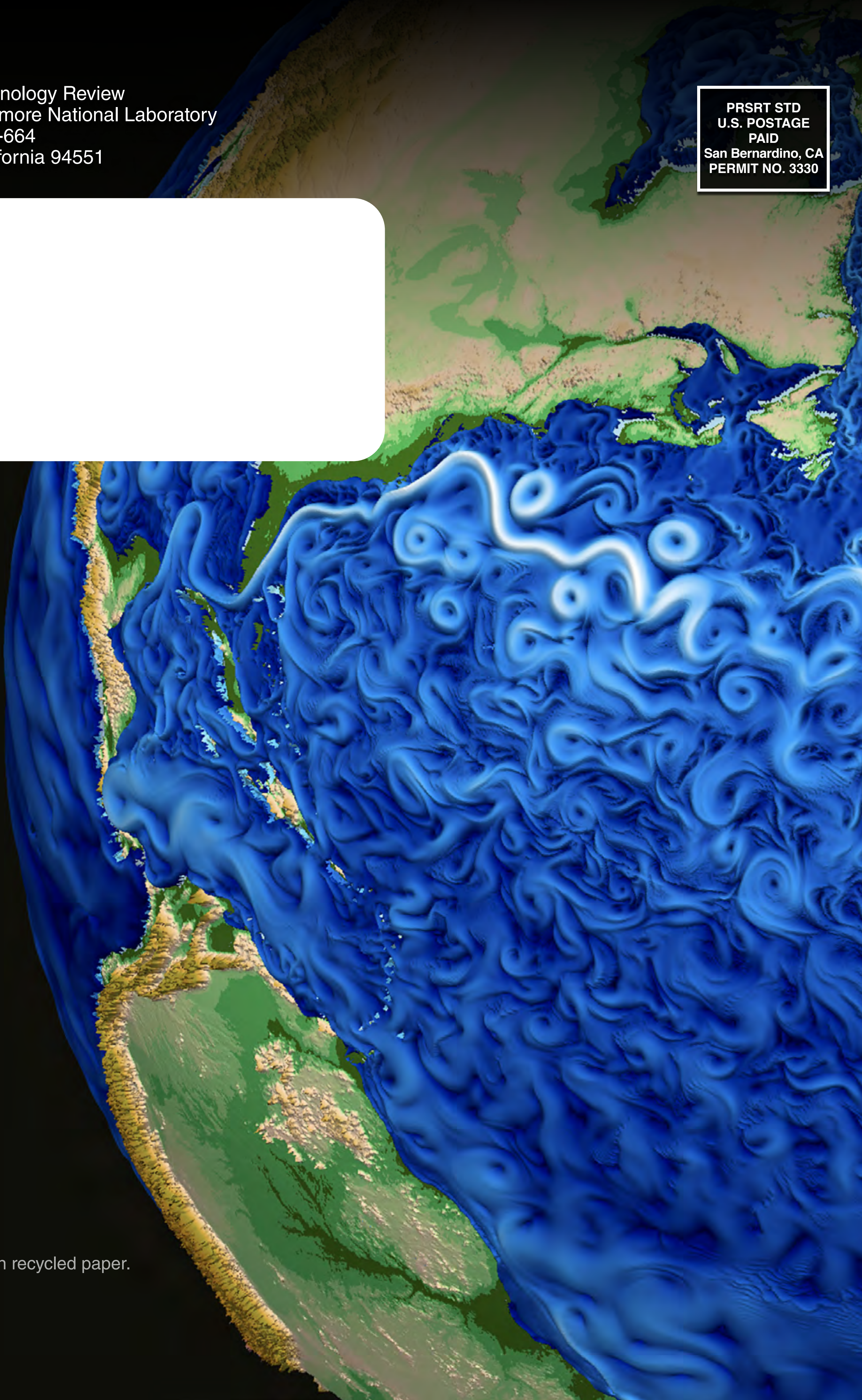

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