Lawrence Livermore National Laboratory

September 2022

Science & Technology REVIEW

Cognitive Simulation

Also in this issue:

Global Material Security Program

High Performance Storage System

X-ray Radiographic Movies

About the Cover

Computer modeling is essential to scientific research. Models simulate natural phenomena to aid scientists in understanding their underlying principles. While the most complex models running on supercomputers may contain millions of lines of code and generate billions of data points, models never simulate reality perfectly. Experiments—in contrast—have been fundamental to the study of natural phenomena from science's earliest days. However, some of today's complex experiments generate too much data for the human mind to interpret. This issue's cover illustrates the researcher's dilemma of processing massive data sets. As the article beginning on p. 4 describes, cognitive simulation unites theory, modeling, and experimentation to solve complex problems.

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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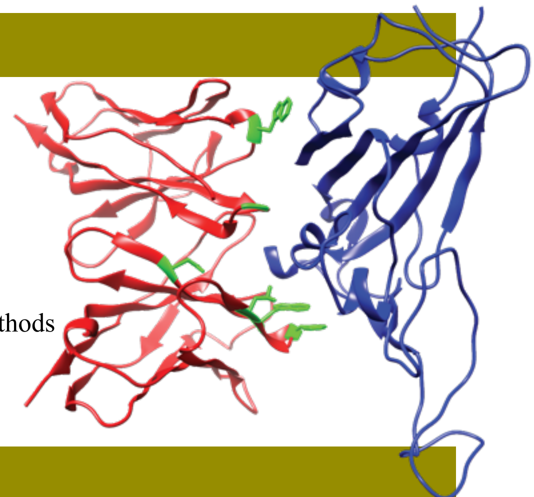

Research Highlights

Departments

Oxygen Effects on Uranium Tested

Uranium and oxygen can form dozens of compounds, each with unique chemical properties. Researchers from Lawrence Livermore and the University of Michigan examined the formation of uranium–oxygen compounds following a nuclear explosion in different environments. Their study, published March 7, 2022, in *Scientific Reports*, found that both the cooling timescale and the local concentration of oxygen significantly influenced formation of uranium oxide species.

Determining the compounds likely to emerge post-detonation is crucial for refining computational models essential to Livermore's predictive and nuclear forensic capabilities. As part of a Laboratory Directed Research and Development Program strategic initiative, a team led by Livermore chemist Mark Burton used a laser to ablate a small uranium metal target at different oxygen gas levels. Applying infrared and Raman spectroscopy to analyze particulates, the team found that ambient oxygen concentration strongly affected the type of compounds formed. In addition, the structural composition of uranium oxides depends on whether the plasma cools from 10,000°C over the course of microseconds or milliseconds.

"We have improved our understanding of gas-phase chemical reactions between uranium and oxygen as hot plasmas cool," says Livermore co-author and lead of the strategic initiative Kim Knight. "Our findings can inform models of nuclear explosions to refine predictive capabilities of particle formation and transport." In a related project, team members developed a tabletop reaction chamber to study small amounts of uranium in reproducible experiments.

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Seismic Models Improved

Scientists with Livermore's Geophysical Monitoring Program have developed an improved Earth model for seismic waveform simulation. With Mondaic, a start-up from the Swiss Federal Institute of Technology in Zurich, Livermore employed full waveform inversion using the Lassen supercomputer (left) to infer seismic models of the Earth for improved simulations. Their research, published July 7, 2022, in *Journal of Geophysical Research,* demonstrates new modeling capabilities by detailing the seismic structure of the Western United States.

Traditional seismic tomography relies on measurements derived from waveforms such as travel time and surface wave dispersion. However, limited knowledge of subsurface structure—3D variations in wave speed, attenuation, and density—has hindered higher accuracy seismic simulations. Research led by Livermore scientist Artie Rodgers inverted observed waveforms and iteratively updated models of subsurface Earth structure to reduce misfits between simulated and observed seismograms. This multiscale approach first fit long-period waveforms with long-wavelength Earth structure, then gradually reduced the minimum period to analyze finer scale structure. With Lassen, the researchers performed 256 model iterations for 72 earthquakes, updating the model to fit the real-world waveform data of 100,000 seismograms.

"The combination of Mondaic's software for managing workflow, Lassen's fast GPU-accelerated nodes, and Livermore's high-performance computing ecosystem and support enabled us to perform many more inversion iterations and resolve more detailed structure than previous studies," says Rodgers. The model's ability to simulate waveforms from small seismic events makes it a promising resource for improving earthquake-explosion identification, aiding nuclear monitoring efforts.

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Diamond Formation Detailed

A multi-institutional team headed by Livermore scientist Michael Armstrong capped off decades of theoretical and experimental efforts by observing the transformation of graphite into an elusive phase of diamond known as lonsdaleite on a picosecond timescale. The team's results were published August 1, 2022, in *Journal of Applied Physics*.

Inside the familiar diamonds used in jewelry and industrial applications, carbon atoms are arranged in a cubic diamond crystal achieved by compressing graphite. Under immense, instantaneous pressures, such as those produced during meteorite impacts, carbon can instead assume the lonsdaleite phase with hexagonal diamond structure. The team replicated these cataclysmic criteria by bombarding graphite samples with picosecond (trillionths of a second) bursts of laser light to achieve 80 gigapascals of pressure (roughly 800,000 atmospheres). Using femtosecond (quadrillionths of a second) x-ray pulses emitted from the Matter in Extreme Conditions instrument at SLAC National Accelerator Laboratory, the team identified lonsdaleite's mechanics of formation through time-resolved diffraction analysis.

"Lonsdaleite structure is likely an intermediate state in the phase transition (of graphite) to cubic diamond," says Armstrong. The researchers observed formation of highly textured lonsdaleite crystals 20 picoseconds after compression that reverted to a distorted graphite structure upon release. Observations confirmed earlier conjecture that lonsdaleite's formation is diffusionless, whereby atoms rearrange cooperatively and simultaneously. The study furthers understanding of dynamic materials response and enhances weapons physics.

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Commentary by Jim Brase

Strengthening Scientific Outcomes

ARTIFICIAL intelligence (AI) is fast becoming one of the most important tools for analysis of scientific data. Uniting AI with high-performance computing simulations yields entirely new capabilities that amplify researchers' abilities to solve complex national security and science problems. This integration—called cognitive simulation (CogSim)—is the subject of this issue's feature story.

The article beginning on p. 4 describes how Lawrence Livermore uses machine learning—one of AI's most important components—to analyze scientific data across a wide range of applications. Combined with high-performance computing simulations long central to Livermore's scientific applications, researchers observe outcomes arguably greater than the sum of their theoretical and experimental parts.

CogSim can amplify computing capabilities by speeding up simulations. Replacing a time-consuming physics calculation with a fast machine-learning model can, in some cases, greatly accelerate the code while maintaining the quality of the simulation. As a result, CogSim improves the predictive power of models and guides optimization methods for unique designs and superior performance in multiple Laboratory applications.

CogSim strengthens the Laboratory's approach to fundamental research and development as well. Advances in scientific discovery occur only when researchers challenge their own theories and previous understanding with experimental results. For complex questions, theory-based predictions require computational simulations with many variables and complex conditions. Comparing simulation predictions to experimental outcomes can validate understanding or, alternatively, provide clues to incorrect or missing parts of scientific theories. Until now, this comparison has taken place in a scientist's mind, limiting the complexity of the evaluation, as multidimensional simulations and experimental results are often reduced to single quantities for comparison. As a result, information in data products such as time series, spectra, or images can be lost. Machine learning offers approaches to systematically unite simulation and experiment in a computational framework that enables scientists to retain more of the complex data for comparison.

Today at Lawrence Livermore, CogSim is used across many applications from U.S. nuclear stockpile stewardship to designing inertial confinement fusion experiments to developing new SARS-CoV-2 therapeutics—several of which are detailed in the feature article. Looking ahead, CogSim promises faster and higher quality answers to complex analysis and design problems that inform improvements in national security, health care, and the economy.

The research highlights in this issue touch on other Laboratory programs and research aimed at maintaining nuclear safety, preserving valuable scientific data, and improving experimental capabilities. The first story beginning on p. 12 describes efforts by Livermore's Global Material Security Program to continue critical work securing nuclear and other radioactive materials despite travel restrictions during the COVID-19 pandemic. Once solely a boots-on-the-ground program to lead nuclear forensics workshops, train international partners in developing their own capabilities, and network internationally with forensics experts, the program pivoted to establish virtual inspection, learning, and conference platforms plus new approaches to joint sample analysis and facility upgrade planning without in-person interactions. The second highlight beginning on p. 16 presents a nearly 30-year collaboration across multiple national laboratories to ensure data storage and retrieval systems match the growing data output of supercomputers. The High Performance Storage System, designed to serve the world's fastest supercomputers as well as protect sensitive data, has met its mission by evolving over the decades, reliably storing data long term for government, academic, and commercial organizations around the globe. The final article beginning on p. 20 details a Livermore diagnostics system designed to capture images of instantaneous experimental effects. Improving on earlier technologies to capture images of material behavior across nanosecond timescales, the Bipolar Reset Experiment—called BiRX—acquires far more images from a single experiment than predecessors, eliminating the need for multiple experiments, reducing cost and potential variability.

Each highlighted achievement reflects how the Laboratory and its people grow and evolve ideas, just as CogSim has grown to advance scientific research and national security. Combined, these stories provide a snapshot of Lawrence Livermore's ongoing commitment to scientific excellence and discovery.

■ Jim Brase is the deputy associate director for Computing.

COGNITIVE SIMULATION SUPERCHARGES SCIENTIFIC RESEARCH

Adding machine learning and other artificial intelligence methods to the feedback cycle of experimentation and computer modeling can accelerate scientific discovery.

COMPUTER modeling has been essential to scientific research for more than half a century—since the advent of computers sufficiently powerful to handle modeling's computational load. Models simulate natural phenomena to aid scientists in understanding their underlying principles. Yet, while the most complex models running on supercomputers may contain millions of lines of code and generate billions of data points, they never simulate reality perfectly.

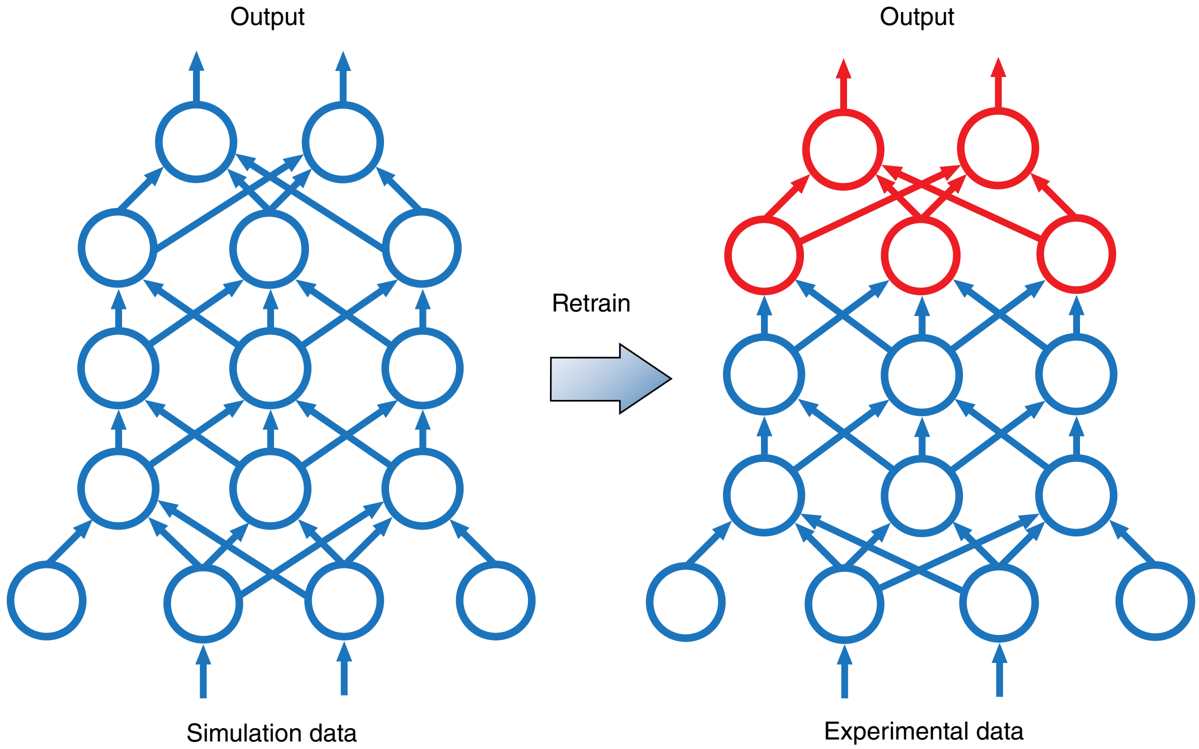
Experiments—in contrast—have been fundamental to the study of natural phenomena from science's earliest days. However, some of today's complex experiments generate too much data for the human mind to interpret, or they generate too much of some data types and not enough of others. The inertial confinement fusion (ICF) experiments conducted at Livermore's National Ignition Facility (NIF), for example, generate large volumes of data; but fusion physics is complex, and connecting the underlying physics to the available data is a difficult scientific challenge. Researchers increasingly face the problem of how to process data so that the underlying physics emerges into light.

To improve the fidelity of complex computer models, and to wrangle the growing amount of data, Livermore researchers are developing an array of hardware, software codes, and artificial intelligence (AI) techniques such as machine learning (ML) they call cognitive simulation (CogSim). Researchers will use CogSim to find large-scale structures in big data sets, teach existing models to better mirror experimental results, and create a feedback loop between experiments and models that accelerates research advances. CogSim's goal is ambitious—to transform itself into a fourth pillar of scientific research, joining the three pillars of theory, experiment, and computer modeling, as tools of discovery.

A New Feedback Loop

"Our wonderful simulations, as good as they are, are not perfect representations of our experiments," says Brian Spears, a physicist and leader of the Laboratory

In a deep neural network embedded within a modeling software code, simulation data flows through linked nodes (shown as circles) that numerically represent underlying physical behavior and train the software on the simulation data (left). The software is then retrained with experimental data, producing a model that both represents the physics and replicates experimental data (right). Red layers represent the retrained data subset.



Director's Initiative in CogSim. "We make approximations in these models. They have shortcomings." Models cannot incorporate physics that is not yet known. Scientists use data from experiments and simulations, evaluate these results together and incorporate their learning into the model to help design the next experiment. The model's accuracy at representing the experimental results is a measure of how well the models replicate the science behind the experiment. "The process has worked well for 50 years," Spears notes. Now, however, AI–ML tools offer a way to better analyze the results, incorporate them more completely into the modeling framework, and use the "retrained" model to improve the design of experiments with the goal of accelerating discovery.

A deep neural network (DNN) is a sequence of computing layers that transforms the inputs until they produce the desired output. A node, also called a neuron, is the basic unit of computation in a neural network. It accepts external inputs from other nodes and applies a mathematical function that results in an output. "A distinctive layer in the interior (of the DNN) we call the latent space," explains Spears. "This space is the most distilled representation of the physics in the data that we can get our hands on. In the latent space, we've preserved all the correlations in the physics that we can use to reduce the amount of data we need to accelerate the training." With the input of the large data set through the DNN, the modeling software is now trained on the simulation data. Then, researchers retrain a portion of the DNN on experimental data.

"We can train AI's deep-learning models on our simulations to make a perfect surrogate that knows exactly what the model's software code knows. However, the model is still not good enough because of the shortcoming of the code to predict the experiment," explains Spears. "We then retrain part of this model on the experimental data itself. Now we get a model that knows the best of both worlds. It understands the theory from the simulation side, and it makes accurate corrections to what we actually see in the experiments." The new improved model is now a better reflection of both the theory and the experimental results.

Applying CogSim to a wide range of research could benefit many fields. "At its highest level, we can build cognitive simulation into the Laboratory's research strategy, and all of its missions," says Spears. "We're already applying it to inertial confinement fusion and the Laboratory's stockpile stewardship mission, as well as in bioscience research. But we're driving it into other areas."

Laboratory researchers are developing three technologies to transform how scientists predict the results of experiments through CogSim. The first is refined models that fully use available data sets, estimate uncertainty, and are further improved through exposure to experimental data.

Software tools to develop and guide application of those models are the second need. These tools include workflows that guide simulations, learning frameworks that scale to the largest platforms at Livermore, and an environment in software that allows users to work productively without the hurdle of building the software stack and understanding the interface.

The third need is for computational platforms to support these tools. The Laboratory anticipates that its first exascale computer, El Capitan, arriving in 2023, will be a driving force of CogSim.

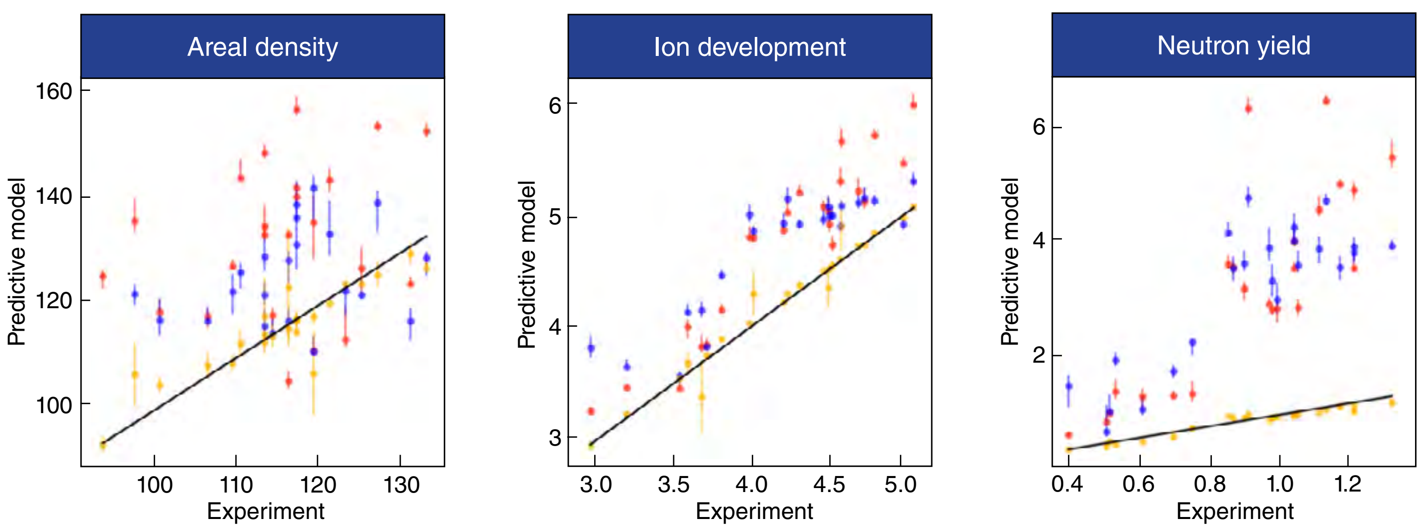
Improving ICF Experiments

Laboratory researchers already use Livermore-developed CogSim tools to design new ICF experiments to achieve nuclear fusion ignition. During a NIF shot, as many as 192 lasers fire into a holhraum, a hollow cylinder open at the ends that holds a 2-millimeter-diameter fuel capsule containing a mixture of the hydrogen isotopes of deuterium and tritium.

The lasers strike the interior walls of the hohlraum, converting their ultraviolet-wavelength light into x-ray wavelengths, bathing the fuel capsule in an intense burst of energy. The capsule shell explodes, compressing the fuel inside into a pinpoint-size area of high-energy-density plasma. The implosion causes hydrogen atoms to fuse, releasing energy. According to the widely used National Academy of Sciences definition, fusion ignition takes place when the energy output from the shot is greater than the energy input. NIF researchers have developed software to model these experiments. The model inputs include factors such as the thickness of the fuel capsules, the geometry of the hohlraum and size of its laser entry holes, the fuel mix and gas fill inside the capsule, and the energy and pulse shape of laser shots. Physical parameters affect the energy output, and researchers measure quantities such as the intensity of emitted radiation, number of neutrons, and the evolution of ion temperature inside the plasma with time to see how their design affected the shot results. By modeling experiments with different inputs, the researchers can try to increase critical outputs that approach fusion ignition and avoid spending time and money on setups that won't improve the outcome.

A CogSim method called transfer learning is helping researchers improve ICF models. "Transfer learning is a two-step process," explains physicist Kelli Humbird. "First, we need to train a neural net from scratch on a really large data set relevant to the problem. Neural nets are data-hungry, so they need many examples of how to solve a given problem to learn effectively. Second, we take a small data set that we care about, that should be related to the large set, and partially retrain the neural net on that data. The large data set should give the net a general idea of the problem it's trying to solve. The small data set fine-tunes its predictions on the more targeted task."

ICF simulations can be used to create large data sets. "This gives the model a good idea of how ICF implosions change



Blue dots in the graphs represent low-fidelity model predictions of an inertial confinement fusion experiment model before the experiments took place; red dots represent a higher fidelity model's pre-shot predictions. Yellow dots represent the cognitive simulation (CogSim) model's ability to predict the results of each experiment based on transfer learning from the aggregate set of collected experimental data.

as you change input conditions—the target, the laser pulse, and so on," says Humbird. "However, our simulations are not perfect—physics approximations mean that what our simulation predicts is sometimes not what we see in the experiment. So, we can take our neural net with 'general knowledge' about ICF, and our small set of experimental data, and retrain just a portion of the model with the experiments. Now, our neural net has basically learned how to take the simulation predictions and adjust them to be more in line with what we really see in experiments."

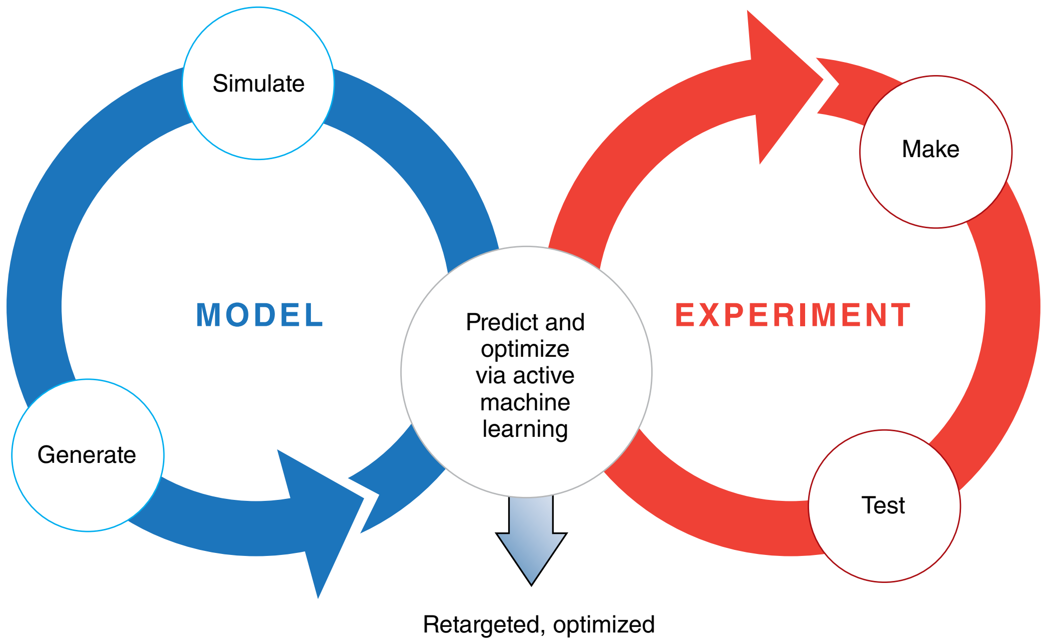
In an experiment applying CogSim to ICF experiment simulations, Humbird modeled a series of laser shots conducted at the University of Rochester's Laboratory for Laser Energetics. Before the experiments, they modeled measurable parameters such as the areal density of a shot's plasma cloud, the ion temperature, and the neutron yield and then used the data from a portion of the shots to retrain their model using a DNN. The retrained model more correctly predicted the results of the other experiments. Their paper, "Transfer Learning to Model Inertial Confinement Fusion Experiments," reported in *IEEE Transactions on Plasma Science* won the 2022 Transactions on Plasma Science Best Paper Award from the IEEE Nuclear and Plasma Sciences Society. The model in this proof-of-concept experiment used just three hidden layers (DNN layers between the input and output layers) with a few dozen neurons, nine inputs, and five outputs. In fall 2022, *HPCwire* magazine awarded its Editor's Choice award to the Livermore team for Best Use of HPC in Energy, recognizing the application of CogSim to ICF research.

The group also ran simulation and experimental data from ICF shots at NIF using transfer learning, and a larger amount of data. The results indicate that the DNN-trained model provided the best match with the experimental results. "We've been making predictions with the NIF model routinely and updating it as we acquire more data. We're observing that it generally improves over time, and we're hoping to add new diagnostic data, such as capsule quality, and other metrics we think impact performance," Humbird notes.

In August 2021, a NIF shot yielded an output of about 70 percent of the input energy—the threshold of ignition. (See *S&TR*, April/May 2022, pp. 4–15.) A second NIF shot in September 2022 that applied record-high laser energy produced about 1.2 megajoules (MJ) of fusion energy yield, compared with the 2021 experiment that produced 1.35 MJ. Later in the fall, CogSim techniques predicted that a specific experiment conducted at NIF had a greater than 50 percent probability of surpassing the ignition threshold. The model was correct; the record yield observed in the December 2022 experiment fell within the range predicted by the CogSim

Livermore researchers trained a model to design mutations to a SARS-CoV-1 antibody that enabled it to bind to and neutralize SARS-CoV-2, the virus that causes COVID-19. Illustrated is a structural model of the receptor binding domain (blue) of SARS-CoV-2 spike protein in complex with modified m396 antibody (red) and designed antibody mutations (green).

model. "The ability to predict the outcome, with credible uncertainties, of such a significant experiment demonstrates great improvements in simulation capabilities and physics understanding," says Humbird. "The growing use of CogSim techniques strengthens predictive capability, enabling a push into high performing regions of the design space at NIF."



In the biosciences, a cycle of simulating mutated antibody reactions with a virus and improving mutations through simulation coupled with synthesizing and testing antibodies can speed antibody developments from years to months or weeks.

Faster Discovery for Bioscience

CogSim tools can work across a range of scientific endeavors. Laboratory bioscience researchers have been applying CogSim to produce predictive models for biology since the 2000s. One example is the Accelerating Therapeutic Opportunities in Medicine (ATOM) consortium, a partnership of GSK (formerly known as GlaxoSmithKline), Lawrence Livermore, Frederick National Laboratory for Cancer Research, and the University of California at San Francisco. ATOM develops a preclinical design and optimization platform to help shorten the drug discovery timeline. The consortium uses ML to predict the properties of proposed drug molecules, and screens them virtually for safety, pharmacokinetics, manufacturability, and efficacy.

Jim Brase, deputy associate director for Computing, leads Livermore's ATOM efforts, and the Laboratory's work applying HPC to life science and biosecurity. "There isn't enough data for some parameters to build the high-fidelity model we want," he says. "The chemical space is so wide open. Current models can't predict a protein structure to have the properties that enable it to, for example, penetrate the blood–brain barrier. So, we have to build a machine-learning model to teach the simulation how a protein penetrates the barrier and use this understanding to predict the proteins that might do a good job at the task."

Another Laboratory effort to apply CogSim to countering biothreats was accelerated by the COVID-19 pandemic. (See *S&TR*, June 2021, pp. 4–11.) Daniel Faissol led a team to design antibodies capable of binding to SARS-CoV-2 using ML algorithms and Livermore's high-performance computers. The team took antibodies known to be effective against SARS-CoV-1 and retargeted them by proposing mutations of amino acid sequences on the antibody they thought would work against SARS-CoV-2. ML algorithms helped identify promising sequences, and high-fidelity simulations tested how well the antibodies bound to a SARS-CoV-2 antigen to inactivate it. Faissol, who leads Livermore's program in Computational Design of Antibodies, says, "We did this with three different SARS-CoV-1 antibodies and successfully retargeted them to neutralize SARS-CoV-2, sometimes maintaining full potency against SARS-CoV-1."

When the COVID-19 pandemic hit, the team had been working to extend the protective effects of a meningitis-B vaccine by modeling the meningitis virus' antigen proteins. To combat SARS-CoV-2, Faissol says, "We flipped this model around—we modeled different candidate antibodies to SARS-CoV-2, while keeping the antigen the same. It was a different approach compared to what others were doing. The method is very fast and can potentially result in broadly protective antibodies against COVID variants." Laboratory development of antibodies normally takes years. "Because we're doing this computationally, we can do this work rapidly, in principle. We didn't have to wait for a patient who was infected with and recovered from both SARS-CoV-1 and -2 to design a protective antibody," he notes.

Later, the team was asked by Department of Defense (DOD) sponsors to redesign a clinically used SARS-CoV-2 antibody—part of AstraZeneca's antibody drug product for COVID-19 that suffered significant potency losses against Omicron variants. "We performed a lightning computational sprint over two weeks that successfully identified antibody variants with potency that bound Omicron-variant antigens while maintaining full potency against previous strains," says Faissol. "One of the things that distinguishes our work is co-optimization for multiple antibody properties, such as stability, together with binding to multiple viral variants. The Omicron antibody binds with multiple Omicron antigens—we can optimize it for manufacturability at scale."

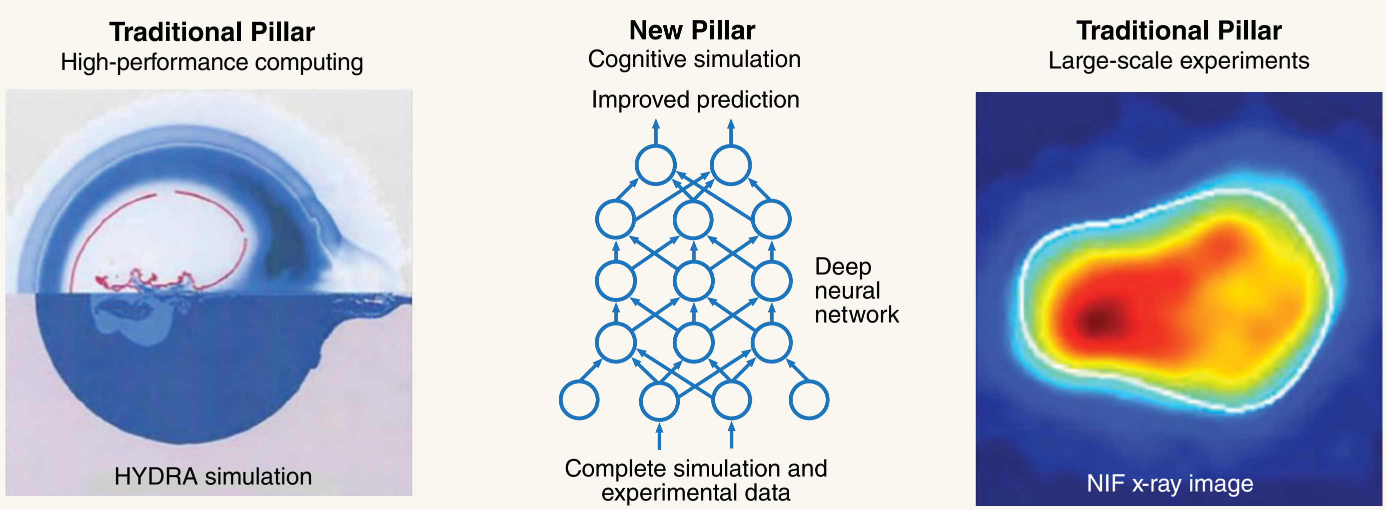
Thanks to this work, DOD has funded a six-year effort to further develop this CogSim-based optimization platform called Generative Unconstrained Intelligent Drug Engineering (GUIDE). The goal of the GUIDE program is to develop the predictive tools, data, and experimental capability to enable rapid response to new pathogens and to design broadly protective anitbody and vaccine candidates against entire classes of viral pathogens. The platform will also help accelerate the time required to design robust medical countermeasures to days or weeks, and it will provide capabilities for early analysis of emerging biothreats. This work aligns with the Laboratory's mission focus area in bioresilience—the use of data and CogSim tools to greatly improve the response to biothreats. The Laboratory's cooperative work with AstraZeneca is just one example of a collaboration furthering CogSim.

Collaboration Speeds AI–ML

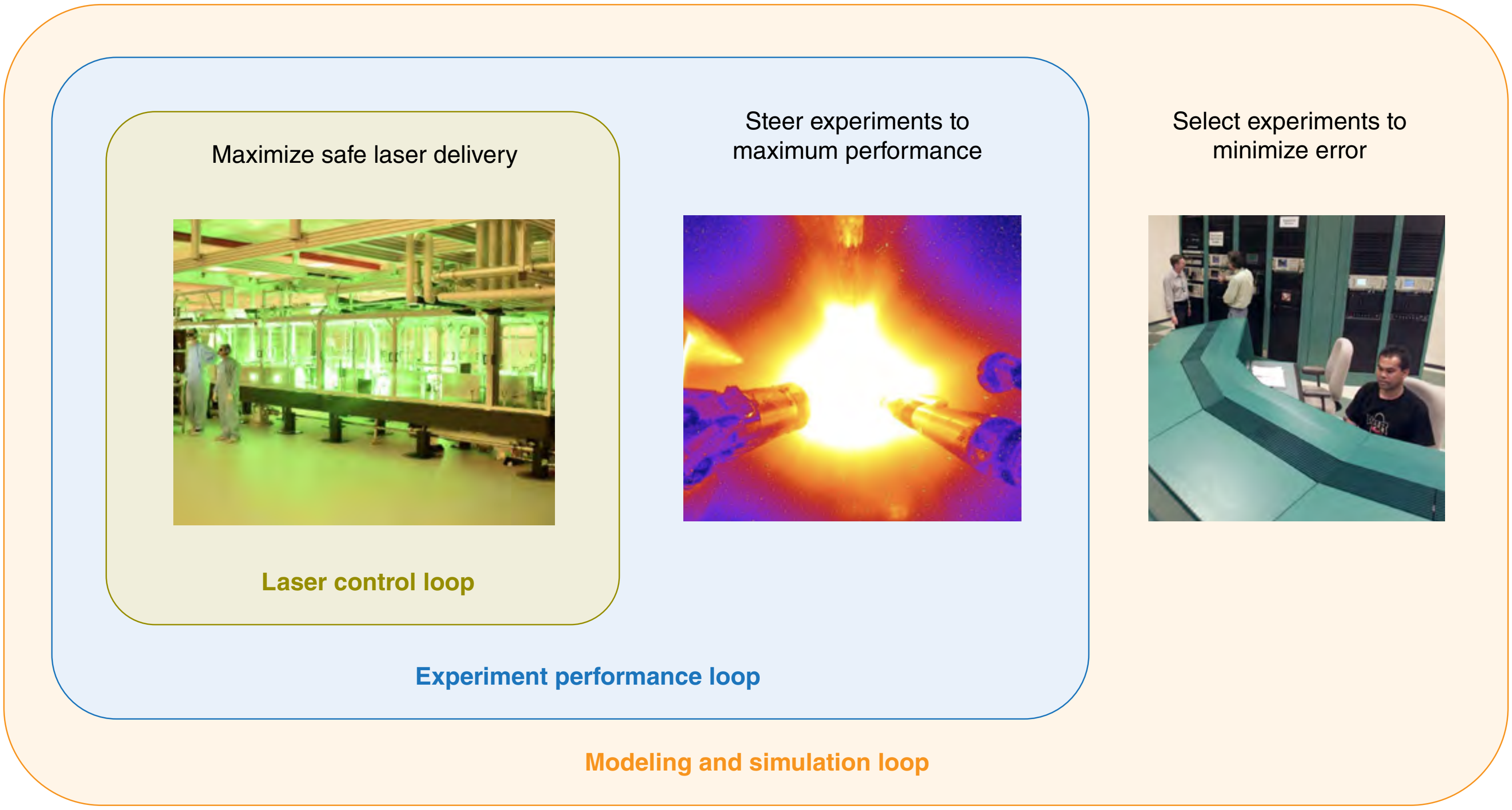
In December 2021, the Laboratory announced the founding of the Artificial Intelligence Innovation Incubator (AI3), a collaborative hub aimed at uniting experts in AI from Lawrence Livermore, industry, and academia to advance AI for large-scale scientific and commercial applications. The Laboratory is driving AI3 to advance scientific solutions using AI tools—building partnerships with Google, NVIDIA, Hewlett Packard Enterprise, Advanced Micro Devices, and others. Tools developed can be brought back to the Laboratory to advance its missions.

Laboratory scientists will apply CogSim tools to stockpile stewardship and other missions through discovery, design exploration, manufacturing and certification, and deployment and surveillance. Laboratory researchers will use CogSim tools to design new molecules and materials vital to national security priorities. Design exploration tools will help them accelerate development of technologies used in the nuclear stockpile. Manufacturing tools will help increase the speed and efficiency of manufacturing parts and reduce materials waste.

With these tools, Livermore researchers will answer the question, "How can we design a material that performs well in the component we're building and is also easy



Adding a new pillar of cognitive simulation, researchers use machine learning to apply the results of a model, such as those from the hydrodynamic simulation code HYDRA (left), to results of an experiment, such as an x-ray image from the National Ignition Facility (NIF) (right). Running the improved model helps guide the design of the next experiment.



Livermore is working with chip manufacturer NVIDIA to develop CogSim-based software to control and steer laser experiments for maximum performance.

to manufacture?" Researchers will develop a new material, design a part for the stockpile or for ICF experiments and then apply CogSim tools to develop efficient manufacturing processes. AI offers the ability to pull these tasks closer to each other. Next, in considering performance over the component's lifetime, researchers will answer questions such as, "How will systems change over their lifetime? What's the impact of aging? Are the materials compatible with each other?" Says Spears, "Cognitive simulation tools will ensure that we can design for the lifetime of the technology so that, for example, a material won't degrade early in a device."

Self-guided Laser Experiments

Work is also underway to use CogSim to help drive the future of high-power laser experiments for ICF and basic science. Laboratory researchers are working with chip manufacturer NVIDIA to develop a CogSim-based automated control system for laser experiments. NVIDIA's research on self-driving cars has produced hardware and software that the Laboratory is adapting in partnership with the company to build a self-driving laser control system. "We'll be able to control laser experiments sufficiently well to perform one every minute, and we know how to scale this rate up to one shot per second," says Spears. CogSim embedded in a computer-controlled system could quickly reset the parameters of a laser shot to achieve a desired result. The goal is to accelerate discovery through high-energy, high-repetition rate laser-driven experiments (See *S&TR*, July 2021, pp. 20-23.)

In just a few years, CogSim has gone from small-scale studies to a promising tool that is poised to broadly impact Livermore's missions and research. New discoveries will not trail far behind.

—Allan Chen

Key Words: Accelerating Therapeutic Opportunities in Medicine (ATOM) consortium, artificial intelligence (AI), Artificial Intelligence Innovation Incubator (AI3), AstraZeneca, cognitive simulation (CogSim), COVID-19, deep neural network (DNN), El Capitan supercomputer, exascale computing, hohlraum, inertial confinement fusion (ICF), machine learning (ML), National Ignition Facility (NIF), NVIDIA, Omicron variant, SARS-CoV-1, SARS-CoV-2.

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OPERATIONAL RESILIENCE DURING THE COVID-19 PANDEMIC

As COVID-19 pandemic travel bans were imposed in March 2020, the U.S. Department of Energy's (DOE's) National Nuclear Security Administration's (NNSA's) Global Material Security (GMS) Program, which works overseas to provide partners with the capacity to secure nuclear and other radioactive materials and deter smuggling efforts, faced a serious challenge. "When the pandemic started, the stakes were already high. We had to come up with solutions—and fast," says GMS Program Leader for Lawrence Livermore Melinda Lane. "GMS was a 'boots-on-the-ground' program in every sense of the word. We relied heavily on our most important asset—the physical presence of our subject matter experts (SMEs)—leading nuclear forensics technical workshops, research, and training; building relationships and growing networks; and supporting the security and protection of nuclear materials around the world. In March and April of 2020 alone, we cancelled dozens of in-person engagements."

Initially, travel restrictions severely impacted GMS activities. By creatively using virtual communication platforms and adopting a new, more flexible approach to program implementation and execution, GMS cultivated an innovative operational resilience that supported mission fulfillment. Despite the absence or restriction of in-person engagements, this approach continues to enhance the program's mission delivery.

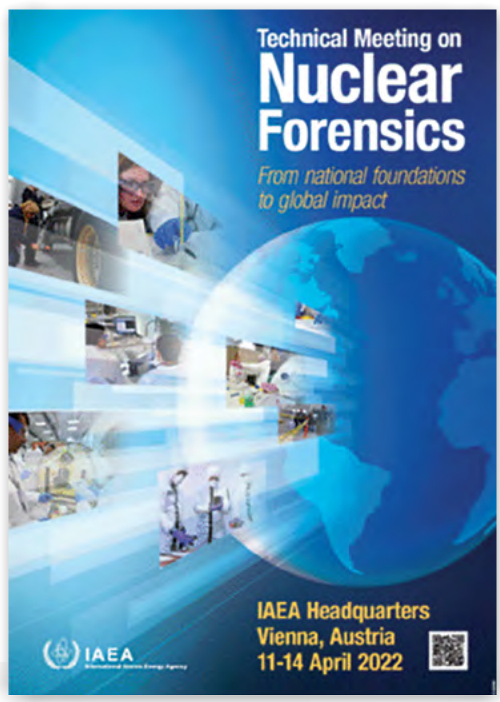
One of several DOE national laboratories supporting GMS efforts, Lawrence Livermore provides leadership and expertise in nuclear forensics, support for the International Atomic Energy Agency's (IAEA's) Information Circular/908 (INFCIRC/908) "Joint Statement on Mitigating Insider Threats" and its International Working Group, and good practices for the protection and security of nuclear and radioactive materials. The Laboratory also works collaboratively with its NNSA sponsor, NA-21, and other national laboratory SMEs to advance capacity building across all aspects of the nuclear security regime and state-of-the-practice in nuclear nonproliferation.

Virtual Nuclear Forensics

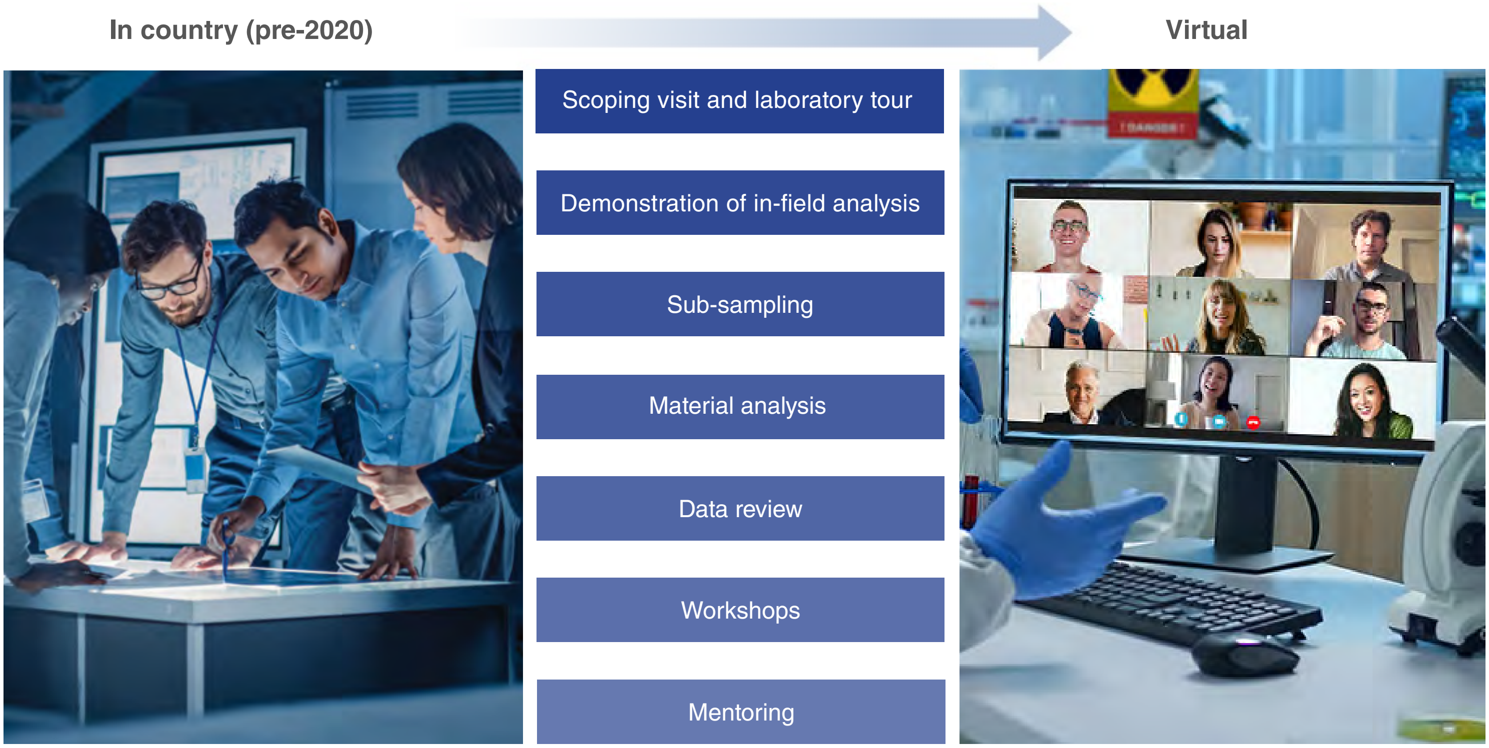
Nuclear forensics—the science of analyzing and identifying the origins of illicitly trafficked nuclear or other radioactive materials—plays a critical role in keeping the nation safe. GMS assists partners in developing their own nuclear forensics capabilities by conducting technical workshops, trainings, and benchmark studies. "If there ever was an example of necessity driving invention, this transition to virtual nuclear forensics training and workshops applies," says Ruth Kips, deputy associate program leader for Nuclear Smuggling Detection and Deterrence at the Laboratory. "We had to identify virtual communication tools to teach and perform joint science, something we had never done before. We learned so much during this process, and our program is stronger because of it."

To accommodate the new virtual learning environment, course content was streamlined and complemented by pre-recorded presentations. Course instructors also encouraged virtual participation by crafting polls and quizzes. "We realized that some of the work we perform in person could be done virtually. From initial introductions with our international partners and overviews of laboratory capabilities to technical demonstrations, data review, and mentoring, we used virtual video conferencing platforms for the first time."

For joint sample analyses, part of international nuclear forensic capacity building efforts, all participating laboratories measure a small part of the same nuclear material and compare results and methods. Prior to the pandemic, at the start of a joint sample analysis, Kips and her team would typically meet in person at a partner laboratory and discuss what sample would be analyzed, how to organize the sample shipment process, and what techniques each laboratory would apply to evaluate the material. "Our first joint sample analysis with Romania on a set of highly enriched uranium (HEU) samples started early in the pandemic,



The International Atomic Energy Agency (IAEA) held its first hybrid Technical Meeting in April 2022. The event was co-chaired by Lawrence Livermore and INTERPOL and attended by more than 118 in-person and 79 virtual participants, 64 member states, and four international organizations.



The COVID-19 pandemic curtailed nearly all travel, requiring the Global Material Security (GMS) Program to shift from exclusively in-person to virtual engagements. Using virtual tools and platforms, GMS successfully collaborated with its partners around the world to continue to build capacity across all nuclear security domains including support for nuclear forensics training and collaborative research.

and we were not able to travel to the laboratory in Bucharest for those initial discussions and laboratory visits. So, we observed the subsampling process of a set of HEU metal samples through prerecorded demonstrations and virtual meetings performed by our partners in Romania, which resulted in a well-documented record of the material sampling in preparation for shipment to Los Alamos and Lawrence Livermore national laboratories," says Kips.

More Engagements, More Participants

As with in-person workshops and hands-on research performed prior to the pandemic, GMS team members have maintained a presence at international conferences and nuclear security summits for decades. SMEs from Lawrence Livermore and Pacific Northwest National Laboratory provide technical leadership and support for the IAEA's INFCIRC/908 and its International Working Group to mitigate insider threats for nuclear security. "After the initial travel hiatus, we realized we can conduct more engagements with more participants," says Livermore nuclear engineer and former policy director Frank Wong. "In June 2021, we launched a webinar for INFCIRC/908 subscribers so they could receive updates on the International Working Group's efforts since the last IAEA International Conference on Nuclear Security in 2020. We were thrilled because there was so much pent-up demand. INFCIRC/908 subscribers are passionate and engaged. We now have INTERPOL and 32 country subscribers including Slovenia and Switzerland, which subscribed during the pandemic. That's huge. Travel costs can limit in-person attendance, but virtual attendance can be almost limitless."

Wong and other GMS team members coordinated and executed virtual sessions and side events at several IAEA conferences and meetings, including transforming Argentina's in-person-only event, "Leadership in Nuclear Security: Women Supporting the Amendment to the Convention on the Physical Protection of Nuclear Material," into a hybrid format featuring Mirela Gavrilas, director of the Office of Nuclear Security and Incident Response for the U.S. Nuclear Regulatory Commission. The event hosted 50 in-person attendees as well as 40 virtual attendees from around the world.

GMS teams also supported the Nuclear Forensics International Technical Working Group's (ITWG's) Annual Meeting in June 2021. This first, virtual annual meeting included more than 100 nuclear forensics practitioners from 30 countries and highlighted the working group's notable contributions to international nuclear security. The 25th anniversary meeting of the ITWG, originally planned for June 2020, took place in June 2022—the first time the ITWG Annual Meeting has convened in the United States since its first meeting at Lawrence Livermore in 1995. Lawrence Livermore hosted the meeting as a hybrid event combining virtual and in-person engagements.

Securing Nuclear and Radiological Materials

Pre-pandemic support for the GMS mission included site assessments, progress reviews, and assurance visits to identify and improve nuclear material security systems and practices at nuclear or radiological facilities. Before the pandemic, SMEs conducted in-person walk-throughs to evaluate security systems, touring site perimeters and access control points and examining cameras, sensors, barriers, and material storage containers. "Gaining a complete understanding of how a site operates and maximizing security system effectiveness without seeing the location firsthand presented a major obstacle," says Adam Houlihan, international security specialist and portfolio leader at Lawrence Livermore. After the pandemic curtailed travel, GMS stakeholders determined how to conduct virtual walk-throughs using facility diagrams, photos, and videos filmed by partners and submitted via secure digital portals. "These virtual visits allowed GMS to support the design and implementation of crucial security upgrades at nuclear and radiological facilities around the world despite the absence of travel."

Continuously engaging partners on security improvements and operations throughout the pandemic ensured continuity of the GMS mission and presented an opportunity to understand the challenges partner facilities and organizations face in maintaining secure operations under pandemic conditions. In response, Lawrence Livermore SMEs documented their feedback and developed a comprehensive report assessing the lessons learned to better inform security planning and foster resilience during disruptive, large-scale events.

The Best of Both Worlds

Crafting creative, virtual solutions led to more frequent communication among GMS partners. Lane says, "Our relationships are stronger because now we interact with partners on a much more frequent basis." While beneficial to existing relationships, virtual engagements still present limitations when forging new partnerships. Wong adds, "Many of the successful international engagements continued through the pandemic due to the solid foundation of our established networks and relationships." By developing operational resilience during the COVID-19 pandemic, GMS team members determined that they can successfully execute trainings, joint research, and workshops remotely; increase SME and senior leader participation in engagements due to fewer travel commitments; and improve opportunities for mentoring and coaching by including junior staff at limited cost.

GMS Program team members coordinated and executed virtual sessions and side events for several International Atomic Energy Agency conferences and meetings.

In a post-pandemic world, Lane and her team anticipate an optimum hybrid of virtual and in-person engagements. The success GMS achieved during the pandemic is based on everyone's willingness to be flexible and think creatively. "The hybrid model is here to stay. Our engagements are more interactive and inclusive because we're using the robust communication tools we developed during the pandemic. Going forward, GMS will benefit from the best of both worlds."

– Sheridan Hyland and Genevieve Sexton

Key Words: Department of Energy (DOE), Global Material Security (GMS) Program, Information Circular/908 (INFCIRC/908), International Atomic Energy Agency (IAEA), International Technical Working Group (ITWG), National Nuclear Security Administration (NNSA), nuclear forensics.

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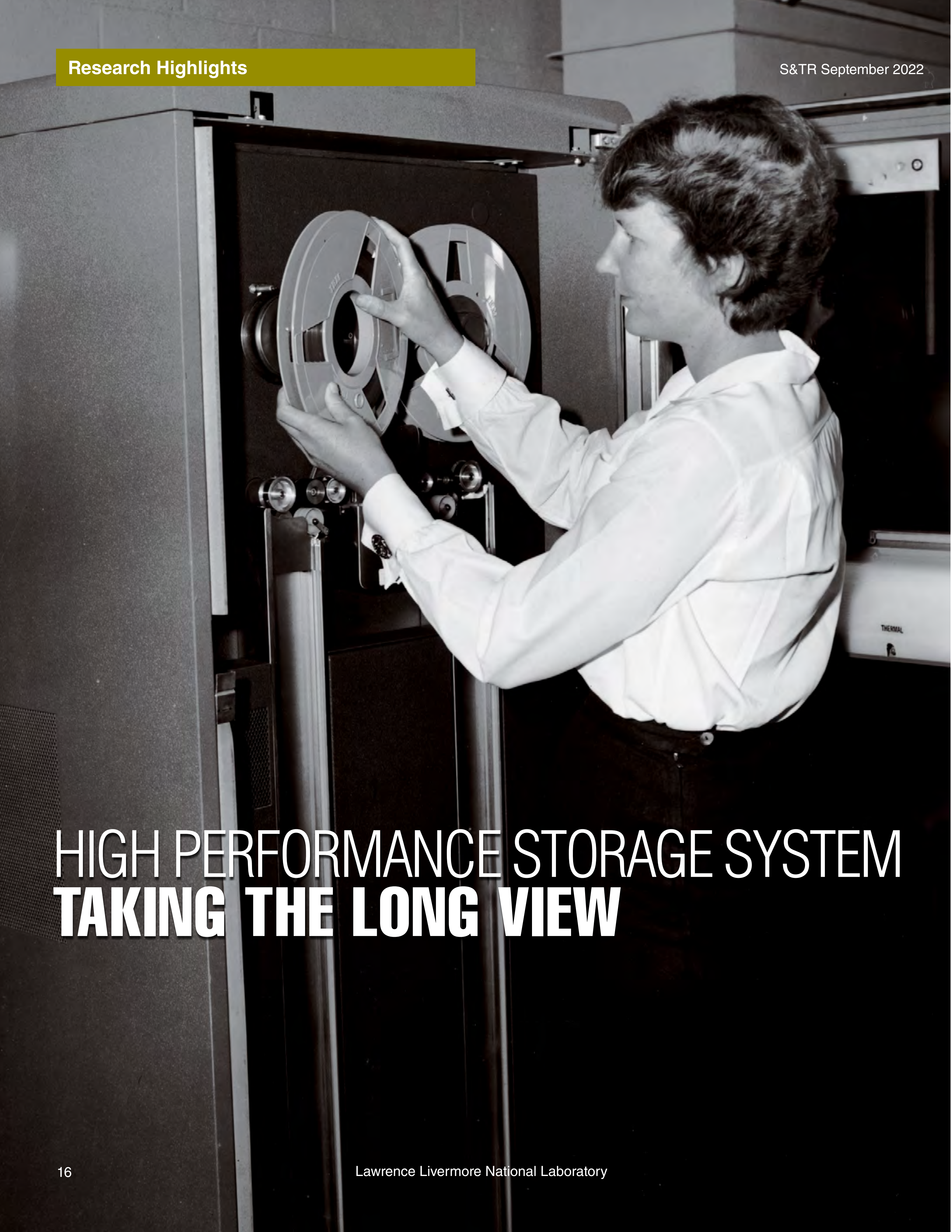


HIGH PERFORMANCE STORAGE SYSTEM
TAKING THE LONG VIEW

THE world of high-performance computing (HPC) is ever advancing with software updates, new hardware, increasingly data-heavy challenges, and the need to access and store immense amounts of data. Today's data dilemmas can be summed up in two simple questions: "Where should all this data go? How should it be managed?" Easy questions to ask, but not so easy to answer.

About three decades ago, Lawrence Livermore and four other Department of Energy (DOE) national laboratories working in HPC collaborated with IBM to tackle this issue. The laboratories and IBM recognized that issues around data storage constantly progress, requiring new and innovative solutions as supercomputing environments evolve. The result of their collaboration was the High Performance Storage System (HPSS), a scalable software solution that addresses the ever-changing data storage challenge facing the worldwide HPC community.

Lawrence Livermore plays a key role in the HPSS collaboration, significantly contributing to the original inspiration for the technology as well as being a co-developer and early adopter. The Laboratory had experience building distributed networked computing, printing, and storage shared environments long before this became commonplace. Engaging with other supercomputing centers that had similar experience, such as NASA and Los Alamos National Laboratory, led to the idea of standardizing how distributed storage could be achieved in the form of the Institute of Electrical and Electronics Engineers (IEEE) Mass Storage Reference model. HPSS was built on that scalable model.

The Laboratory's experience in data storage system development dates back to the 1953 delivery of its first computer system, the UNIVAC-1. Then, computers used vacuum tubes to perform calculations and stored data in mercury tanks and on magnetic tapes. (See *S&TR*, March 2002, pp. 20–26.) Now, supercomputer systems run calculations using thousands of powerful processors and store data on solid-state disks, magnetic disks, in the cloud, and on tape cartridges—high-tech descendants of historic magnetic tape reels.

The Data Conundrum Timeline

Before the advent of 3D simulations, the largest storage management systems at leading HPC sites archived a total of less than 10 terabytes each. (Today, Livermore's HPC archives allow individual files 10 times that size.) Beginning in the late 1980s, data storage became a concern for national laboratories involved in HPC, including Lawrence Livermore. These HPC leaders arrived at hierarchical storage management (HSM) as an archival system that could meet supercomputer performance requirements. HSM automatically moves data between expensive storage media—for instance, solid-state drive arrays—and low-cost media such as hard disk drives and magnetic tape cartridges. The HSM system helps keep costs down by keeping frequently accessed data on fast devices and moving "less used" data to slower devices.

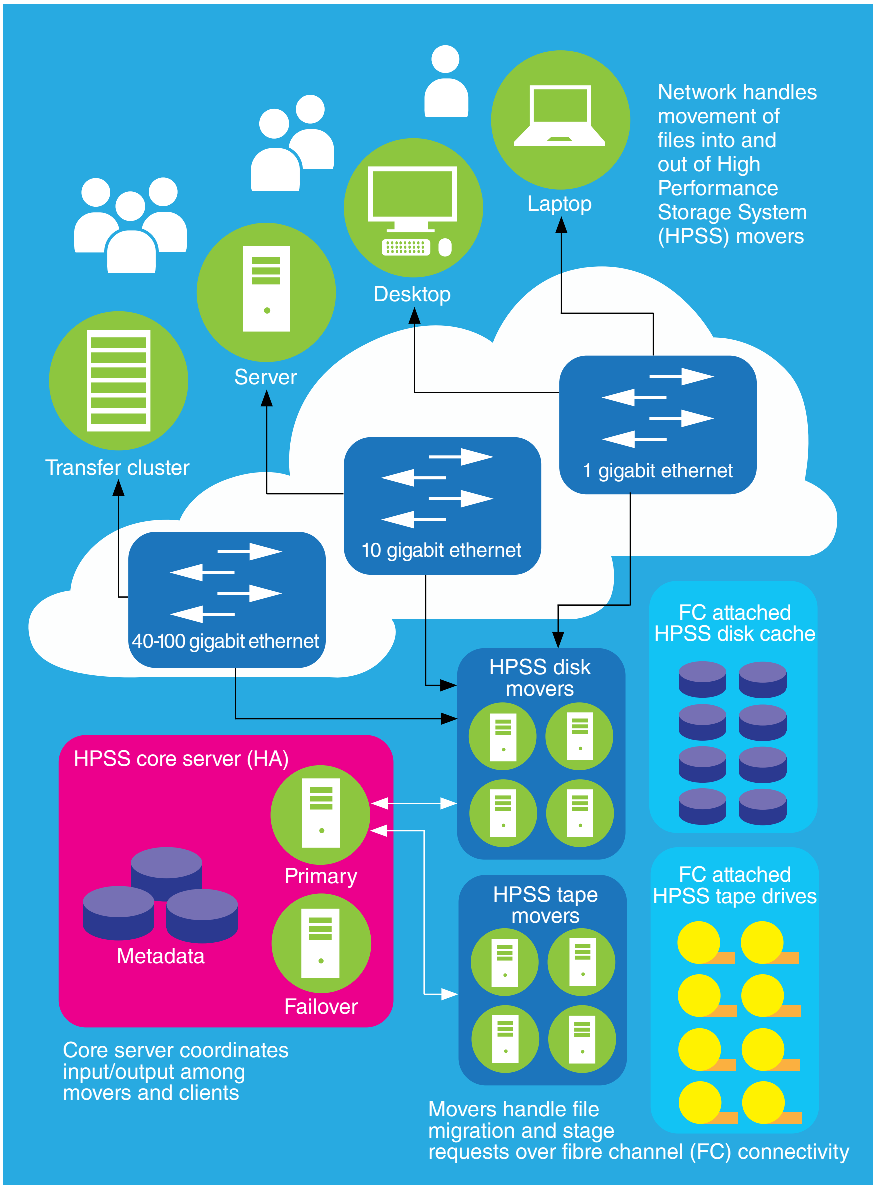
In 1992, predating HPSS, Lawrence Livermore, Los Alamos, Sandia, and Oak Ridge national laboratories along with IBM and other industry partners pooled resources to develop a scalable and efficient data archiving system. These organizations formed the National Storage Laboratory (NSL) Cooperative Research and Development Agreement, setting out to investigate, demonstrate, and commercialize high-performance hardware and software storage technologies that would remove network computing bottlenecks. "The HPC community foresaw a data storage explosion and realized that no single organization had the necessary experience and resources to meet all the challenges involved. This realization fueled the birth of the HPSS collaboration," says Todd Heer, Lawrence Livermore's representative on the HPSS Steering Committee and the committee's co-chair representing DOE. An additional national laboratory, Lawrence Berkeley, joined the other laboratories and IBM in this venture.

The inaugural HPSS-based archive drew heavily on NSL's results and the IEEE's Mass Storage Reference model, which NSL and others helped to create. Spearheaded by Livermore Computing's Dick Watson, who came to Livermore from Stanford Research Institute (SRI), that first HPSS could store billions of objects long before any competing systems, earning it an R&D 100 Award in 1997. (See *S&TR,* October 1997, pp. 18–19.) When the collaboration formed, the terascale era—with computers capable of 10^{12} floating-point operations per second (flops)—was still five years away. The collaboration met the challenge and those that followed by evolving storage architectures to meet the needs of the supercomputing community. In the three decades since, the collaboration has provided more than 10 major releases, with the most current release addressing storage needs for computations at petascale—one quadrillion (10^{15}) flops. Each release focuses on increasing operational efficiencies, performance, and storage capabilities while providing the ever-greater speeds required by its users. Heer notes the rarity of software that thrives for three decades. Yet, HPSS has achieved that milestone and continues to deliver.

Tape has been one of the go-to media for storing and archiving computer data since the early days of the Laboratory. This photo shows Livermore computer programmer Edna Vienop, who worked on a project calculating the return of Halley's Comet, loading a tape on the IBM 704 in 1959.

The Nuts and Bolts of Now

One of the founding tenets of HPSS was to take magnetic tape—the most economical form of digital media—and scale it up and out. “Using physical storage tapes may seem old-school,” says Heer, “but in actuality, advancements in tape technology have kept tape further than disk from the super paramagnetic limit where it can no longer grow in density.” Heer notes that the tapes used today are quite different from the old eight-tracks in their capacity and capabilities. “Unlike 1970s-era Neil Diamond eight-track audio tapes, today’s digital tapes have upwards of 7,500 tracks spanning their width,” he continues. “The HPSS application must be similarly advanced to handle this technology. We were the first to successfully develop the technology of using redundant arrays of independent tapes—‘RAIT.’ RAIT gives us the ability to write different chunks of a given data set to any number of tape drives simultaneously, providing cost-effective redundancy.” Tape drives have other benefits as well: they save energy, maintain data integrity longer than disks, and are inexpensive compared to cloud storage and hard disk drives.



“Clients,” which can be anything from laptops to supercomputers, have their own disk-based file systems suitable for short-term data storage. When a user selects files for archiving, copies of the files are transferred by disk movers to the first tier of the archive—the fast access disk cache. Files stored in the cache can be instantaneously retrieved. If a file stored on tape is requested, a robot grabs the relevant tape, mounts it on a nearby drive, and the data is transferred up through the disk cache and out to the user.

Today, approximately 40 sites around the globe including Japan’s High Energy Accelerator Research Organization, Germany’s Max Planck Computing and Data Facility, the National Oceanic and Atmospheric Administration, Indiana University, and Australia’s University of Tasmania use HPSS. Roughly 20 organizations have contributed to the HPSS effort over the years, including the core team of five U.S. national laboratories and IBM. Heer says, “The value of the feedback mechanism from some 40 sites cannot be overstated. These scaled-out production sites—a few even bigger than Lawrence Livermore’s archive—report back on bugs and features yielding a battle-hardened codebase worthy of keeping DOE’s most important data long into the future. DOE benefits significantly from this model compared to a model in which only national laboratories ran the software. At the same time, DOE keeps its HPC national interests at the fore by co-developing the codebase.”

From the start, HPSS was designed to be an HSM application to meet the high volume and speed requirements of the world’s fastest supercomputers while providing the security to protect data at multiple sensitivity levels. The application is hardware-agnostic, allowing a smooth transition to new devices and systems as the industry evolves and permitting users to choose from the best vendor technologies available. Worldwide, HPSS serves a total of more than 4.5 exabytes (4.5 quintillion bytes) of production data.

Pictured (left to right) are Lawrence Livermore High Performance Storage System team members Todd Heer, Debbie Morford, and Geoff Cleary in front of a Laboratory tape storage system. (Photo by Garry McLeod.)

Accelerating into the Future

At Lawrence Livermore, where more than 50 terabytes of data are produced daily for the archive, HPSS runs on a scalable and lightning-fast, clustered architecture. The Laboratory's HPSS features multiple storage tiers including a fast access disk cache in front of a tape-based archive. Livermore's team leverages economies of scale to deploy an archive disk cache that enables files placed in the archive to be immediately retrievable from a disk cache within a year (on average) before needing to be read from tape.

The Laboratory has five Spectra Logic TFinity tape libraries, including the world's largest, capable of holding half an exabyte of data. Livermore's HPC center boasts a total of 1 exabyte of on-premise storage capacity. "We have archive data dating back to the late 1960s that—along with everything stored since—must be saved in perpetuity," says Heer. "HPSS makes it possible for us to do so, knowing that no matter what new storage technologies are available in the future, the data will remain accessible. HPSS continues to play a key part of a total HPC center storage solution, lifting the burden of the more expensive storage closer to the computer."

The collaboration keeps a steady eye on the challenges ahead as it celebrates impressive accomplishments to date. The amount of data that user sites need to archive continues to accelerate. For example, archiving rates are expected to increase by more than 500 petabytes per year for DOE HPC sites as a whole. Meanwhile, the demands of the exascale computing era bring significant speed requirements to HPSS. "Parallelization of the data retrieval process—that is, increasing the number of tapes we can simultaneously pull data from and the speed at which we can spin the drives and thus access the data—is helping HPSS match the data bandwidth of these systems," says Heer. "Looking forward, the team is also working to incorporate more open-source software, exploring integration of cloud-native technologies, and increasing data discoverability so users can better understand data trends and patterns." In these ways and more, the HPSS collaboration continues to create ever-evolving, software-defined, scalable datastore systems, honoring its primary mission of long-term data stewardship for government, academic, and commercial organizations worldwide.

— Ann Parker

Key Words: archive, data storage, data retrieval, disk cache, exascale, high-performance computing (HPC), High Performance Storage System (HPSS) collaboration, IBM, magnetic tape libraries, Los Alamos National Laboratory, National Storage Laboratory (NSL), Oak Ridge National Laboratory, Sandia National Laboratories, Spectra Logic TFinity, tape drive.

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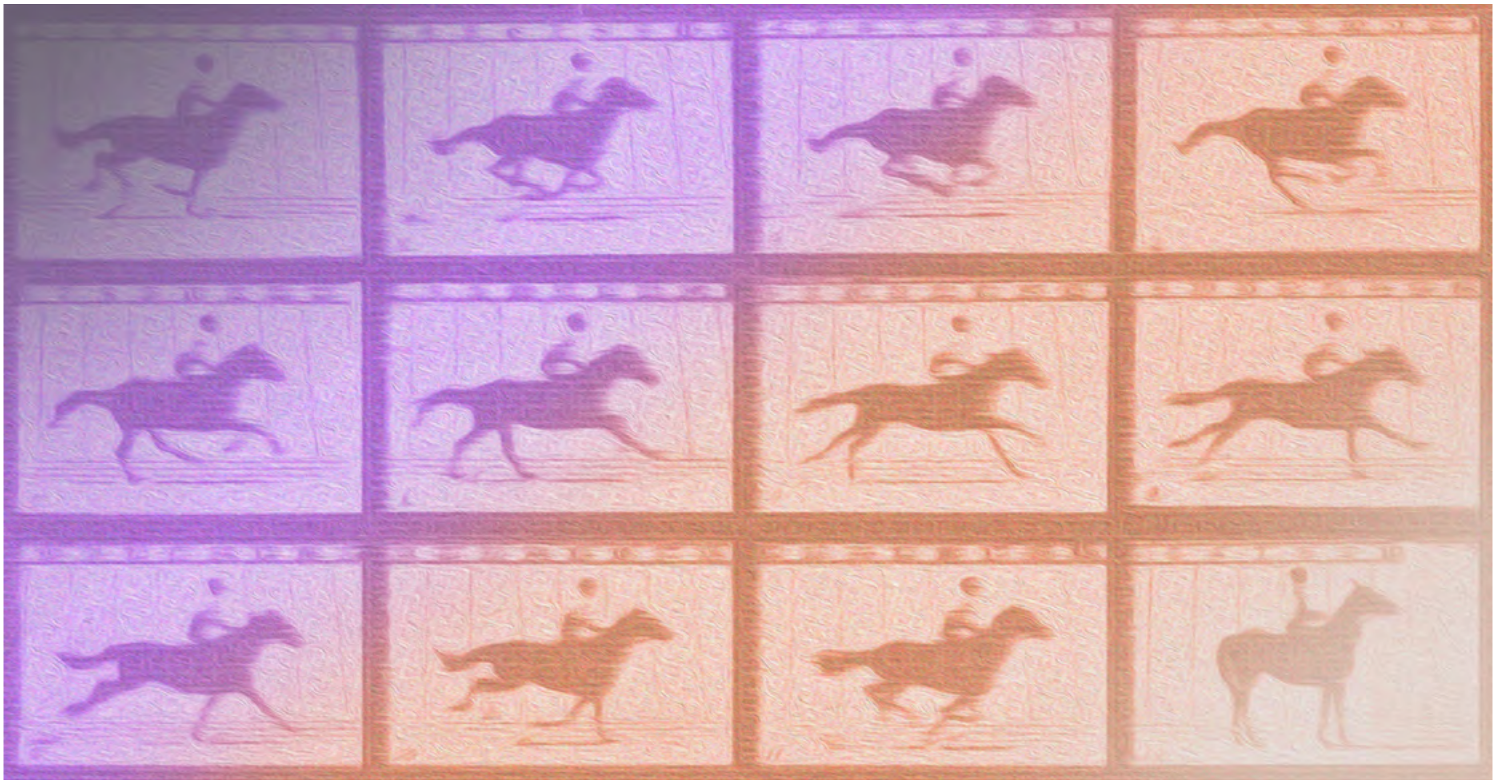


CINEMA IN A NANOSECOND

JUST as sports photographers must clearly capture chaotic movement on the playing field, Lawrence Livermore personnel must photograph experimental detonations in action. In the Laboratory's hydrodynamic tests, devices experience temperatures and pressures that imitate the initial stages of a nuclear explosion—conditions so extreme that rigid materials instantaneously exhibit fluid properties. Such tests, which are essential for studying material dynamics and informing computational models, would be impractical if only the aftermath of an explosion could be analyzed. Instead, scientists must study the entirety of implosion behavior, in high detail, to assess nuclear stockpile operability and longevity, a core directive of the Stockpile Stewardship Program.

To analyze nearly instantaneous effects, pulses of x-ray light just nanoseconds in duration are fired off at microsecond intervals, penetrating objects to examine their interior effects similar to a medical x-ray procedure. Successfully acquiring even one snapshot represents significant scientific and engineering developments and a collection of complex instrumentation. But one image only reveals so much. A Livermore team headed by Jennifer Ellsworth, the Linear Induction Accelerator (LIA) Program group leader, is developing a method to obtain dozens of back-to-back diagnostic images. The technology—an improvement over earlier attempts to achieve multiple images—will drastically reduce the time and cost associated with testing while capturing more data than ever before.

"If we want to understand the evolution of these systems, we need to take a series of images," explains engineer Katherine Velas, part of the LIA group and a member of the Pulsed and Electrical Power Group in the Laser Systems Engineering and Operations Division. She displays Eadweard Muybridge's iconic work, *The Horse in Motion*—famed photographs that settled an age-old debate by revealing that all four horse's hooves are, at one point, simultaneously airborne during gallop. Velas establishes parallels between the 150-year-old images, considered by some to be the birth of moving film, and the team's current endeavor toward x-ray movies. "For the longest time," she says, "acquiring multiple images meant performing multiple experiments, each of which demands immense investment and coordination. Think about all the variables that may change just slightly between tests. By acquiring a multitude of images from a single experiment, we're eliminating variability, obtaining more precise data, and significantly reducing the cost of testing."

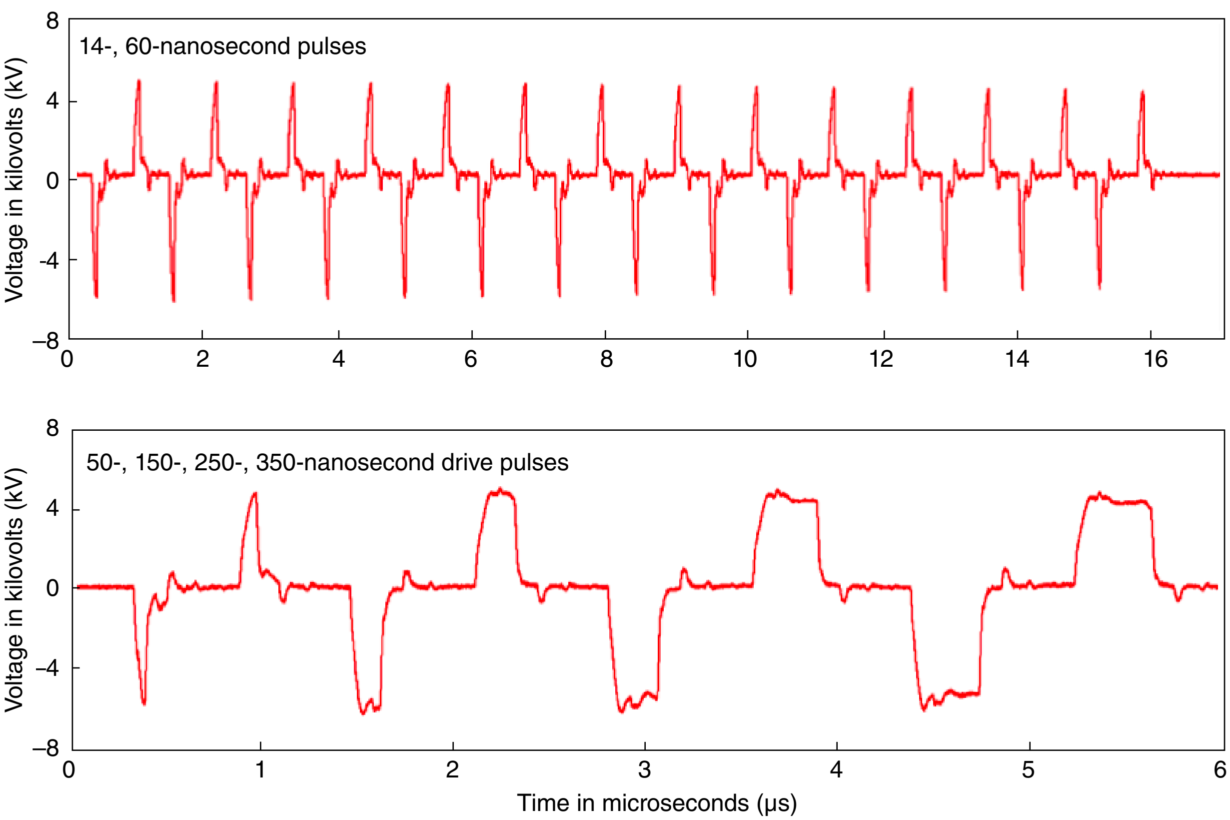
Freeze Frame

X-ray diagnostics for nuclear-related testing dates back as far as the explosive devices themselves. However, x-ray imaging requirements have posed significant limitations on the types of tests conducted and the information gleaned. Early systems yielded only one image—or "radiograph"—of experiments, leaving uncaptured dynamics to be inferred by modeling. Given the substantial cost incurred with each experiment, the pursuit of ever more frames has continued. Livermore's Flash X-Ray (FXR) system housed at Site 300's Contained Firing Facility generates two diagnostic frames for each experiment. (See *S&TR*, July/August 2018, pp. 12–15.) A multilaboratory accelerator effort, Project Scorpius, will provide four images at flexible intervals once installed at the Nevada National Security Site.

To image hydrodynamic experiments, FXR first creates an initial electron beam and channels it into an accelerator. (See *S&TR*, May 1997, pp. 15–17.) Like other linear induction accelerator models, its accelerator is a meters-long shaft encircled by ring-shaped compartments containing hunks of magnetic material. As the electron beam proceeds through the accelerator, the electrons are steered by electromagnets and sped up by precisely timed electric field fluctuations. FXR's downstream transport section then narrows the electron beam onto a thin target of dense metal, usually tantalum. Upon impact, electrons passing near the target's atomic nuclei are deflected, and their resulting kinetic energy loss is converted via emission of a continuous spectrum of high-energy light known as "Bremsstrahlung," which is perceived by a gamma-ray camera to image the experiment.

In 2017, Ellsworth's accelerator team began work on the Bipolar Reset Experiment (BiRX, an homage to accelerator design pioneer Daniel Birx) seeking to support rapid-fire pulses. Within a year of obtaining funding and approval and amid the COVID-19 pandemic, they designed, built, and tested a prototype device by integrating it into Livermore's FXR facility, the first time it was used with a live beam. "That test was a big deal," says Nathaniel Pogue, technical lead for the BiRX accelerator cell design and Accelerator Physics group leader. "The setup worked exactly as we wanted."

The diagnostic capabilities achieved with BiRX soar past those of its predecessors. Rather than divide a single microsecond



Plots of voltage over time depict 14 rapid electron-beam pulses, 60 nanoseconds in duration (top) and variably timed (bottom) achieved with the Bipolar Reset Experiment. This data was obtained at reduced operating voltage.

beam pulse into multiple subintervals like other systems, the newly developed hardware generates and accelerates multiple beams in rapid succession. With BiRX, nanoseconds-long pulses can be executed at arbitrarily spaced intervals on the order of microseconds, revealing behavior on the smallest of timescales. Pogue is convinced the new system can outdo itself yet. He envisions a powerful movie machine serving as a second axis to Livermore's FXR facility. The new instrument would supplement FXR's existing two shots with another 20 shots taken from a different angle, creating a 3D image series—a leap after nearly 70 years of incremental improvement. "We're not simply aiming to provide the next *evolution* of linear accelerator technology," says Pogue. "This work is a complete *revolution* in radiography. Without that singular image taken by Muybridge, we'd never know whether horses left the ground. Unexpected behavior can't be extrapolated; we just have to see it."

Pulsed-Power Potential

The lightning-quick nature of flash radiography requires compression of large energies into small timescales. BiRX ultimately confirmed viability of a bipolar solid-state pulsed-power (BSSPP) system, the key innovation for realizing x-ray cinema. Energy is first accumulated as electrostatic potential within a large capacitor bank where it is stored as if in a battery. The built-up charge is released on cue almost instantaneously to generate and accelerate the electron beam. Because power is inversely proportional to elapsed time, discharging the stored energy in a matter of nanoseconds maximizes the peak power achieved.

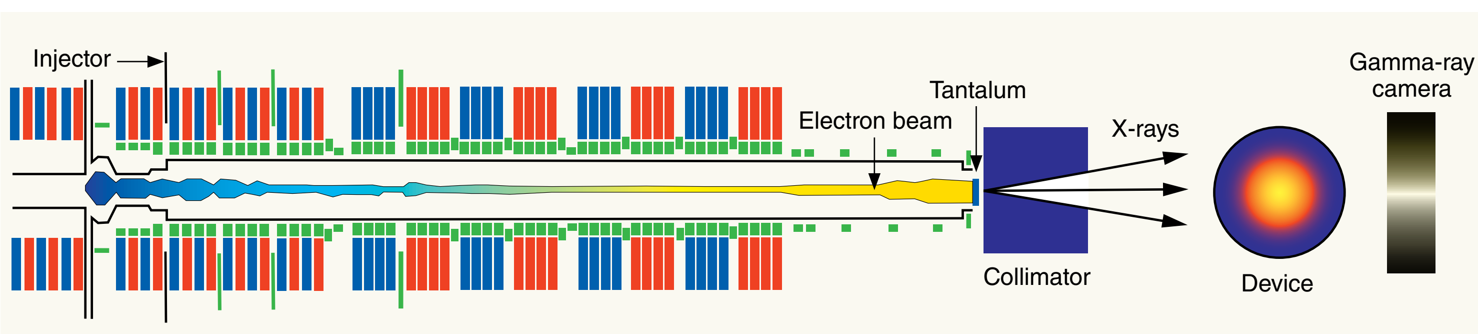
Livermore's multidisciplinary team reimagined pulsed power by introducing solid-state components. "Solid-state refers to the use of semiconductor devices such as the silicon carbide components found inside your home appliances," explains Velas. Previous generations used a combination of water-filled pipes and spark gaps to provide single, fixed-duration pulses. Employing millions of solid-state components affixed to printed circuit boards provides researchers unprecedented experimental customization. In addition to the number, duration, and rate of pulses, the amplitude and shape of each pulse in a sequence can be altered as well.

The notion of using solid-state materials to power accelerators was hypothesized decades ago, but, until recently, schematics were more theoretical than realistic. "Innovation in the electric vehicle market paired with federal investment in semiconductor technology has given us high-quality, readily available components," says Velas. "I'm fascinated that linking loads of tiny semiconductor chips together in the right way can generate gigawatts of power. Millimeter-size differences on a circuit board can make or break the entire system."

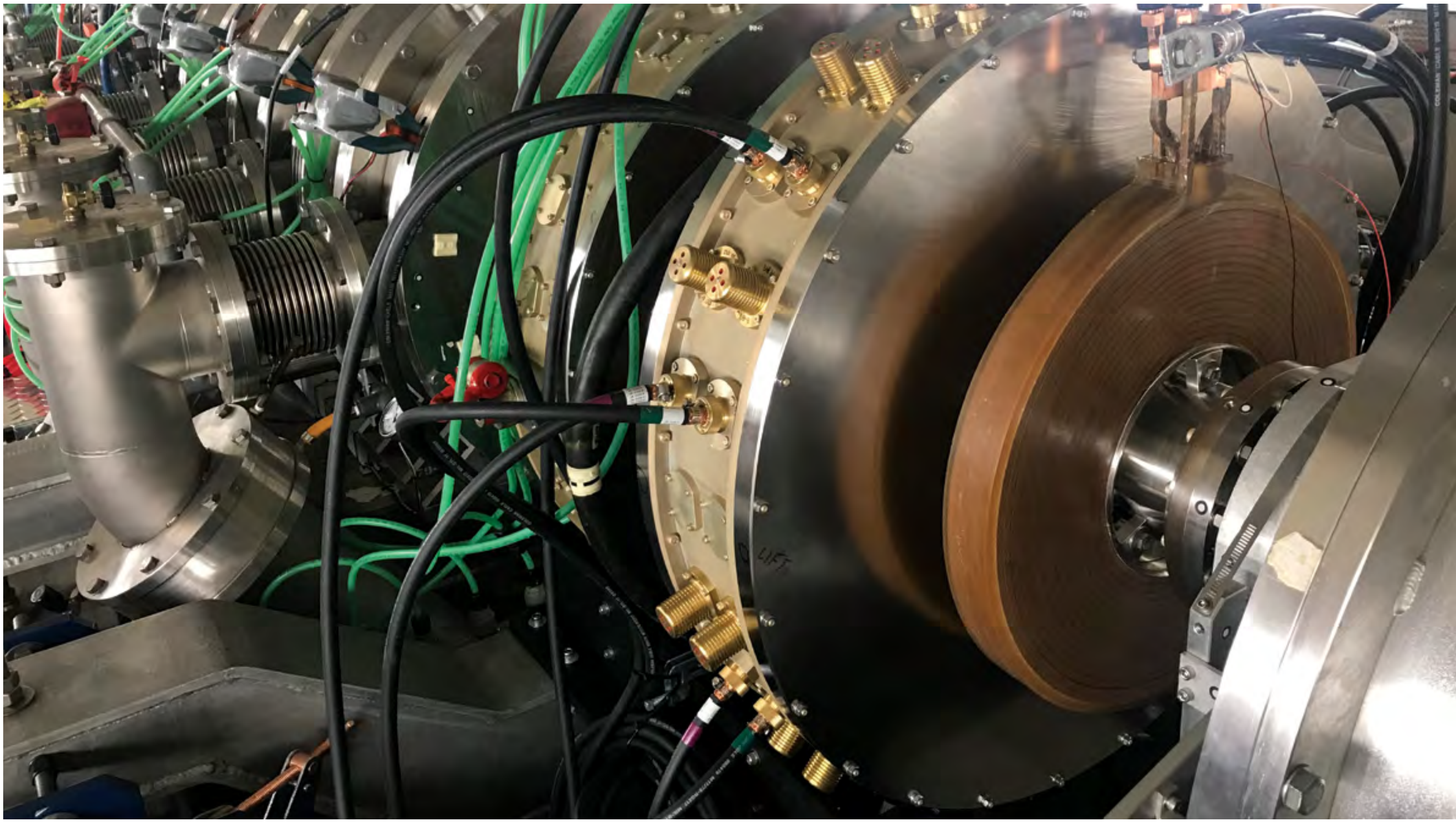
Fire and Reset

The other revolutionary principle validated by BiRX was its eponymous bipolar reset functionality. Electron beams conceived at high voltage experience high initial velocity. Rather than endlessly generate ever-higher voltages, however, the beam is further accelerated using magnetic induction. Upon entering the accelerator portion of the system, the electron beam passes through rings of magnetic cores. These fine-tuned composites of ferromagnetic material are electrically charged to generate alternating polarity electric fields along the length of the accelerator. Exploiting the electromagnetic tenet of "like repels like," the propensity for negatively charged electrons to accelerate away from a negative electric field ultimately propels the beam.

The magnetic cores, however, can withstand only so much use before becoming energetically saturated and shorting the system. Once too much voltage has been applied over time, the cells require cool-down time to neutralize and reset their



A simplified schematic illustrates how a linear induction accelerator creates diagnostic x rays. The process unfolds from left to right: an energetic pulse supplied by the injector is compacted and accelerated through a series of induction cells before striking the tantalum target to produce x rays, which then interact with the sample and are imaged by a gamma-ray camera.



Active reset cells, seen here installed at Livermore's Flash X-Ray Facility, are key enabling components for rapid-fire x-ray capabilities. The cells take the shape of large, metal cylinders at the injector side of the accelerator (foreground).

storage capacity. This "passive reset" requirement has hindered prior experiments seeking a greater number of pulses. BiRX's success ushered in "active reset" technology. Once a beam is fired using one polarity to obtain an x-ray image, a second pulse opposite in polarity shortly follows, releasing the magnetic cores' accumulated internal energy.

Pogue's team has so far designed an injector that supports bipolar capabilities, but Livermore's FXR facility is still limited to passive reset overall. "Marrying active reset to the existing pulsed-power system is challenging," admits Velas, who leads design of a bipolar pulsed-power source. Obtaining a bipolar active reset system will require a separate machine with purpose-built components, including new magnetic cells and a more resilient target. Pogue lauds the achievement thus far. "We started with arguably the most difficult part," he says. "Now that we've proven the pulsed-power system performs just as we hoped, the remaining parts of the system should be less complicated to devise and construct."

Pogue and Velas attribute their success to working with a diverse, fast-paced team. "The agility and multidisciplinary talents of our group prove we have exactly the people we need working on our national security mission," says Velas. "We're likely to uncover problems and solve them before other projects even know they're there."

— Elliot Jaffe

Key Words: accelerator, active reset, Bipolar Reset Experiment (BiRX), electromagnet, Flash X-Ray Facility (FXR), hydrodynamic testing, linear induction accelerator, pulsed-power, semiconductor, Site 300, solid-state material, Stockpile Stewardship Program, target, x-ray diagnostic, x-ray movie.

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Patents and Awards

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

High-Contrast, Convergent X-Ray Imaging with Laser-Compton Sources
Christopher P. J. Barty
U.S. Patent 11,357,458 B2
June 14, 2022

System and Method for Computed Axial Lithography for 3D Additive Manufacturing
Brett Kelley, Robert Panas, Maxim Shusteff, Christopher Spadaccini, Hayden Taylor, Indrasen Bhattacharya
U.S. Patent 11,370,173 B2
June 28, 2022

Multifunctional Reactive Inks, Methods of Use, and Manufacture Thereof
Kyle Sullivan, John M. Densmore, Eric Duoss, Alexander E. Gash, Joshua Kuntz, John Vericella
U.S. Patent 11,370,927 B2
June 28, 2022

Deformable Mirror with Integrated Microchannel Support
Andrew J. Pascall, Kerry G. Krauter
U.S. Patent 11,372,235 B2
June 28, 2022

System and Method for Plasmonic Control of Short Pulses in Optical Fibers
Eyal Feigenbaum, Graham S. Allen, Jay W. Dawson, Mikhail A. Noginov
U.S. Patent 11,374,378 B2
June 28, 2022

Shape Memory Polymer Foams for Endovascular Therapies
Thomas S. Wilson, Duncan J. Maitland
U.S. Patent 11,376,009 B2
July 5, 2022

Porous Materials via Freeze-Casting of Metal Salt Solutions
Michael Bagge-Hansen, Patrick G. Campbell, Jeffrey Colvin, Sergei Kucheyev, Thomas E. Felter
U.S. Patent 11,376,657 B2
July 5, 2022

System and Method for Rapid, High Throughput, High Pressure Synthesis of Materials from a Liquid Precursor
Michael Robert Armstrong, Sorin Bastea
U.S. Patent 11,383,218 B2
July 12, 2022

Hierarchical Triply Periodic Minimal Surface Structures as Heat Exchangers and Reactors
Pratanu Roy, Du Nguyen, Joshuah K. Stolaroff
U.S. Patent 11,389,765 B2
July 19, 2022

Awards

Tom Kohut, an operations manager at the National Ignition Facility (NIF), received the **"Managers Who Get Safety" Award** presented by the San Francisco Chapter of the **American Society of Safety Professionals**. Recipients demonstrate superior commitment to the safety and well-being of employees, the environment, and the community. Kohut was recognized for his significant contributions to ensuring the security of NIF's complex and high-risk operations by engaging collaboratively with multiple Laboratory resources and encouraging employees at all levels to think about safety during routine meetings.

Livermore researchers claimed first place in an international symbolic regression competition hosted by SRBench at the 2022 **Genetic and Evolutionary Computation Conference**. The group, led by **Brenden Petersen**, applied their Unified Deep Symbolic Regression (uDSR) algorithm to real-world COVID-19 data to predict and interpret epidemiological effects in New York state. The work emerged as part of a Laboratory Directed Research and Development Program project aimed at integrating several deep learning and search methods into a unified framework. The uDSR method garnered high scores based on algorithmic accuracy and simplicity, and the team also placed third in the competition's synthetic track.

Livermore physicist **Debbie Callahan** received the **2022 Leadership Award** from **Fusion Power Associates (FPA)**, a nonprofit fusion and plasma science research and education organization. The FPA Board of Directors highlighted Callahan's decades of contribution to hohlraum designs used for implosion experiments at NIF. Since joining Livermore in 1987 as a graduate student, she has authored and co-authored more than 200 refereed journal publications related to fusion energy. Callahan was also praised for her dedication to cultivating scientific talent through recruiting, training, and mentoring researchers who will lead the coming era of NIF target design.

The Institute of Electrical and Electronics Engineers Nuclear and Plasma Sciences Society honored a team that included three Livermore researchers. Lead author **Kelli Humbird** was joined by **Luc Peterson** and **Brian Spears** in receiving the **2022 Transactions on Plasma Science Best Paper Award** for introducing hierarchical transfer learning (TL) to calibrate inertial confinement fusion experiments at NIF. Humbird's team described a novel TL approach that first calibrates implosion physics models based on simulations, then fine-tunes models given high-fidelity experimental data, ultimately providing models that predict implosion dynamics more accurately than simulations alone.

Abstract

Cognitive Simulation Supercharges Scientific Research

The Cognitive Simulation (CogSim) initiative at Lawrence Livermore adds a new toolkit of machine learning, artificial intelligence, and data science to scientific discovery. Researchers will use CogSim to find large-scale structures in big data sets, teach existing models to better mirror experimental results, and provide pathways to designing new materials and technologies. The initiative's goal is ambitious: to transform CogSim into a fourth pillar of scientific research, joining theory, experiment, and computer modeling as tools of discovery.

Contact: Brian Spears (925) 423-4825 (spears9@llnl.gov).

Coming Next Issue

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 an 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.*

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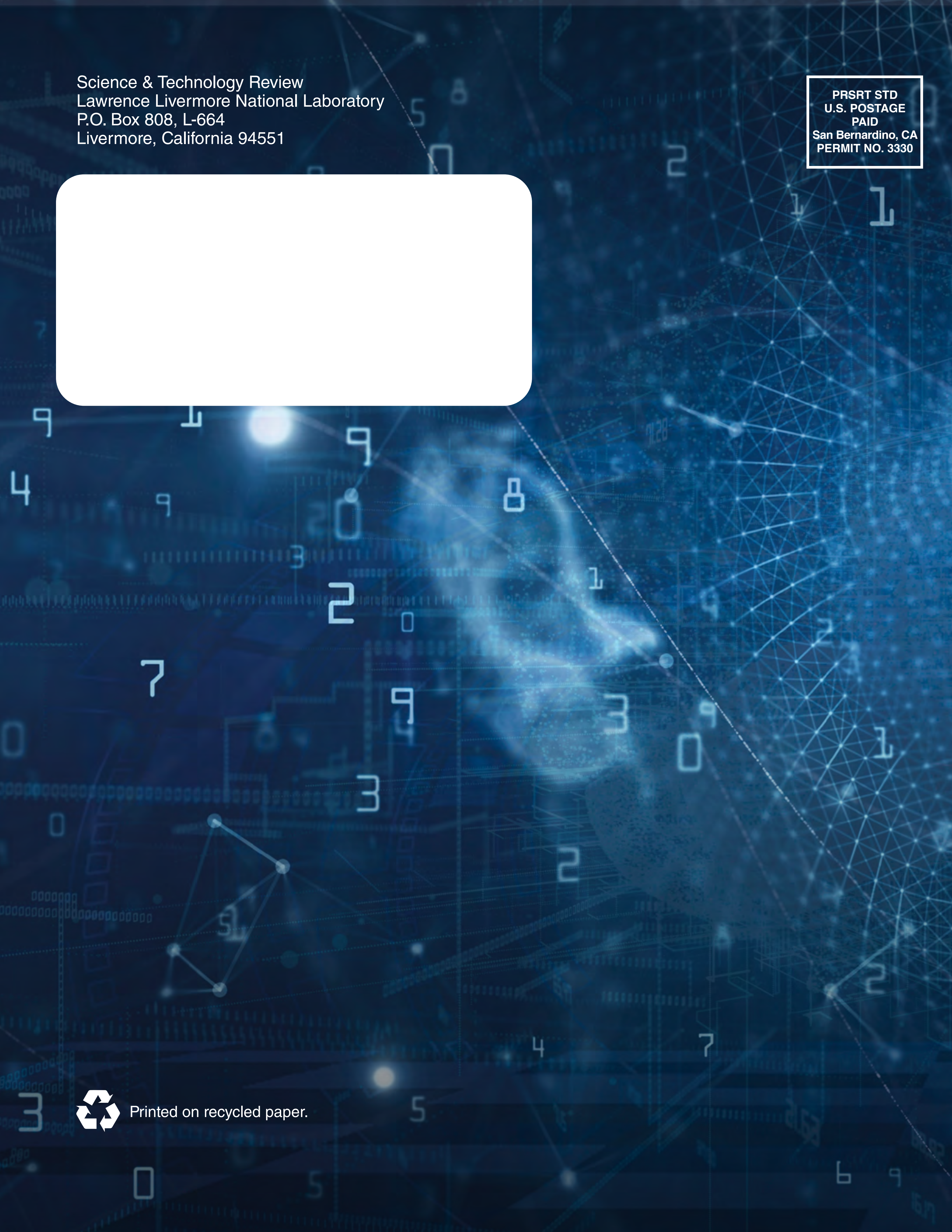

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