

July/August 2022

Science & Technology

REVIEW



AWARDS FOR **LIVERMORE INNOVATION**

Also in this issue:

Simulator for Nuclear Response Training

Exascale Computing Infrastructure

Flexible, Implantable Probes

About the Cover

In 2021, Lawrence Livermore technologies received three R&D 100 awards, which honor the year's top 100 innovations from around the world. The feature article beginning on p. 4 describes the Laboratory's winners: the Multiplicity Counter for Thermal and Fast Neutrons, Flux, and the Optical Transconductance Varistor. The 2021 awards raised the Laboratory's total R&D 100 awards to 173 since 1978. The R&D 100 logo is reprinted in this issue with permission from *R&D World* magazine.



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 (S&TR)* 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 Amentum Environment & Energy, 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' 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) 422-1651. Our e-mail address is str-mail@llnl.gov. *S&TR* is available online at str.llnl.gov.

© 2022. 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.

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.



Prepared by LLNL under contract
DE-AC52-07NA27344

Contents

S&TR Staff

SCIENTIFIC EDITOR

Amanda Askin

MANAGING EDITOR

Mitch Vander Vorst

PUBLICATION EDITOR

Suzanne Storar

WRITERS

Shelby Conn, Lily Forest,
Sheridan Hyland, Elliot Jaffe, Caryn
Meissner, Ann Parker, Genevieve
Sexton, and Stephanie Turza

ART DIRECTOR

Alii Diaz

PROOFREADERS

Caryn Meissner and Deanna Willis

S&TR ONLINE

Jason Barrett, Pam Davis Williams,
and Cyndy Willis-Chun

PRINT COORDINATOR

Chris Brown

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-52000-22-7/8
Distribution Category UC-99
July/August 2022

Feature

3 A Powerful Innovation Ecosystem

Commentary by Elsie Quaite-Randall

4 A Tradition of Excellence in Technology Innovation

Lawrence Livermore earned three 2021 R&D 100 awards in the annual, global competition.

6 Real-Time Detection of Nuclear Threats

An advanced multiplicity counter provides critical real-time data to identify nuclear threats.

8 Optimizing Workflow with Flux

A scalable workflow manager maximizes utilization of computing resources for complex research.

10 Improving the Electrical Grid with the Speed of Light

A light-activated technology significantly improves electricity delivery for smart grid applications.



Research Highlights

12 A Serious Game for Incident Response Training

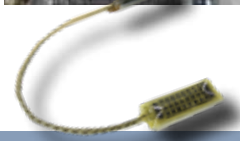
A Livermore-developed interactive simulator provides real-time gamma and neutron data for cutting-edge nuclear emergency response training.

16 Charging Up and Rolling Out

Livermore's Exascale Computing Facility Modernization project team delivered the infrastructure required to bring exascale computing online in 2023.

20 Taking Implantable Microsystems to the Next Level

Flexible probes utilize light and chemical sensors to study and treat conditions of the eyes, ears, and brain.



Departments

2 The Laboratory in the News

24 Patents and Awards

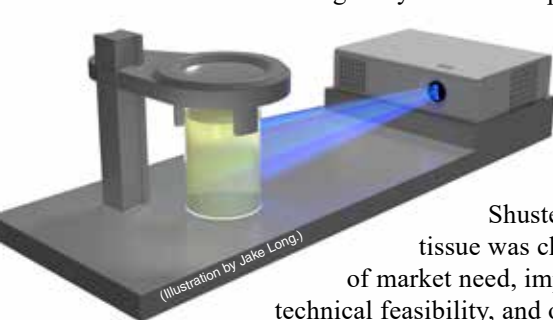
25 Abstract

Printing Materials for Space Applications

NASA is funding a Livermore project to further develop the Laboratory's volumetric additive manufacturing (VAM) printing technology for producing artificial tissues in orbit. Alongside private space and life sciences company Space Tango, Livermore researchers will refine VAM system prototypes specialized to produce artificial cartilage tissue in low gravity.

Departing from traditional 3D printing methods that deposit layer upon layer of material, Livermore's VAM technique forms complete objects at once. Devised jointly with researchers from the University of California at Berkeley, the revolutionary system projects computed tomography (CT) images of an object onto a volume of photosensitive resin. The CT views, obtained by scanning the object to be replicated from all angles, rapidly advance as they are cast onto the rotating container of resin, similar to a video being projected onto a surface (see image below). Sufficient interaction between the resin and incident light causes the resin to solidify into the desired 3D shape.

The fabrication technique is well suited to experiments aboard the International Space Station because the environment eliminates the risk of gravity-caused complications such as



polymer settling and convection flows, allowing for more precise prints than on Earth. Principal investigator Maxim

Shusteff adds, "Cartilage tissue was chosen as a good balance of market need, impact to patients, technical feasibility, and our available expertise."

Similarly, artificial tissues grown in microgravity are expected to exhibit inimitable structural properties, making them valuable medical resources.

Contact: Maxim Shusteff (925) 423-0733 (shusteff1@llnl.gov).

Livermore Supercomputers among Top Performers

Three of Lawrence Livermore's computing systems placed among the 200 highest performing supercomputers worldwide, as announced by Top500 following the International Supercomputing Conference in May 2022. "We're proud to add three machines to the Top500 list of the world's most powerful supercomputers, where we were already well represented," says Chief Technology Officer for Livermore Computing Bronis de Supinski. Lawrence Livermore now claims nine slots among the Top500 list, the most of any U.S. high-performance computing center. Lawrence Livermore's highest ranked system is Sierra at No. 5.

Tested individually, Livermore's lauded systems—rzVernal, Tioga, and Tenaya—will each serve as components for the

National Nuclear Security Administration's (NNSA's) first exascale computer, El Capitan. Garnering the highest rank of the three, rzVernal executed 4.1 petaflops (4.1 quadrillion floating-point operations per second) as measured by the High-Performance Linpack (HPL) benchmark. While no single metric can fully capture a system's design and performance, HPL reflects a machine's ability to solve systems of linear equations served in variably sized batches of problem sets.

These three systems were constructed by Hewlett Packard Enterprise (HPE) and are equipped with state-of-the-art AMD processing units and HPE accelerator blades. Each machine serves as a supercomputing test bed to experiment with hardware combinations, elements of which might later reside within El Capitan. The forthcoming system's unparalleled computing power will aid NNSA affiliate laboratories in carrying out mission-critical research and simulation projects.

Contact: Bronis de Supinski (925) 422-1062 (desupinski1@llnl.gov).

Facility Helps Understand Aging Plutonium

A key part of the nation's nuclear warheads is plutonium "pits." The new plutonium target fabrication facility at Lawrence Livermore will help advance understanding of the physical characteristics of plutonium as it ages, research crucial to maintaining the reliability of the U.S. nuclear deterrent without underground testing. Researchers have developed experiments at the National Ignition Facility (NIF) to help determine plutonium's equation of state (EOS)—the relationship between pressure, temperature, and density—as well as its strength and phase transitions. The results are integrated with data from related experiments at Los Alamos and Sandia national laboratories as part of the National Nuclear Security Administration's science-based Stockpile Stewardship Program.

NIF offers the world's largest and highest energy laser system, creating pressures up to 50 million times Earth's ambient air pressure, and state-of-the-art diagnostics capable of making dynamic measurements of plutonium. "Combined, these unique capabilities are key to exposing plutonium's least known properties," says Heather Whitley, associate program director for High-Energy-Density Science. The new facility is intended to rapidly produce plutonium targets for experiments designed to understand plutonium's EOS under different conditions. Target production must meet precise specifications for dimensions, surface finish, and alignment. The facility will achieve this goal with equipment including diamond-turning lathes and an integrated team of physicists, materials scientists, chemists, engineers, technicians, and machinists. Targets to measure changes in plutonium's crystal structure and strength under pressure are also fabricated at the new facility.

Contact: Heather Whitley (925) 422-1741 (whitley3@llnl.gov).



A Powerful Innovation Ecosystem

In each issue of *Science & Technology Review*, readers learn about Lawrence Livermore research and technologies pushing beyond the state of the art. This issue continues that trend, but with a touch of glitter and gold. The feature article, beginning on p. 4, presents the Laboratory's ongoing success in achieving an industry-wide indicator of innovation excellence: R&D 100 awards. In 2021, Lawrence Livermore received three awards, raising the Laboratory's total awards to 173 over nearly 45 years of participation.

While our mission motivates the range of research conducted at Livermore, awards and recognition confirm that the work done here truly merits the title "innovative." Livermore research is frequently cited in peer-reviewed journals—a mark that our scientific outcomes have broken new ground. Our people receive professional society awards as well. Adding to this list, R&D 100 awards acknowledge Laboratory research nurtured and developed from the earliest stages into devices or software that benefit unique users as well as society as a whole. Beneficial and broad impact is clear for each of our 2021 winners. The Multiplicity Counter for Thermal and Fast Neutrons advances radiation detection technology to better support emergency response to suspected nuclear devices. By optimizing how computing resources are used to solve complex scientific problems, the Flux workflow manager speeds important developments in areas such as effective treatments for disease, among others. The Optical Transconductance Varistor holds the promise to improve electricity delivery on the nation's electrical grid and speed integration of renewable resources into the power mix.

Stepping back to view the success of the Department of Energy (DOE) national laboratory complex as a whole in achieving R&D 100 awards points to the incredible contribution of the enterprise. DOE national laboratories consistently receive approximately one-third of the awards, which are chosen by expert judges reviewing an international pool of industry and research institution nominations. Such consistent outcomes reflect that DOE national laboratories live up to their mission of tackling the critical scientific challenges of our time by translating basic science into innovative applications. The expertise and one-of-a-kind facilities within DOE yield research

that, when developed in partnership with industry and with other academic institutions, address worldwide concerns. The power of DOE's innovation ecosystem to advance federally funded research into beneficial products and services cannot be understated.

The three research highlights in this issue further demonstrate the Laboratory's strengths and ingenuity. The first highlight beginning on p. 12 presents TARANTULA (Tactical Augmented Reality Applications for Nuclear Emergency Support Team Training Using Livermore Analytics), an interactive simulator set to change the course of nuclear emergency response training. Unlike devices that focus on contamination after a nuclear device is detonated, TARANTULA simulates response in seeking and preventing a nuclear explosion and subsequent fallout. The second highlight beginning on p. 16 describes the Laboratory's multiyear project to complete infrastructure upgrades required for exascale computing and the introduction of the El Capitan supercomputer. Livermore teams delivered utility-scale power, sequenced controls, and an energy-saving cooling solution that eliminates traditional chillers. The final highlight starting on p. 20 details implantable probes that reveal never-before-seen views of human brainwaves. Building off a 2009 R&D 100 Award-winning technology, Livermore's latest probes are designed to be uniquely flexible, small, and light weight.

I am delighted to close my commentary with news that reached the Laboratory as this issue went to print: Lawrence Livermore received three 2022 R&D 100 awards for technologies advancing 3D printing and laser science. DOE national laboratories earned 40 R&D 100 awards in 2022 and seven Special Recognition awards, some of which included multilaboratory collaborations. Overall, national laboratory winners offer improvements in clean energy, clean water, spectroscopy, epidemiology, cybersecurity, artificial intelligence, optical sensors, manufacturing, and many other fields. The trend of innovation—at the Laboratory and across the DOE complex—continues.

■ Elsie Quaite-Randall is acting director for the Innovation and Partnerships Office.

A Tradition of **EXCELLENCE** in Technology Innovation

Cutting-edge Livermore technologies have garnered prestigious R&D 100 awards for more than 40 years.

NEARLY 60 years ago, *R&D Magazine*, now called *R&D World*, began recognizing the top 100 technological advances from industry, government, research institutes, and academia that revolutionize the state of the art in a specific field, or have potential to usher in a new one. Before the digital wristwatch, antilock brakes, and high-definition television became household names, they were recognized as R&D 100 winners. Today, the program remains the only industry-wide, international competition that rewards the practical application of science.

Over the years, Lawrence Livermore's track record in the R&D 100 competition has been exceptional, enjoying a 60 percent success rate since 1978, when it earned its first award for diamond machining—a process used to fabricate precision optics. "R&D 100 awards recognize the impact that Livermore

innovation, in collaboration with industry partners, can have on the U.S. economy as well as globally," says Hannah Farquar, a business development executive in the Laboratory's Innovation and Partnerships Office (IPO).

In 2021, the Laboratory added three winners to its roll call. First, Livermore's Multiplicity Counter for Thermal and Fast Neutrons (MC-TF) detects both types of neutrons to help first responders discriminate between special nuclear material and non-special nuclear material in the field—data that informs the emergency response strategy to potential nuclear threats. Next, Flux, a scalable workload management software framework, maximizes the utilization of computing resources through workflow optimization so applications run faster and more efficiently. Finally, the Optical Transconductance Varistor (OTV) is a light-activated, electricity-delivery

control device, which if deployed for the U.S. electrical grid, could save 1 billion kilowatt-hours of electricity and reduce carbon emissions by more than 10 percent. Articles beginning on p. 6 discuss each of these winners in detail.

A Winning Legacy

In the 1980s, Livermore engineered award-winning innovations such as coated diffraction gratings (1989) and a highly dispersive x-ray mirror (1987), among others. A few years later, DYNA3D (1994)—a sophisticated finite element code for analyzing the transient dynamic response of 3D solids and structures—revolutionized crash simulation in the auto industry by accurately predicting vehicle behavior in a collision. In the next decade, Livermore's laser peening system for strengthening metal parts (1998)—marketed as the Lasershot Peening System—made its debut, and the technology continues to be used extensively in the aviation industry for extending the useful life of critical parts, such as airplane fuselages and turbines.

More recently, the Lawrence Livermore Microbial Detection Array (LLMDA, 2017) offered a high-throughput, pan-microbial mechanism for

detecting pathogens. In its commercialized form, the device is used in clinical settings to assess co-infection with other diseases, allowing health care providers to plan more specialized patient treatment options. In 2020, Livermore scientists adapted LLMDA technology to detect COVID-19 during the evolving pandemic.

The Laboratory's technological innovation also extends to software development. Spack (2019), an open-source software package management tool, simplifies and accelerates building, installing, and customizing complex software stacks, and unifies software deployment. Thanks to Spack, thousands of users can share and leverage more than 3,200 scientific software packages.

Livermore's depth and breadth of expertise in wide-ranging disciplines make it a hub for innovative thinking. From the beginning, the Laboratory has stressed the benefit of a multidisciplinary approach to research that has led to many scientific and technological advances. In many cases, Lawrence Livermore also partners with collaborators to enhance exploration and development of new ideas, concepts, and technologies. Indeed, all three R&D 100 winners in 2021 resulted from collaborations with external partners, including another national laboratory, a university, a federal agency, and private companies. These awards also show how products developed in support of the Laboratory's mission have relevance in the marketplace for societal benefit.

Technical Competitiveness

To be eligible for consideration of an R&D 100 Award, the nominated products must have been made commercially available to the marketplace within the previous year. Entry categories include analytical/test, information/electrical, mechanical/materials, process/prototyping, software/services, and other (for technologies falling outside the other groups). Nominees can also submit their entries into five Special Recognition categories—corporate social responsibility; green technology; market disruptor for products; market disruptor for services; and a new category last year, battling COVID-19. A judging panel that includes international technical experts in a range of disciplines reviews and rates each submission. Awards are based on the entry's technical significance, uniqueness, and usefulness compared to competing technologies.

R&D 100 awards captured by Livermore are a testament to the innovative quality of the work done by Livermore's talented and dedicated staff and illustrate how a team approach to research yields significant dividends. Notably, including three recently announced

winners for 2022, Livermore has garnered 176 of these prestigious awards. The Laboratory's success also demonstrates the importance of IPO, which works with Livermore staff and external partners to describe the principal applications and benefits of a new product or technology and transition it successfully to the marketplace. "Lawrence Livermore is a technologically exciting place to work," says Farquar. "In IPO, we get to see the wide breadth of technological diversity and watch innovation move from the lab bench toward industrial and market impact with the support and validation of industry partners." The Laboratory looks forward to the many scientific and technological breakthroughs yet to come as it continues its tradition of excellence in technology innovation.

—Caryn Meissner

2021

**R&D
100**

WINNER

2021

**R&D
100****WINNER**

Real-Time Detection of Nuclear Threats

A 2021 R&D 100 Award-winning detector technology gives first responders a faster, more accurate tool for determining whether an unknown source of radiation contains core materials used in nuclear weapons. The field-deployable Multiplicity Counter for Thermal and Fast Neutrons (MC-TF) rapidly detects, in real time and with high confidence, both fast (high-energy) and thermal (low-energy) neutrons emitted by special nuclear materials (SNM), such as plutonium and uranium. These data are used to determine features of interest,

including the material's type, shape, and size—important data that emergency personnel and decision makers need to develop a response strategy.

Developed by scientists from Lawrence Livermore; Radiation Monitoring Devices, Inc.; the Defense Threat Reduction Agency; and Johns Hopkins Applied Physics Laboratory, the instrument builds off the 2019 R&D 100 Award-winning MC-15 portable neutron multiplicity detector for measuring signals from thermal neutrons. (See *S&TR*, July 2020, pp. 4–5.) MC-15 offered users a smaller, lighter, faster, and more intuitive device compared to conventional multiplicity detectors. MC-TF is an even bigger technological step, utilizing more available components and providing enhanced data at a much faster rate, all of which boost its operational effectiveness.

Better Detection When It Counts

Although other materials emit radiation, SNM is unique in its ability to sustain a fission chain reaction—a self-propagating process in which neutrons emitted from a fission event collide with other nuclei,

which in turn fission and emit more neutrons. The process occurs repeatedly, perpetuating the fission chains.

Livermore physicist Sean Walston, one of the inventors for MC-15 and MC-TF, explains that the neutrons resulting from a fission chain are closely spaced in time and come in bursts separated by gaps, whereas neutrons emitted from non-SNM sources stream out in a steady flow. MC-TF uses this temporal correlation to distinguish between neutrons emitted from the different sources. The MC-TF system records the “timestamp” of each neutron detection event to determine the total number of neutrons produced per fission-chain burst. The data can then be used to estimate the chain length and the rate at which the chains occur to extract features of interest and quantify the magnitude of danger. The pattern of neutron arrival times can reveal the size and shape of the nuclear material as well as the material's composition.

MC-TF offers several advantages over its award-winning predecessor, MC-15. Most notably, it can detect fast neutrons in addition to thermal neutrons. Walston notes, “MC-TF's ability to detect fast neutrons from a fission chain provides the opportunity to witness the chain's evolution, which is a powerful capability for nuclear diagnostics.” The detection medium has also been improved. MC-15 utilizes tubes filled with helium-3 to effectively detect thermal neutrons, leading to an inherently slow response time to fission-chain events. This time



The assembled Multiplicity Counter for Thermal and Fast Neutrons (MC-TF) instrument is about the size of a small suitcase and is modular in construction, allowing it to be scaled up or down, as needed.



Livermore physicist Sean Walston is a co-developer for MC-TF.

is about the size of a small suitcase and is modular in construction, allowing it to be scaled up or down, as needed.

Critical Real-Time Data

The Laboratory developed the algorithm that performs MC-TF's data analysis and detailed source characterization. Conceived in 2013 by Walston, Jim Candy, Neal Snyderman, Dave Chambers, and Hema Chandrasekaran, the On-line Statistical Analysis of Neutron Time Correlation (OSANTC) algorithm estimates the mass and multiplication of SNM given relatively few neutrons.

The technique can be used for fission chains initiated by either a single neutron or by the spontaneous fission of another isotope. In neutron detectors, OSANTC interprets temporal multiplicity information to provide insights about the material being analyzed. The Livermore-developed algorithm is self-calibrating, quantifies uncertainties, and reduces measurement times by as much as a factor of 100.

MC-TF is one of only two instances where the algorithm has been run on the detector itself. OSANTC can operate online, and having it on the detector eliminates the need for multiplicity data to be transmitted to remote personnel for batch analysis. OSANTC also directly estimates MC-TF's detection efficiency from the time-tagged neutron data, rather than relying on human analyses or data gathered from additional "on the scene" neutron detection equipment. Furthermore, OSANTC provides first responders and decision makers with confidence intervals on its estimates of SNM mass and multiplication—a first for this type of detector technology.

The new capabilities provided by MC-TF offer first responders a more advanced technology for quickly assessing in real time and with high confidence the threat level posed by a suspected nuclear weapon. Recognizing the importance of ever-more reliable neutron data, the team is hard at work on further enhancements that will include detection of neutron-capture gamma rays, which can be used as surrogates for thermal neutrons. With MC-TF's ability to detect thermal neutrons, fast neutrons, and gamma rays, first responders facing a potential nuclear threat will have the information they need much more quickly, when it counts.

—Ann Parker

Key Words: MC-15 portable neutron multiplicity detector, Multiplicity Counter for Thermal and Fast Neutrons (MC-TF), neutron, nuclear threat, On-line Statistical Analysis of Neutron Time Correlation (OSANTC) algorithm, R&D 100 Award, special nuclear materials (SNM).

For further information contact Sean Walston (925) 423-7364 (walston2@llnl.gov).

lag is due to the detector's need to wait for the fast neutrons from the fission chain to thermalize—that is, to scatter multiple times until they lose enough energy to become detectable. Another drawback with MC-15 is the gas itself, which is becoming increasingly rare and difficult to obtain. Alternatively, MC-TF detects thermal neutrons with scintillators made from CLYC (cerium-doped cesium lithium yttrium chloride) crystals. For fast neutron detection, the team incorporated stilbene scintillators, enabling MC-TF to detect both slow, thermal neutrons, and fast neutrons in one device.

The MC-TF system contains 90 individual radiation detectors that are evenly split between stilbene and CLYC scintillators. Each detector includes a stilbene or CLYC crystal coupled to a solid silicon photomultiplier array and associated electronics. These improvements allow MC-TF to directly digitize incoming pulses with a timing accuracy of 12 nanoseconds compared to MC-15, which records data in blocks of 100 nanoseconds. The detector is also more portable and adjustable. MC-TF

2021

**R&D
100****WINNER**

Optimizing Workflow with Flux

TODAY'S supercomputers enable researchers to simulate phenomena and investigate data across vast spatial scales—from the smallest atoms to the largest objects in the universe. Scientific applications in the exascale era will grow more diverse and complex as researchers seek to accomplish simultaneous tasks, such as combining large-scale simulations with in situ visualization, data analysis, machine learning, and artificial intelligence. Such efforts create advanced workflows that span not only individual supercomputers but multiple high-performance computing (HPC) clusters to dramatically increase the scale of computation and data analysis.

Resource management and workflow scheduling software help monitor hardware availability and assign access to HPC systems as researchers submit requested jobs, which encapsulate dependent and independent tasks from a workflow. However, traditional resource managers and workflow managers cannot keep pace with increasing system scales

and interplays such as those occurring between multiple compute clusters and file systems nor are they designed to address converged computing, in which HPC and supercomputing sites leverage cloud infrastructure to improve performance, portability, and accessibility of scientific applications. A framework is required to manage resources and complex workflows efficiently and seamlessly while adapting to various operating scales and infrastructure ranging from exascale supercomputers to medium-scale HPC clusters to on-demand cloud platforms.

Honored with a 2021 R&D 100 Award, Flux is a scalable, flexible next-generation workload management framework that meets this need—maximizing resource utilization while allowing scientific applications and workflows to run faster and more efficiently. Developed in collaboration with university partners, Flux also enables new resource types, schedulers, and services to be deployed at data centers as they continue to evolve. Former Livermore

computer scientist and principal investigator for Flux, Dong H. Ahn,

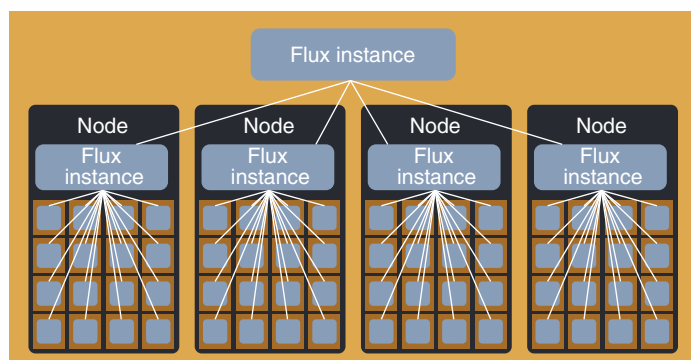
says, “Flux is a low-level piece of software that makes high-level computing possible.”

Beyond State-of-the-Art

Flux's first major advantage over competing technologies is the software's hierarchical approach to resource management and workflow scheduling. Flux breaks down bundled user requests into subtasks and then manages each subtask with an individualized sub-scheduler. For example, a workflow requiring high throughput of many small jobs could submit a larger, longer running parent job and use a specialized scheduler to maximize small sub-job throughput. Higher throughput allows users to run larger job ensembles, generating more simulation data. This hierarchical design allows any workflow to use Flux as a component layer of a larger workflow.

Next, Flux's graph-based scheduling uses directed graphs to model system resources, check states, and manage allocations to manage resources with complex relationships. Users can spin up their own personal Flux instance and fine-tune the Flux scheduler to fit their needs rather than be tied to specific schedules and settings. Becky Springmeyer, Livermore Computing (LC) division leader and Flux project leader, says, “Users benefit from pluggable schedulers with deeper knowledge of network, I/O (input/output), and power interconnections, and the ability to dynamically shape running work.”

Finally, Flux offers portability to different computing environments, particularly



Any Flux instance can spawn child instances to aid in scheduling, launching, and managing complex compute job sequences until the lowest level instance manages a single core.



Development team for Flux: (from top left) Thomas Scogland, Albert Chu, Tapasya Patki, Stephen Herbein, Mark Grondona, Becky Springmeyer, Christopher Moussa, Jim Garlick, Daniel Milroy, Clay England, Michela Taufer, Ryan Day, Dong H. Ahn, Barry Rountree, Zeke Morton, Jae-Seung Yeom, and James Corbett.

new HPC systems with heterogeneous architectures, such as Livermore's upcoming exascale system El Capitan—projected to be the world's most powerful supercomputer when fully deployed in 2023. Workflows can also be enabled on other computing systems, at remote locations, on laptops, and in the cloud. Workflows requiring multiple sites no longer need to code to each site-specific scheduler. Instead, they can rely on Flux to handle the nuances of each site.

Flux was the brainchild of LC systems software experts, who recognized that existing resource managers and workflow managers would not handle the scale and complexity of future HPC systems. The team initiated Flux's foundational project in 2014 and expanded the research to include other researchers from the Laboratory as well as the University of Delaware and the University of Tennessee at Knoxville. Active involvement among researchers, operational specialists, users, and vendors in the design phase ensured a workable framework for both researchers and developers. "We tried to create an environment in which the production side and the research side could talk to each other. A tremendous level of trust exists between the two teams, and they truly understand that they need one another to produce the best possible product," says Springmeyer.

Real-World Applications

Flux has been instrumental to several scientific discovery projects, including efforts geared toward combatting the COVID-19 pandemic. In 2020, to improve understanding of the disease and help develop response strategies, the Department of Energy formed the National Virtual Biotechnology Laboratory (NVBL), a consortium of several national laboratories. NVBL urgently needed computing cycles to model the spread of COVID-19 but did not have time to tailor coding to different schedulers at each supercomputing site. Instead, NVBL researchers used Flux to program their complex workflows and manage the intricacies of running jobs at each site while simplifying site-specific resource managers.

For Livermore's COVID-19 antiviral small molecule project, a multidisciplinary team was tasked with developing a highly scalable, end-to-end drug design workflow to produce potential COVID-19 drug molecules for clinical testing. When creating an end-to-end solution based on the existing components presented workflow limitations, Flux's fully hierarchical framework allowed researchers to overcome scalability issues to continue drug design research. Flux has also been a foundational component of Livermore's Merlin workflow, enabling

machine learning-ready HPC ensembles; the American Heart Association Molecular Screening workflow; and the Laboratory's Autonomous Multi-Scale Strategic Initiative advancing embedded machine learning for smart simulations.

Flux is open-source software available on GitHub that can be used freely by HPC centers, cloud providers, and users around the world. The Flux team continues to harden the framework ahead of widespread production deployment at the Laboratory while adding enhancements to support cloud computing environments such as Kubernetes. Research collaborations with other academic institutions may yield greater improvements, and industry collaborations to develop best practices include Amazon Web Services, IBM, and Red Hat OpenShift. As Ahn says, winning the R&D 100 Award "is just the starting point."

—Stephanie Turza

Key Words: Flux, high-performance computing (HPC), National Virtual Biotechnology Laboratory (NVBL), open-source software, R&D 100 Award, workflow manager.

For further information contact Dan Milroy (925) 424-4419 (milroy1@llnl.gov).



Improving the Electrical Grid with the Speed of Light

TECHNOLOGY improvements and investments for modernizing the nation's electrical grid can help mitigate a multilayered set of challenges that impact both utilities and end users. Planned and unplanned outages and loss of power due to extreme weather events put unnecessary stress on grid infrastructure and utilities. Emergency services, system maintenance, and increased demand from a growing public reliance on electric devices, further adds to the strain. Interactive smart grid technologies sense and respond to energy demands to integrate renewable energy suppliers, speed power restoration after blackouts, and improve grid security. However, smart grid devices such as transistors used in the inverters and breakers that control electricity delivery experience electrical losses and limits to the voltage and current levels they can handle.

A 2021 R&D 100 Award-winning device, co-developed by Livermore engineers and commercial partner Opcondys, Inc., could help address grid reliability. The development team's technology, called the Optical Transconductance Varistor (OTV), maintains higher output power at higher switching speeds—more than 10 times faster—for more efficient grid-scale power conversion than traditional power electronics. By shortening the transition from off to on and vice versa when managing grid demands, OTV can reduce expensive energy losses that also contribute unnecessarily to greenhouse gas emissions.

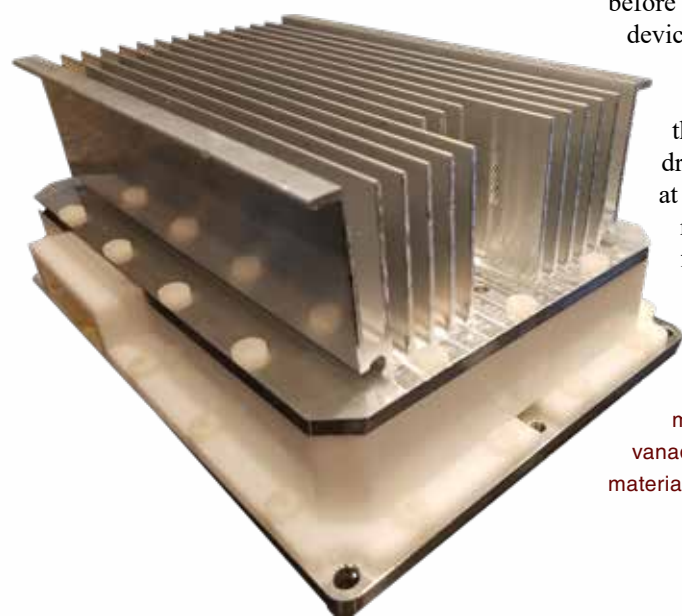
Speed and Resilience

Existing smart grid control technologies rely on the reaction between dissimilar materials to carry a charge for a distance before current can flow through the devices. The longer a device takes to transition from off to on, the more energy is lost to heating within the device. In addition, the voltage drop across the device occurs only at the narrow junction of dissimilar materials, increasing electric field concentration and ultimately

breaking down some materials. For example, typical silicon-based devices are limited to approximately 2,000 volts. Devices using wide bandgap materials (bandgap is a classification based on how different materials conduct electricity) such as silicon carbide (SiC) and gallium nitride (GaN) can handle higher voltages, but only by combining devices in series. Using multiple devices at grid levels adds expense not only in terms of the equipment required, but in the space needed to accommodate a large equipment footprint.

At the heart of the patented OTV design is a bulk piece of vanadium-doped SiC, a wide bandgap semiconductor. A software-controlled laser or LED illuminates the device, exciting electrons in the vanadium dopants within the self-insulating SiC to become instantly conductive and close the switch, delivering voltage. OTV eliminates the semiconductor junction used in existing smart grid devices. Instead, the voltage drops across the entire device, reducing the concentration of the electric field. When the light is removed, the rapid recombination of the carriers opens the switch. The linear response of the OTV to the control light allows for a high level of control over device conductivity and electrical output that is not available from conventional electronics.

OTV's design enables devices to be combined to virtually any voltage and current, reducing the size, weight, and capital cost for smart grid equipment. The simplified design and lack of a junction is expected to translate to a faster and



A 20-kilovolt, 10-amp Optical Transconductance Varistor (OTV) module contains the light source, vanadium-doped silicon carbide switching material, and heat dissipation fins.



Lawrence Livermore team for OTV: (left to right) Brad Hickman, Rebecca Nikolic, Eric Strang, Paulius Grivickas, Steve Hawkins, Peter Thelin, Craig Brooksby, Lisa Wang, Lars Voss, Hoang Nguyen. Opcondys development team for OTV: (inset) Kristin Sampayan (top) and Steve Sampayan (bottom).

less expensive manufacturing process than competitive technologies requiring complex, high-power-consumption manufacturing with less readily available materials. Looking longer term, the reduced cost and manufacturing time and the elimination of additional, stacked devices to achieve grid control could facilitate faster integration of renewable energy resources into the grid, encouraging greater adoption of renewable energy sources such as wind and solar. The design team estimates that, if widely adopted on the grid, OTV could, by 2050, save 1 billion kilowatt-hours of electricity and eliminate 750 tons of greenhouse gases each year.

Switching for the Future

Livermore materials engineer Lars Voss, group leader for High Power Electronics Research in the Materials Engineering division, directs the Laboratory's contributions to OTV. Industry partner Opcondys is moving OTV to the marketplace and exploring other applications. In addition to the technology's importance for energy security, OTV can be applied to human health applications such as air disinfection and medical proton therapy because it can sustain higher voltages than other switches.

The Livermore–Opcondys team has demonstrated OTV's advantages over other high-voltage power switching devices used in grid modernization projects. By supporting higher temperatures and electric fields than the silicon used in metal-oxide-semiconductor field-effect transistors (MOSFETs), the OTV can be a smaller, more efficient device. By operating at more than 30 kilovolts (kV) compared to 10 kV for MOSFETs and 6.5 kV for typical insulated gate bipolar transistors (IGBTs), using OTV reduces the number of devices required in each application to lower capital costs and space requirements. Its significantly faster switching time—10 nanoseconds (ns) compared to 200 ns for MOSFETs and 500 ns for IGBTs—saves electricity costs by reducing energy losses, ultimately reducing greenhouse gas emissions as well.

Voss and his team recently received funding from the Laboratory Directed Research and Development (LDRD) Program to experiment with other ultrawide bandgap materials, such as diamond, which would offer superior optical qualities for OTV. As can be the case with disruptive technologies, adoption does not always come easy. Despite OTV's effectiveness, Voss sees challenges in encouraging stakeholders to choose a

technology that operates differently than traditional devices. The R&D 100 Award recognition and continued LDRD funding may provide future opportunities to discuss OTV applications with potential users.

The R&D 100 Award is an important recognition for Voss and his team, acknowledging the timeliness and importance of this kind of work. "Many people have contributed to OTV, including current and former Livermore scientists and engineers as well as our colleagues at Opcondys," says Voss. "This technology would not have been successful without all of their contributions."

—Lily Forest

Key Words: energy grid, grid modernization, insulated gate bipolar transistor (IGBT), metal-oxide-semiconductor field-effect transistor (MOSFET), R&D 100 Award, ultrawide bandgap material.

For further information contact Lars Voss (925) 423-0069 (voss5@llnl.gov).



A Serious Game for INCIDENT RESPONSE TRAINING

NUCLEAR emergency responders called to a scene involving an unknown radiological device must quickly locate, identify, and defeat the threat using specialized detectors and equipment. To prepare for real-life nuclear incidents and improve operational decision-making, nuclear emergency responders require realistic exercises. Unfortunately, training with nuclear material is logistically challenging, expensive, and can only involve sources that emit low levels of radiation and are carefully prepared and actively monitored to ensure the safety of the participants. The ideal solution to this problem is a new training capability that can simulate high radiation dose events without causing harm to trainees.

To address the need for realistic high-fidelity training, a multidisciplinary team at Lawrence Livermore has worked to establish the new gold standard simulator called TARANTULA (Tactical Augmented Reality Applications for Nuclear Emergency Support Team (NEST) Training using Livermore Analytics). TARANTULA is a scientifically accurate, fully functional, field-deployable simulator that provides an immersive training experience unlike any other. At the technology's core is its ability to calculate and display real-time gamma and neutron data from

virtual radiological sources on simulated handheld detectors for trainees and instructors to use for developing skills and practicing response tactics.

Recognizing the importance of a cost-effective, feature-rich, flexible training capability for the nuclear emergency response community, the Department of Energy (DOE) Office of Nuclear Incident Response has funded a small team of Livermore developers, scientists, and engineers to develop the TARANTULA project since 2019. This new capability is intended to support NEST, which addresses DOE's and the National Nuclear Security Administration's (NNSA's) radiological and nuclear response functions.

Pre-detonation Simulations

As part of the Computing Directorate's Global Security (GS) Computing Applications division, visualization and simulation developer Ryan Chen conceptualized TARANTULA and leads its ongoing development. Chen also created its predecessor, the Radiological Dispersal Device (RDD) Studio, which simulates response to the detonation of an RDD, a so-called "dirty bomb"



(above) This visualization shows a setup of the TARANTULA (Tactical Augmented Reality Applications for NEST (Nuclear Emergency Support Team) Training using Livermore Analytics) augmented reality (AR) platform inside a large warehouse. An array of cameras above the training area tracks a simulated detector using infrared light sources (visually represented by the path of purple lights streaming from the cameras to the markers around the edge of the detector). The simulated item of primary concern (black case) is also marked and tracked by the cameras. The screen in the background provides instructors with a real-time view of everything the trainee sees during the training exercise. (Images by Ryan Chen.)

that combines explosive and radioactive materials with the intent of causing widespread radioactive contamination. RDD Studio tracks the cumulative radiation dose received by simulated first responders in a dirty bomb scenario. The tool uses empirical data collected from real-world explosive tests and a computational fluid dynamic atmospheric dispersion model, provided by the National Atmospheric Release Advisory Center, to simulate a post-blast, radiologically contaminated urban environment to help responders learn to minimize their dose exposure while performing critical lifesaving rescues.

RDD Studio and earlier training tools such as the Radiation Field Training Simulator (RaFTS)—a 2017 R&D 100 Award-winning technology developed by Steve Kreek, former leader of the Laboratory's Nuclear Detection Research Program, and project leader Greg White—focus on RDD post-blast scenarios and responding to environmental contamination following an RDD explosion. (See *S&TR*, April/May 2018, pp.12–13.) TARANTULA takes a different approach. “In contrast to RDD Studio and RaFTS, this new technology simulates radiation from an improvised nuclear device and focuses on pre-detonation scenarios where

responders work to prevent a nuclear device from producing a potential nuclear explosion with fallout debris,” explains Anthony Jackson, GS associate program leader for Render Safe Operations. While RDD Studio deploys virtual responders into a simulated training environment, TARANTULA makes the trainees active participants in the interactive simulation. Chen says, “Our design was born out of the need to provide real-time simulated radiological exposure information to real people as they train in the real world.”

Accounting for Variations

TARANTULA provides an integrated multiplayer training experience across multiple platforms including smartphones, tablets, and augmented reality (AR) and virtual reality (VR) headsets. The ability to simulate real-world detector user interfaces and detector response behaviors from virtual sources on a custom smartphone application allows trainees to exercise their skills in a fundamentally new way.

The project team created the proxy detectors for training by 3D printing handheld enclosures that resemble the look and feel of



Visualizations show the TARANTULA training set up in a remote field (top), office (middle), and warehouse (bottom). Cameras in a circle formation optically track everything inside a space (boundaries indicated in blue) where a trainee holds a detector and walks around the object(s) of interest to locate and determine the nature of the nuclear threat(s). (Images by Ryan Chen.)

a radionuclide identification device. A smartphone, which runs a custom application that displays simulated detector response data for trainees, is embedded into the front of the enclosure to emulate an actual detector's user interface. During a training exercise, simulated radiological data is calculated in real time by the system by using optical tracking data of the virtual radiological source, people, and simulated detectors. Livermore signal processing engineer Karl Nelson established the method for producing this detector-specific data to simulate the behaviors and functions of detectors in the field. In the past, the software that performed real-time gamma calculations was single-threaded, meaning the program was not designed to efficiently provide data to multiple entities, for example, people and detectors, in a real-time application. To address TARANTULA's needs, Nelson developed a new multi-threaded gamma calculation service to replace the older training standard. This capability allows the technology to support dose tracking and simulated detector response for multiple individuals and detectors simultaneously.

Most radiological training tools are limited to identifying gamma radiation alone, but TARANTULA is unique in that it can also support simulated neutron radiation. This capability is essential to support a variety of training scenarios; while some source types may only emit gamma or neutron radiation, others emit both. In addition, understanding how an environment's intervening layers—such as walls or flooring made of wood, brick, concrete, iron, lead, water, or other materials—can affect the way radiation particles move and interact is an important feature. For example, gamma radiation is primarily attenuated and scattered, while neutrons tend to move around as they diffuse, spread, and bounce around a space. Livermore nuclear engineer Bonnie Canion, who developed the technology's neutron simulation component, says, "Interpreting the neutron signature from a source object is key to assessing the threat, particularly for those involving special nuclear material. The neutrons provide information about whether an item is a criticality concern or if it is suspected to have high explosives in conjunction with nuclear material."

TARANTULA can calculate real-time gamma and neutron exposure rates based on a room's dimensions, intervening layers, and even the orientation of the detector relative to the radiological material. To perform these calculations, optical tracking cameras are stationed above the training area to track the location and distance of the simulated radiation source from the handheld detector, the trainees, intervening layers, and any other equipment in the training environment. These cameras use submillimeter-accurate optical tracking technology to capture 120 to 240 frames per second—the same motion capture technology used in video games, television shows, and movies. Chen says, "The simulation is so realistic because we can perform context-specific calculations in real time and account for variations and changes in the real world. As the scenario evolves, we can continue to simulate the



detector's response in real time, even if the source's location is adjusted or intervening layers are added or removed."

Unlimited Possibilities

The TARANTULA program is completely customizable and can support both single player and multiplayer-multidetector training. The technology's flexible and interactive design will provide the nuclear emergency response community with an unlimited number of training scenarios for years to come.

Training can be conducted in a large room, a warehouse, or outside in a remote field. Along with simulated detectors, TARANTULA provides an AR experience for instructors to watch on a tablet device where real-time information such as dose rate and total accumulated dose of trainees are superimposed on the real-world view of the participants. "The system records individual trainee performance and produces video and data files for after-action reports and post-training analysis," says Jackson. "This feature provides trainees with the opportunity to replay their simulations, receive feedback from their trainer, and improve their nuclear response skills." The emphasis on providing enhanced real-time situational awareness during training exercises, as well as additional material for classroom discussions, is all designed to give students the best training experience possible. What TARANTULA provides is a significant leap forward from current training methods that rely on verbal announcements read from pre-calculated datasheets on a clipboard.

More advanced AR tools are in development, as are VR applications enabling individuals or a team of responders to train in their offices, classrooms, or homes. Since the COVID-19 lockdown in early 2020, and a shift to remote work practices, Chen's team has started developing a custom application to support high-quality

During a TARANTULA training exercise, a tablet application provides instructors with an AR experience of the live simulation. The black case contains the simulated radiological source, and the superimposed circles represent a handheld detector's reported radiation dose rates as the trainee moves around the training area. (Image by Ryan Chen.)

training through teleconferencing. In these tabletop exercises, trainees observe virtual responders in a lifelike simulated environment as they discuss tactics, make choices, and study the outcomes and consequences of their decisions.

Laboratory researchers continue to expand on the technology's capabilities, working with DOE and NNSA partners to help inform and prepare the nation's emergency responders to recognize, understand, and appropriately address nuclear and radiological threats. In support of these efforts and to encourage hands-on training opportunities among all sponsors, stakeholders, and potential end users, the team plans to build new TARANTULA-supported training facilities at Lawrence Livermore and other federal sites. "The community has desired a solution such as TARANTULA for a long time, and we aim to deliver on this need," says Chen.

—Shelby Conn

Key Words: augmented reality (AR), detector, gamma radiation, neutron radiation, Nuclear Emergency Support Team (NEST), nuclear incident, optical tracking, pre-detonation, Radiological Dispersal Device (RDD) Studio, simulator, TARANTULA (Tactical Augmented Reality Applications for NEST Training using Livermore Analytics), threats, training, virtual reality (VR).

For further information contact Ryan Chen (925) 423-0360 (chen74@llnl.gov).



Charging Up AND ROLLING OUT

LAURENCE Livermore's El Capitan supercomputer will come online in early 2023 with a peak performance of more than 2.0 exaflops (2 quintillion floating-point operations per second). The massive computing capabilities of El Capitan and anticipated follow-on computing systems will require correspondingly massive infrastructure, cooling, and power. In response, the Laboratory's Exascale Computing Facility Modernization (ECFM) project team has planned, designed, and executed a project to nearly double the power available for computing systems.

Providing a dedicated utility-power electrical substation and cooling towers to add 40 megawatts (MW) to the 45 MW capacity already allotted to high-performance computing (HPC) required multilevel government approval, stakeholder coordination including state and local governments as well as local constituents, partnerships with local and regional utilities providers, and strategies to stay on schedule despite the COVID-19 pandemic and supply chain delays. In a testament to the team's creative thinking, innovative problem solving, and exceptional collaboration, the ECFM project proceeded ahead of schedule and the team met its delivery goals.

(above) Lawrence Livermore's Exascale Computing Facility Modernization (ECFM) project management team ensured that the project stayed on task and on budget. Brandon Hong, Chris Deprater, and Bradley Davis (from left to right) played a critical role in leading the project's implementation, coordinating the many logistics involved, and overcoming the obstacles and challenges that the project faced in the past several years. (Anna Maria Bailey and other project team members not pictured.) (below right) The ECFM project under construction.

Designing for the Future

Long-term planning was vital for a project of this size and scope, and Livermore began preparing for El Capitan's needs in 2004 to ensure site infrastructure would support Livermore's HPC needs. Anna Maria Bailey, program manager for the ECFM project, says, "We understood immediately that the industrial-scale power supply of 13.8 kilovolts (kV) used at Livermore would be insufficient for future HPC needs and that the project would have to upgrade to utility-scale power of 115 kilovolts."

To transition to utility-scale, Livermore embarked on an extensive, phased Critical Decision process in alignment with

Department of Energy (DOE) requirements. The ECFM project cleared three major rounds of DOE approval—mission need, alternative selection and cost range, and performance baseline—before construction could even begin. A utility facility study, site impact study, and environmental impact review were also required by DOE. While similar studies typically take upwards of two years, coordination with utility providers such as the Western Area Power Administration (WAPA), Pacific Gas and Electric, and Hetch Hetchy Water and Power enabled Livermore to complete the studies in half the usual time.

Bailey describes the ramp up to the approval process as intense. “When we started design, project management resources familiar with similar construction projects, such as the Livermore Computing Center, had moved on to other roles or projects at the Laboratory,” she says. “Fortunately, our senior leadership recognized just how critical this project would be for the Laboratory’s mission, and we were able to draw on experienced people in other areas of the Laboratory, bring people back from retirement to help with project controls and risk assessments, and hire new staff to increase our capability.”

The project included design of transmission lines, core-type transformers, cooling towers, and pumps as well as intricate control features hidden from view. Bailey says, “Since we’re operating at utility-scale power to meet the Exascale Computing Facility’s needs, we’ve moved beyond localized electrical controls and data acquisition systems. The large relays and controls we have in place for this facility must be timed and programmed

for the right electrical sequencing.” Checks and balances ensure efficient, safe, and steady energy distribution. For example, WAPA operates the 115 kV tie line feeding the electrical substation, enabling the system to automatically carry and transfer the load between two power sources while maintaining the transformer’s connection to the load. Brandon Hong, systems engineer, says, “Controls are critical for this project. The power will be distributed to a larger sector of the California Independent System Operator grid. Any power swings will be noticed at the utility grid level, not just the Laboratory’s 13.8-kilovolt grid level.”

The cooling system provides an additional 18,000 tons of cooling capacity and incorporates controls including multiple fail safes, function checks, and sequencing. Sensors, control relays, and switches integrated into the Laboratory’s existing building management system adjust to a variety of load conditions. Newer sensors in the control systems create the opportunity to move toward condition-based maintenance, saving future labor costs.

The system is designed to operate without the use of chillers. Instead, water supplied at a temperature typically between 24 and 29 °C flows through cooling distribution units rather than directly to machines. Even if water temperatures rose due to environmental conditions, the system will operate—without chillers—within the American Society of Heating, Refrigeration, and Air Conditioning Engineers’ guidelines for the W32/W40 (between 32 and 40 °C) classification. By eliminating traditional chillers, the new system will save more than 60,000 MW hours annually to meet sustainability and energy efficiency goals.





In March 2020, the site for the substation and cooling towers serving the Exascale Computing Facility had only just been cleared and prepared for construction.

Construction...and COVID

The start of construction signaled that the approval stage was complete and potential planning and design challenges had been overcome. At the same time, the team appreciated the gargantuan task ahead. Bradley Davis, deputy project manager for the ECFM project, says, “We basically combined five large projects to support the facility—the transmission lines, substation, cooling towers, processing cooling loop that brings water to and from the building, and the power distribution.” To meet the production scope, the team added four construction managers and two project managers to keep the work on task, on time, and on budget.

Construction began in 2020 and was almost immediately impacted by the COVID-19 pandemic. Hong says, “The procurement process alone was a whole different beast with long lead times for absolutely everything we needed due to supply chain delays.” The ECFM project team also encountered equipment delivery challenges. One piece of equipment was so large, California Highway Patrol coordination and support was required for transport from southern California to the Laboratory. In another case, a cooling tower change sent the team back through the

procurement process midstream. Systems engineer Chris Deprater says, “We had to switch to a completely new cooling tower design with different specifications and sequence of operations because the original vendor could not meet the required California structural code standards. On top of that, we needed to continue operating within the same schedule, no delays.”

Workers’ health and safety requirements ramped up as the construction managers developed and implemented an effective COVID-19 plan with protocols such as mask wearing, social distancing, and communication by hand signal in close quarters. Bailey says, “The construction management team treated COVID-19 as another potential job hazard that required careful planning. They met the challenge with excellent handling of the additional safety measures. While we saw some cases of COVID-19 among the construction workers, we were able to mitigate rapid spread by quarantining where necessary, bringing additional crews onsite as needed, and staggering the different tasks around discrete areas.”

COVID-related travel restrictions also posed significant challenges for specialty contractors traveling to and working at the

A little more than a year into construction, the new cooling towers and pump system had been built, and work to install the electrical substation progressed.





project site. Bailey says, “These contractors are one-in-a-million subject matter experts. Most people aren’t putting in a substation every day. We partnered with an expert team in extremely high demand to do the utility-scale work.” When the specialty contractors were inadvertently exposed to COVID-19 during the 2020 holiday season, the ECFM project management team had to revisit its safety controls to find alternative solutions. As a result, people who did not need to be onsite were asked to work remotely, and Livermore provided a COVID coach to work with contractors to ensure updated safety plans were feasible and effective.

Looking to the Future

Despite the construction challenges, the ECFM project team not only met project demands but stayed ahead of schedule. Deprater credits the team and creative problem solving. “No one on the team took ‘can’t’ for an answer,” he says. Hong adds, “We found another solution or a creative, innovative work-around to every obstacle. We planned far enough in advance to provide float when we needed it. In addition, Anna Maria (Bailey) knew every step of the project, how much time it would take, and how early we had to act to make things happen. She was a real asset.”

Although El Capitan has not yet come online, Livermore Computing and the project management team are looking ahead to future, more demanding power, cooling, and infrastructure needs. Ever-advancing HPC capabilities are at the heart of Lawrence Livermore’s stockpile stewardship mission, and efforts to advance supercomputing capabilities are a critical priority. (See *S&TR*, September 2016, pp. 5–11.) The Laboratory has already

By February 2022, construction on the substation, cooling towers, and pump system was largely completed, and the ECFM project shifted focus to ensuring the systems inside the Exascale Computing Facility would be ready for El Capitan’s deployment.

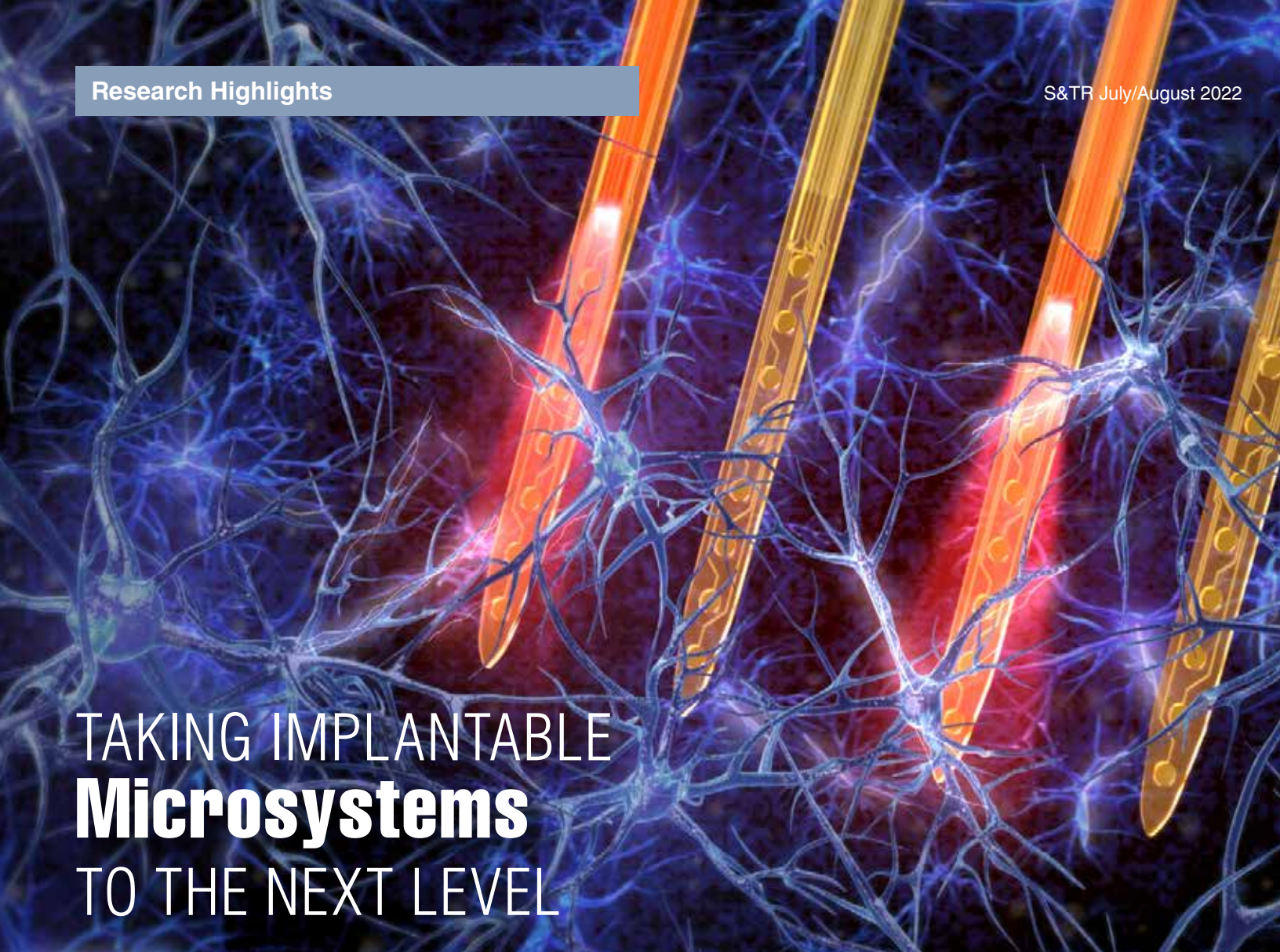
started planning for the next supercomputer, labeled Advanced Technology System 6 (ATS6), and will initiate procurement in a few years. The team’s forward-looking strategic planning to anticipate enduring and growing needs ensures that ATS6 will be able to take advantage of the same infrastructure put in place through the ECFM project.

Moving forward, Bailey emphasizes the ongoing demand for infrastructure growth. “Right now, in addition to the new ECFM transformer lineup, we have three main transformers tied in parallel as the base load for the Laboratory,” she says. “When you consider the potential power and cooling demand of future supercomputers, we will need to add capacity to the entire site. New innovations will be needed. For now, we will meet the expected HPC load for another 10 years.”

– Sheridan Hyland

Key Words: Advanced Technology System 6 (ATS6), Critical Decision, El Capitan supercomputer, exaflop, Exascale Computing Facility Modernization (ECFM) project, high-performance computing (HPC), Livermore Computing.

For further information contact Anna Maria Bailey (925) 423-1288 (bailey31@llnl.gov).



TAKING IMPLANTABLE **Microsystems** TO THE NEXT LEVEL

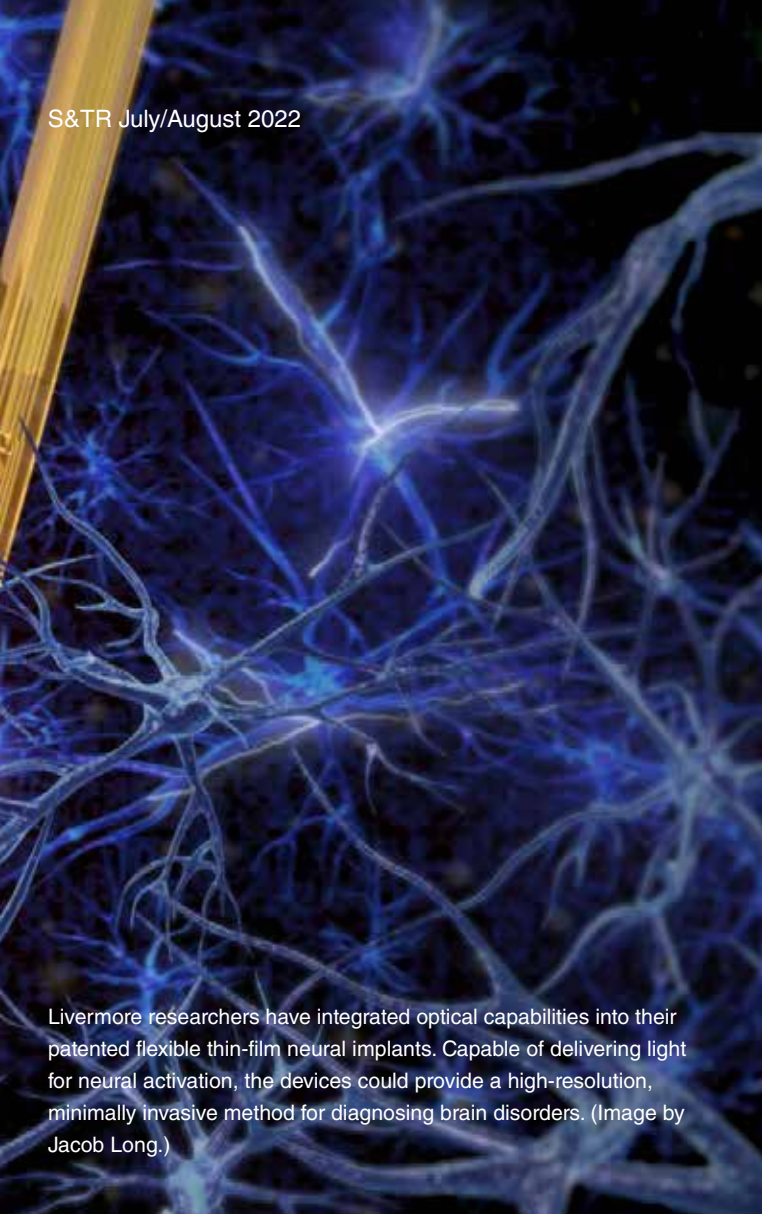
IN 2021, using a flexible thin-film microelectrode array developed by scientists and engineers at Lawrence Livermore's Center for Bioengineering, medical researchers at the University of California at San Francisco, observed a never-before-seen view of how the brain's signals move in a human subject. The high-density grid layout, small size, and ability to conform to the brain's surface offered by the Livermore-developed technology enabled the team to see, for the first time, bi-directional brainwaves traveling across the hippocampi of patients.

Artificial retina technology, developed in the 2000s at Livermore with partners from other national laboratories, universities, and the private sector, served as a very early precursor to making this discovery possible. Components of this earlier project—a patented thin-film array containing electrodes, an implantable hermetically sealed package, and a surgical tool for placing the array—restored basic vision via a miniature video camera embedded in eyeglasses and an electronic imaging system implanted within the eye. This invention was the first Food and Drug Administration–approved retinal prosthesis for individuals with end-stage retinitis pigmentosa and won a 2009 R&D 100 Award in addition to innovation accolades from *Time*

and *Popular Science* in 2013. Expanding on this foundational work, recent versions of the Livermore microelectrode array have pushed the limits of existing technology. These examples—the latest versions of the device type involved in the 2021 findings—are poised to help collaborating researchers make more breakthrough discoveries about the brain's complexities.

Using Light Instead of Electrons

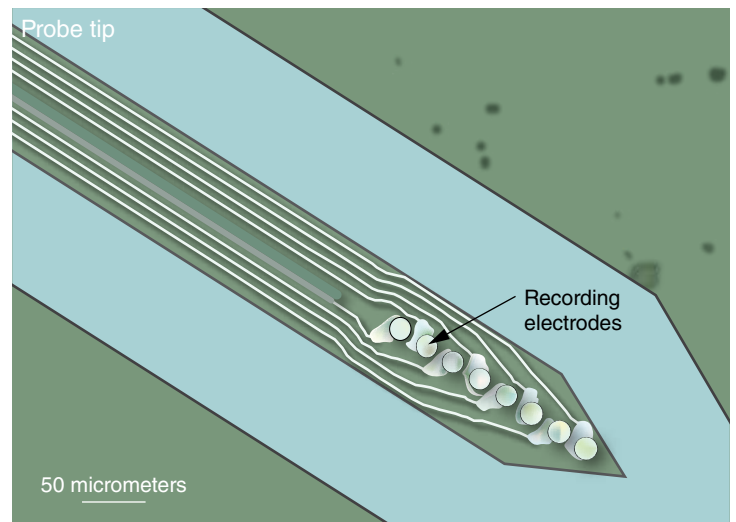
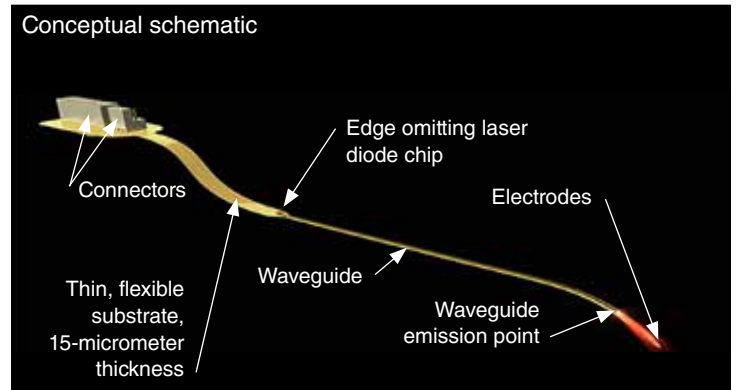
Livermore's first optical implantable devices are built on a novel platform called POEMS, for polymeric opto-electro-mechanical systems. POEMS integrates optical waveguiding capabilities with the previously patented flexible electrode platform technology—a Laboratory first. Using light to activate neurons instead of electrons, these devices could one day be used for high-resolution, minimally invasive therapeutics. "Researchers need better spatial precision and real-time monitoring over long periods of time to study the brain," says Razi Haque, Implantable Microsystems group leader. "With the Laboratory's additive manufacturing and microfabrication expertise and resources, we identified a combination of materials and a design configuration to develop a neural interface that combines optical and electrical capabilities into a single device." POEMS'



Livermore researchers have integrated optical capabilities into their patented flexible thin-film neural implants. Capable of delivering light for neural activation, the devices could provide a high-resolution, minimally invasive method for diagnosing brain disorders. (Image by Jacob Long.)

waveguides can be used for optical delivery or sensing and imaging. The National Institute on Deafness and Other Communication Disorders (NIDCD), part of the National Institutes of Health, and the Laboratory Directed Research and Development (LDRD) Program funded the team's work.

Previous polymer-based implantable waveguides performed poorly compared to waveguides made of rigid materials such as glass. Their reduced optical transparency resulted in increased power levels, hindering use in the brain where minute temperature increases could damage sensitive tissue. Combining recent developments in polymer additive manufacturing with the Laboratory's thin-film neural interface advancements, researchers incorporated hybrid polymer-based, microscale waveguides onto flexible polyimide substrates. The hybrid polymers offer both polymerlike flexibility and glasslike transparency, making them more suitable for optical implantable microsystems. The resulting waveguides are more optically transparent than conventional polymers while also remaining flexible. POEMS-based neural interfaces cause less damage to surrounding tissue over time than rigid glass waveguides or silicon neural implants, enabling researchers to conduct longer term animal studies. In vitro testing



The POEMS (polymeric opto-electro-mechanical systems) neural interface and components, pictured in a schematic (top), provide a compact, implantable option for brain function research. Details of the probe shank and implantable area are pictured (center). The middle of the probe tip (bottom) includes a waveguide emission site and platinum iridium recording electrodes. (Reprinted from *Materials Letters*.)

of the hybrid polymers indicates reduced degradation of the waveguide compared to the conventional polymer waveguides. “We engineered a solution that instantly expands the capabilities of our neural probes without negatively impacting our core technology foundation,” says Haque. “Our work also leverages the Laboratory’s Biomedical Foundry, within the Center for Micro and Nanotechnologies clean room, which is capable of building human-grade implants.”

A Better Cochlear Implant

More than one million severely to profoundly deaf individuals have received a cochlear implant (CI) to restore some of their hearing. However, CI performance varies due to poor frequency discrimination and limited frequency range, making the devices less effective in noisy environments. An advanced CI, manufactured using techniques developed in the Biomedical Foundry, could help overcome these challenges and bring down the significant cost of commercial CIs.

Recent research indicates that the cochlea may be stimulated with light as well as electrical signals, possibly sending the right signal more precisely to the cochlea. This approach would provide greater control across the spectrum of sound frequencies compared to adding acoustic channels. “An optical cochlear

implant that transmits light into the cochlea and produces a high-definition hearing response is next-generation technology,” says Haque. “While we don’t know if this approach will perform better than existing devices, we are working with collaborators who can conduct the studies necessary to determine the potential of this new technology.”

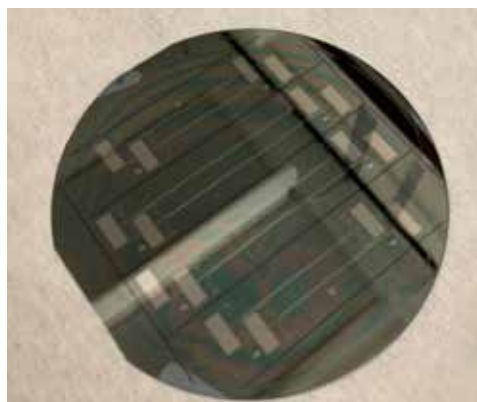
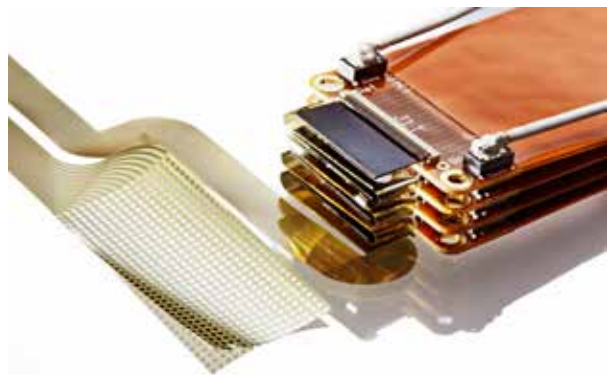
Researchers in Haque’s group are also developing an open-source CI design, with support from NIDCD, consisting of a 32-electrode array, the required custom electronics in a behind-the-ear package that controls and powers the implant, and accompanying software. In consultation with a scientific advisory panel, the group will support the hearing research community and related commercial sector in using the specifications to develop standardized hardware and algorithms for stimulation coding to improve the overall design and function of the device. The team is also working to make better, more affordable CIs by replacing the manual production process for traditional CIs with microlithography.

High-Resolution Neural Interfaces

Research staff engineer Travis Massey aims to further extend the Implantable Microsystem group’s efforts by increasing an array’s electrode channel count and the number of electrodes within a given



Added flexibility of the latest Livermore-developed thin-film arrays helps the electrode better conform to the brain's cortex, establishing more intimate contact between the brain and the array so neural activity is more readily transmitted.



A 512-channel array (left) electrically records speech activity from the surface of the brain to decode the fundamental building blocks of spoken language. Time to test this array has been reduced from days to hours through the team's automated process. Carbon nanotube electrodes are incorporated into prototype devices (right) to enable detection of a wider variety of neurotransmitters.

brain volume or area. Scaling channel count and density requires developing a new nanofabrication process leveraging Livermore's electron-beam lithography capability. Massey says, "We must also address how we handle, amplify, and digitize 1,000 or even 10,000 signals. Part of that challenge is physically getting the signals to the electronics. Either we need a compact thousand- or ten-thousand-channel connector, which doesn't yet exist, or we integrate a microchip directly into the probe."

Another consequence of increasing spatial density to accommodate the increased channel count is crosstalk between the channels that must be managed through careful design and modeling. Electromagnetic interference (EMI) from the noisy operating room environment and sterilization process present a related challenge that Massey has mitigated by developing integrated electromagnetic shielding and a compatible, conductive fabric wrap, or Faraday cage. Massey's solution was presented at the 2022 Neuroelectrical Interfaces Gordon Research Seminar. Both EMI and crosstalk are also alleviated by digitizing the signals as closely to the brain as possible.

Rigorous testing ensures electrode arrays function properly before they are implanted in animals or in humans. Electrochemically testing 1,000 to 10,000 channels can take days or weeks, but Massey has developed an automated process. "We reduced the time to test a 512-channel array from days to hours," says Massey. "By parallelizing this automated testing, which is still a work in progress, we will be able to further reduce the time by a factor of 1,000. What would have once taken a month, even multiplexed, will someday take less than an hour per device."

Sensing Brain Chemistry

Detecting and quantifying chemical neurotransmitters in the brain's complex signaling system requires modifying the Livermore microelectrode array to measure chemical signals. (See *S&TR*, November 2016, pp. 16–19.) Adding chemical sensors onto the electrodes enables sensing modalities that can provide neuroscientists and other researchers with insight into brain functionality beyond electrophysical signals alone.

Research staff engineer Allison Yorita is developing microfabrication processes with a team of Livermore researchers she led under a separate LDRD-funded effort. The earlier work integrated carbon nanotubes onto the existing Livermore flexible microelectrode

array as an electrode material to enable detection of a wider variety of neurotransmitters. "The polyimide substrate would degrade at the 700 °C temperatures required to grow carbon nanotubes, so we determined how to grow them before any polyimide was introduced into the fabrication process," says Yorita. "In our 'bottom up' approach, we grow carbon nanotubes on a silicon carrier wafer first. Then we deposit, pattern, and etch the remaining materials that comprise our polymer probes."

Yorita sees enormous potential as applications for the team's technology expand. "I'm interested in observing other parts of the body, such as the spinal cord or interstitial fluid, to monitor what's happening chemically, in real time, for biodefense applications. Detecting minute chemical changes in the body now may indicate potentially harmful physiological effects that would present later and point to earlier deployment of possible treatments and therapeutics for improved prognosis."

The Laboratory's unique capabilities and infrastructure combined with resources at the Biomedical Foundry enable the design and fabrication of medical-grade devices and circuits at microscale with fine-grained control all within a Quality Management System (QMS). The Foundry's next step is accreditation in alignment with International Organization for Standardization 13485 for medical device prototyping. "We're one of the few institutions in the nation with a QMS for microfabricated medical devices, and we are working hard towards accreditation. We're committed to maintaining this level of excellence and developing the foundry's capabilities even further," says Haque.

"With growing interest from the scientific community in how these technologies can best be leveraged to better understand the brain and human body, our team stands at an exciting time in implantables research," says Yorita. Adds Massey, "Core Laboratory technological competencies are opening therapeutic avenues that could be life altering for millions of people."

—Genevieve Sexton

Key Words: artificial retina, cochlear implant (CI), Laboratory Directed Research and Development (LDRD) Program, microelectrode, microlithography, neural interface, POEMS (polymeric opto-electro-mechanical systems), polymer waveguide.

For further information contact Razi Haque (925) 422-1172 (haque3@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

Differential Holography

Frank Ravizza

U.S. Patent 11,215,951 B2

January 4, 2022

Burst-Mode Chirped Pulse Amplification Method

Jeffrey D. Bude, David A. Alessi, Maurice B. Aufderheide, John E. Heebner, Andreas J. Kemp, Otto L. Landen, Andrew J. Mackinnon, Raluca A. Negres, Craig W. Siders, Scott C. Wilks, Wade H. Williams, Steven T. Yang, Thomas M. Spinka

U.S. Patent 11,222,734 B2

January 11, 2022

Engineered Microbes for Rare Earth Element Absorption

Yongqin Jiao, Dan McFarland Park, Mimi Cho Young, David W. Reed

U.S. Patent 11,230,750 B2

January 25, 2022

Wavelength Selective Filtering with Non-Radial Array of Microstructure Elements

Leily S. Kiani, Jay W. Dawson, Derrek R. Drachenberg, Michael J. Messerly, Paul H. Pax

U.S. Patent 11,269,137 B2

March 8, 2022

Optical Authentication of Images

Maxwell R. Murialdo, Brian Giera, Brian M. Howell, Robert M. Panas

U.S. Patent 11,271,747 B2

March 8, 2022

Metal-Overcoated Grating and Method

Hoang Nguyen, Jerald Britten

U.S. Patent 11,333,807 B2

May 17, 2022

Non-Circular Optical Fiber and Mode Shape Converter and Method

Derrek R. Drachenburg, Graham S. Allen, Diana C. Chen, Matthew J. Cook, Robert P. Crist, Jay W. Dawson, Leily S. Kiani, Michael J. Messerly, Paul H. Pax, Nick Schenkel, Charles X. Yu

U.S. Patent 11,340,396 B2

May 24, 2022

Mechanical Reticulation of Polymeric-Based Closed Cell Foams

Jennifer N. Rodriguez, Duncan J. Maitland, Thomas S. Wilson

U.S. Patent 11,345,067 B2

May 31, 2022

Emulsion Stereolithography and 3D Printing of Multimaterials and Nanoscale Material Gradients

Xiaoyu Zheng, Joshua R. Deotte

U.S. Patent 11,345,879 B2

May 31, 2022

Parallelized Multiple Nozzle System and Method to Produce Layered Droplets and Fibers for Microencapsulation

Congwang Ye, Julie A. Mancini, Kevin Scott Paulsen, William Smith

U.S. Patent 11,351,514 B2

June 7, 2022

Awards

The **Department of Energy (DOE) Project Leader Institute (PLI)** selected Livermore scientists **Lara Leininger** and **Al Churby** as 2022 cohort members based on project performance and technical program leadership. Leininger leads an array of projects as the Laboratory's Energetic Materials Center director and has led multi-institutional research in high-energy-density physics and explosives. Churby heads Livermore's contribution to the Advanced Sources and Detectors project, a joint effort of DOE and the National Nuclear Security Administration to achieve next-generation x-ray images of subcritical experiments. PLI participants undertake DOE-administered leadership training with instructional resources from Stanford University.

Principal Associate Director for Global Security **Huban Gowadia** was inducted into the 2022 **State of Alabama Engineering Hall of Fame**. Gowadia earned a bachelor's degree in aerospace engineering from the University of Alabama and a doctorate in mechanical engineering from Pennsylvania State University. Gowadia served as acting administrator of the Transportation Security Administration before joining the Laboratory in 2018. Now heading Livermore's Global Security principal directorate, Gowadia manages intelligence, cybersecurity, nonproliferation, and counterterrorism programs with more than 1,200 matrixed employees.

Livermore scientists were inducted into the Laboratory's **Entrepreneurs' Hall of Fame**, recognizing research that generated significant economic impact and new enterprise. Materials researcher **Natalia Zaitseva** developed rapid crystal growth methods for optical components critical to National Ignition Facility operations and crystalline structures used in radiation detection. Physicist **Mary Spaeth** developed and applied tunable dye lasers to produce enriched uranium, a process the U.S. Enrichment Corporation acquired. Physicist **Tony Ruggiero** founded Sierra Photonics, later acquired by Google, based on his work in free-space optical communication with ultrahigh bandwidth lasers.

Employees in Lawrence Livermore's Innovation and Partnerships Office (IPO) were recognized by the **Department of Energy's Technology Transfer Working Group**. IPO business development executive **Annamarie Meike** received the **Innovative Lab Technology Transfer** award for her work securing collaboration between Livermore and science and technology company Millipore Sigma to commercialize next-generation inks for printed device construction. Digital Assets Coordinator **Mary Holden-Sanchez** garnered a **Best in Class** licensing award for her work on Livermore's Numerical Electromagnetic Code Antenna Modeling Software, Livermore's most licensed software to date.

A Tradition of Excellence in Technology Innovation

Lawrence Livermore earned three 2021 R&D 100 awards, building on the Laboratory's strong track record in the nearly 60-year-old competition. Winners include the Multiplicity Counter for Thermal and Fast Neutrons, a neutron detector supporting emergency response; Flux, a workload management framework enabling complex computing workflows; and the Optical Transconductance Varistor, a light-activated control device for electricity delivery on the nation's grid. R&D 100 awards, selected by *R&D World* magazine, recognize the top 100 technological advances of the year. The diversity of projects honored in 2021 reflect the Laboratory's broad research impact and its commitment to collaborative work with partners from other national laboratories, universities, federal agencies, and private companies.

Contacts: Sean Walston (925) 423-7364 (walston2@llnl.gov),

Dan Milroy (925) 424-4419 (milroy1@llnl.gov), and

Lars Voss (925) 423-0069 (voss5@llnl.gov).

W87-1 Modification Program



Lawrence Livermore will deliver the first newly manufactured warhead in three decades—transforming the nuclear security enterprise through innovative collaborations in the process.

Also in this upcoming issue...

- *Strategic latency anticipates how emergent technologies might impact national security.*
- *Discovery Science Program experiments reveal iron's properties under extreme conditions.*
- *A new 3D printing technique supports microbial characterization and function.*

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

PRSRT STD
U.S. POSTAGE
PAID
San Bernardino, CA
PERMIT NO. 3330



Printed on recycled paper.