Searching for the NUCLEAR NEEDLE in a HAYSTACK

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- Johnny Foster: Pushing the Boundaries of Science
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Patents and Awards
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**Lab Develops First-Ever Living 3D-Printed Aneurysm**

Ruptured brain aneurysm affects about 30,000 Americans each year and can lead to serious medical emergencies, including stroke, brain damage, and even death. Existing treatment options are limited, often invasive, and surgical outcomes vary. But clinicians may be able to improve existing treatment, thanks to researchers at Lawrence Livermore and their collaborators at Duke University and Texas A&M who produced the first-ever living, bio-printed aneurysm. Their work appeared in the October 16, 2020, edition of Biofabrication.

The team, led by engineers William “Rick” Hynes and Monica Moya, were able to replicate an aneurysm in vitro by 3D printing blood vessels with human cerebral cells. Hynes then performed an endovascular repair procedure on the printed aneurysm, introduced blood plasma, and observed the formation of a blood clot. The researchers then documented the “post-op” healing process of the endothelial cells within the vessels.

“We thought that if we could pair computational modeling and experimental approaches, maybe we could come up with a method for selecting personalized treatment,” says Hynes. “Now we can start to build the framework of a model that surgical practitioners can use to determine best practices for treating aneurysms.” In addition to patient-specific care and serving as a testbed for surgical training, researchers say the platform will enhance understanding of how metals become stronger when physically deformed or hardened. The root cause of metal hardening remained a mystery until 2020, when it was first proposed that dislocations—curvilinear crystal defects made of lattice disorder—are responsible for crystal plasticity. This gives geophysicists a validated target for locating and mapping distributions of this type of gas hydrate formation in the seafloor. This gives geophysicists a validated target for locating and mapping distributions of this type of gas hydrate formation in the seafloor.

Seafloor Gasification Illuminated

Methane hydrate, a naturally occurring crystalline solid that forms from hydrocarbon gases (commonly methane) and water in the seafloor and continental shelves, is a source of natural gas, as well as a potential contributor to ocean acidification and climate change. Its presence lowers the electrical conductivity of the seafloor, in comparison to hydrate-free formations, allowing the gases to be imaged by geophysical methods. Measurement of seafloor electrical conductivity, either using borehole logs or geophysical prospecting methods, is one of the most reliable ways for estimating hydrate location and abundance, but these methods must be calibrated using laboratory measurements of hydrate-sediment mixtures.

To provide this essential data, Lawrence Livermore scientists and their collaborators at the U.S. Geological Survey and Scripps Institution of Oceanography at University of California, San Diego synthesized methane hydrate in mixtures with sediments in the laboratory to determine their electrical conductivity. Their findings were published in the August 4, 2020, issue of Geophysical Research Letters.

Current estimates suggest there are substantially higher amounts of natural gas associated with gas hydrates than all the continental shelf reservoirs combined. “Determining the global distribution and inventory of petrogenic organic carbon in the crust is important to gaining a basic understanding of the Earth’s deep carbon cycle,” says Wyatt Du Frane, a Livermore materials scientist and contributing author. “Our lab results are consistent with wellbore core samples obtained in the field that show high concentrations of gas hydrate. This gives geophysicists a validated target for locating and mapping distributions of this type of gas hydrate formation in the seafloor.”

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One lesson this reinforces is just how deeply computing is embedded in Livermore’s mission. As we push into extremely difficult problems, and in its approach to innovation. The article beginning on page 12 explores the work of a new research center led by the Laboratory that is creating high-performance computing software to aid in the development of new functional materials, which respond to stimuli such as voltages, light, or magnetic fields. We need this new class of materials in such applications as quantum computers (a technology required to counter a variety of threats), sustainable energy applications such as solar cells, and next-generation solid-state data storage technology. Again, we have recognized a national security need and are building the tools to address it. Finally, in support of its nuclear stockpile stewardship mission, the Laboratory is challenged to assess weapon readiness as systems age and the workforce grows more removed from the last live nuclear weapons tests. Computer simulations can model weapons behavior but require extremely difficult problems, and in its approach to innovation.

**Realizing Solutions to the Nation’s Security Challenges**

In the early 1950s, the U.S. needed a breakthrough to bolster its second-generation nuclear weapons—NNSA, in its infancy, was created to address this technical problem posed by the Soviet Union. That breakthrough took the form of a smaller, lighter atomic device that could be mounted on missiles or launched from submarines and was developed by a group led by Johnny Foster—just 27 years old at the time and a future director of Lawrence Livermore National Laboratory. Foster was known for having the ability to recognize technical problems and the knack for making the tools to fix it. The new device’s development and Foster’s leadership helped launch the Laboratory’s success and its evolution into an innovation powerhouse.

Today, the world faces significant challenges to its security as technological advances have increased the ease with which non-nuclear states might develop nuclear weapons. Greater regional conflict increases the possibility that instabilities could lead to proliferation among neighboring hostile nations. Now more than ever, the U.S. and the international nonproliferation community need tools to identify incipient illicit nuclear weapons development efforts. We need to know about such developments long before they lead to an explosive test, the signature of a long development process.

And once again, as described in the article beginning on page four, Livermore has recognized a technical problem. Possessing the knack for making the tools to fix it, we are developing the technology to address this critical national security need. Artificial intelligence, neural networks, and deep learning—technologies that the Laboratory has unparalleled experience with—offer a possible way to mine open sources of information on the Internet to detect states and non-state actors and track their activities and capabilities. Researchers in our Machine Learning Group developed a neural network trained to look for specific objects in unlabeled data obtained from some known users.

This gives geophysicists a validated target for locating and mapping distributions of this type of gas hydrate formation in the seafloor. The article beginning on page 16 discusses Livermore’s contribution to the development of Scorpion, a 125-meter-long linear induction accelerator diagnostic tool that will generate radiographic images of contained subcritical experiments with fissionable nuclear material, specifically plutonium. Once deployed underground at the Nevada National Security Site, its multi-pulse flash x rays will offer researchers a view of the late stages of a nuclear weapon implosion, help identify the effects of aging and manufacturing on the stockpile, and inform future improvements to the stockpile.

The Laboratory is particularly well-positioned to solve these problems. We can pull together a range of experts with diverse skills into multidisciplinary teams to find solutions to the many security challenges facing the nation today—just as we did in the 1950s, when a young physicist led a group that provided the tools to meet the challenge of the Cold War.®
A nuclear nonproliferation analyst searches for evidence that can help detect and characterize the status of a state’s nuclear fuel cycle activities, including those that could assist in the clandestine development of nuclear weapons. In addition to information derived from classified intelligence or other confidential means, an increasingly relevant information source for analysts is the rapidly growing body of information openly available on the Internet. A hypothetical example might be an image of a gas centrifuge, which can be used to enrich uranium, in an obscure technical newsletter published by a research institution.

Although the publication may be freely available on the Internet, the image of a centrifuge might be unlabeled, or the caption only identifies the names of the VIPs touring the facility. The article may be only one of millions of Internet-searchable links, in many publications and languages.

In that sea of information, how could the analyst find the article with this vital clue? How to sort through billions of bytes of data to get straight to the evidence?

One of Livermore’s mission research challenges is to develop innovative technologies to prevent, detect, counter, and respond to the use or threatened use of weapons of mass destruction. The Laboratory supports the work of the National Nuclear Security Administration (NNSA), other U.S. government agencies, and international bodies such as the International Atomic Energy...
Agency (IAEA) to advance the nuclear nonproliferation mission. All the players in the nuclear nonproliferation community have a common goal: identifying early warning signs of proliferation—the development and spread of nuclear technologies for weapons—and a detailed, ongoing understanding of the status of extant nuclear weapons programs.

Livermore researchers are developing technologies that use data analytic capabilities to extract valuable nuggets of information from massive data streams to detect, characterize, and track nuclear weapons proliferation. Deep neural networks (DNNs) and machine learning offer a way to sift through these data streams for clues, which might be found in peer-reviewed scientific journals, local newspaper articles, patent applications, purchase orders for materials or equipment, and even job postings for nuclear-relevant skills.

**LBANN Provides the Foundation**

In 2015, a Livermore team led by machine learning researcher Barry Chen and high-performance computing (HPC) researcher Brian Van Essen developed the Livermore Big Artificial Neural Network (LBANN) Training Toolkit for accelerated training of large neural networks on HPC (See SDTR June 2017, pp. 16). An artificial neural network (ANN) is a machine learning model that “learns” a task by exposure to examples. ANNs are simplified mathematical models loosely inspired by biological brain structure. ANNs consist of individual “neurons” organized in multiple layers, each of which learns how to transform inputs into outputs optimized to achieve a task such as categorizing images into those with cars or trucks. Provided with multiple examples of images of cars and trucks, ANN layers progress through the input layer, one or more hidden layers, and finally the output layer, learning to successively detect meaningful aspects from the original images to discriminate between cars and trucks. Earlier layers “learn and remember” how pixels form edges, corners, and texture features. Intermediate hidden layers learn how these features form the bumpers, wheels, and doors of cars and trucks. Finally, the output layer combines everything to learn high-level details that distinguish car images from truck images, like the presence or absence of a trunk, truck bed, or hubcap. ANNs that have many layers between the input and output layers known as DNNs make it possible to model complex nonlinear mathematical relationships and solve large computational problems like image classification or object recognition.

After considering what kinds of problems a neural network could solve among the Laboratory’s missions, Chen and his collaborators recognized a need for nuclear proliferation analysis. “The analysts face a deluge of data. Retrieval of useful information is the challenge,” says Chen. “There’s too much information for any one person to sort through.” Chen imagined that a neural network-based data retrieval system could make life easier for analysts by doing most of the sorting for them if the network could be trained to recognize and retrieve useful information. “There’s a lot of open-source data that we’re leaving on the table because we can’t manually process it,” says Yana Feldman, associate program leader for international safeguards in Livermore’s Global Security Principal Directorate.

**Learning Other Languages**

Discussions with the Laboratory’s nuclear proliferation analysts led to a research project “Large-Scale Multimodal Deep Learning for Nuclear Nonproliferation Analysis” funded by the Laboratory Directed Research and Development (LDRD) Program, begun in 2017. The three-year project goal was to deliver a system that allows analysts to retrieve multimodal open-source data such as text, image, audio, and video relevant to nuclear proliferation.

Developing the system required that the computational engineers, data scientists, and nonproliferation analysts assigned to the project learn new ways of working together, and even new ways of talking to each other. When the neural network experts sat down with the nonproliferation experts, they had to develop a shared lexicon to advance the project’s goals. Even a seemingly simple word like “data” had different definitions for different groups. “Data is a vague term,” says Brenda Ng, Livermore data scientist and machine learning group lead, “For us, ‘data’ is labeled input as well as the target output. To a proliferation analyst, ‘data’ is any video, text, or image. We worked with the analysts to understand how to categorize and label the data. That way, we could derive labeled data that the model can use to learn to map the data from text into specific categories.”

“We had to get enough labeled data to test the system so that we could give the analysts something that would work,” says Carmen Carrano, computational engineer at Livermore who works on image processing, machine learning, and video analytics and developed and tested the software codes for the system. “Coming up with the language for captions or tags for the images was a challenge. The analysts would give us sentences describing an image, but we needed to know which part of the sentence described what we’re actually looking at.” Ultimately, persistence paid off. “Lots of iteration was required,” says Feldman, “Relabeling, re-annotating videos, and so on. We found that working closely with the machine-learning specialists was an important factor in making this project a success.”

**Neural Networks for Nonproliferation**

“People might ask, aren’t companies like Google doing unlabeled image-video search retrieval? To some extent yes, they are. If you’re looking for images, you can perform a keyword search to find images...
labeled with text descriptions. But for unlabeled images, keyword search doesn’t work. That’s why we decided to use neural networks to help us index unlabeled data, and more importantly, specialize the way the neural network index data related to nuclear technologies. This lets us find images and video about specific nuclear technologies that do not have text descriptions,” says Chen.

Central to the system, the team created the “Semantic Wheel.” Each “spoke” of the wheel represents a data modality: text, image, audio, video. “Neural networks are a great way to index and organize data for easy searching,” says Chen. “Data of different modalities would be projected into a classification learning problem with feature vectors called “a joint feature space,” such that the distance between conceptually related data is small. This index provides a search mechanism for the analyst.” For example, images and video of gas centrifuges, and text containing the words “gas centrifuge,” would all reside “near” each other in a feature space, such that the distance between conceptually related data is small. This index provides a search mechanism for the analyst.”

To develop the text spoke, the team first gathered as much data as possible from freely available internet sources using automated tools. “We had to develop methods to clean up the information. For example, to distinguish watermarks in PDF files from relevant information,” says Computational Engineering Division machine learning scientist Sam Nguyen. The other big challenge was to adapt existing natural language processing models to the task of finding what proliferation analysts were looking for. The team needed to develop a compressed, numeric representation, or an “embedding,” specific to nuclear nonproliferation phenomena. “To ‘embed’ means to take a data object and map it to a numeric representation so that data object can be integrated into a neural network for further analysis,” says Ng.

Industry search engine and social media giants have published embeddings for text, but the Livermore team needed to develop embeddings specific to the nuclear proliferation-related content they monitor. “At the time, ours was one of the earliest groups that trained our own models to learn customized embeddings for our application,” says Ng. “Now, this is becoming more common. For example, the biomedical community has come up with BioBERT, which is their customized embedding for medical texts.”

“Entity reconciliation” emerged as another success of the project. Ng’s team tackled this challenge using context-sensitive models. “Analysts may refer to one thing in many different ways,” she says, “So mapping different names to the same concept is a challenge. But in managing this, we were able to deliver a system to analysts that went beyond key word retrieval, which is really remarkable.”

Data representing text, images, and video of like items, in this case cooling towers, are mapped into a feature space in close proximity to one another.

Training Neural Networks to Index

To train the DNN, the team gathered images and schematic diagrams of such technologies as uranium gas centrifuges, flow diagrams, reactors, fuel elements, cooling towers, spent fuel pools, reactor cores, hot cells, and uranium cylinders from a variety of open sources including U.S. Department of Energy and IAEA publications, Wikipedia, and various news sources. The team used both labeled and unlabeled images and video to train the DNNs. The goal was to map raw unimodal features into a feature space where similar data are close to each other. The DNN would project these labeled images, for example of gas centrifuges, in mathematical proximity to one another in the feature space. The learning process generates n-dimensional vectors of numerical features that represent a target object called “unimodal feature vectors,” which mathematically represent individual images, text excerpts, or video clips of the targeted object.

The second phase of the project was to train another DNN to map each of the unimodal feature vectors into a multimodal feature space that maps and aggregates conceptually related data to nearby locations. After the training, the feature vectors representing all text, images, and video of gas centrifuges, for example, are in close proximity within the multimodal DNN’s feature space. Once this learning process is sufficiently advanced, the analyst can execute various searches using text to search for images, an image to search for like images, text to video, and image to video.

The video spoke presented unique data curation and computational modeling challenges. The information conveyed by a video is often greater than the individual frames. As a result, analyst annotations often expressed abstractions not tied to any particular frame or region of interest, such as the outcome of a process. Therefore, the video team and analysts worked together to develop new ways to curate and label video data for training the video spoke. On the work’s computational modeling aspect, engineer Doug Poland, who works on computer vision, video analytics, and machine learning, says, “Video presents a fundamental problem that has not been completely solved. We are developing a new framework based on spatial and temporal modeling for capturing the complexities of video scenes.”

Unimodal Learning Saves Effort Later

One of the innovations emerging from this work is the insight that training the unimodal spokes first saves learning effort later. “You can recycle a lot of relationship data from the unimodal data so that you don’t need as much multimodal data for training,” says Chen. “Consider, for example, the concepts of airplanes and clouds. In images you’d likely see airplanes flying through clouds or flying above clouds. This sort of relationship also manifests itself in text, so when training the multimodal DNN, our system will recycle these pre-learned unimodal relationships in the multimodal feature space.”

In this way, training the neural networks of the unimodal spokes first reduces some of the data required to train the multimodal DNN. “The lack of truly large-scale aligned, multimodal datasets presents a challenge in multimodal training,” says Jeayoung Choi, a graduate student at the University of California, Berkeley-affiliated International Computer Science Institute. “The individual datasets in each modality were not always big enough to train the individual spokes—data collection has been a bottleneck in much of machine learning’s development. One potential solution is to combine multiple datasets for training.” Several issues needed to be addressed such as different semantic coverage between datasets and certain concepts being over or under-represented quantitatively—a lot of text and fewer images for a given element of the nuclear fuel cycle, for example.
The overall question was, "Can we combine multiple datasets and still get a good alignment so that similar multimodal data were close to each other in the hub?" We had two objectives in developing training methods," says Choi. "We did not want to worry about the different characteristics of the datasets. Second, we wanted to make the methodology scalable and efficient." To address the first problem, multitask learning was integrated into the framework with "joint loss weight optimization." This method treated multiple datasets as if they were one large dataset. Uncertainty-based weighting compensated for the loss of matched data as the multimodal dataset was scaled up by combining smaller datasets. During the model training process, these "loss weights" were jointly optimized with other model parameters. The Livermore work was the first to use uncertainty-based weighting to handle the loss-with-scale-up issue between multimodal data sets.

For the second problem, Choi developed a strategy of two-stage, shared representation optimization. In this process, each modality is first optimized individually—text or image or video. During the next step of intermodal optimization, the model's unimodal semantic structure is transferred to a joint semantic space (text, images, and video together). In the joint space, paired data might be imperfectly matched. To deal with this problem, the model uses a "bidirectional quadruplet loss function," so-called because it takes two pairs of aligned data as the input. The model now jointly optimizes the cross-modal semantic relationship of the pairs, compensating for imperfect alignment of data between modalities. This process was crucial to the model’s ability to learn a discriminative joint semantic structure—in other words, learning how to find the object the analyst is looking for whether it is text, image, or video. The result was a robust DNN whose performance showed significant improvement compared to training methods reported by other researchers.

**Working System Delivered**

The system the machine-learning team demonstrated to the analysts can conduct several types of multimodal searches. The input of a sample image of a hot cell successfully returns unlabeled images of hot cells from among tens of thousands of possibilities. Text-to-image and text-to-video searches also show a high degree of accuracy. Image-to-video, text-to-video, and video-to-text searches show promising results. The video spoke, which is still in development, has demonstrated success at executing an image-to-video search, identifying cooling towers within video frames from a sample cooling tower image. Data scientist Steven Samson developed the user interface and the search index that stores, delivers, and displays target information to the user interface as quickly as comparable commercial search engines. "We wanted to make sure that the interface was responsive—delivering with a sufficiently rapid turnaround," says Samson.

"This system gives me the capability to quickly find things that I would not have been able to find manually," says Feldman. "It could potentially alert me to something that might interest me—a two-second frame in a two-hour video. Without it, I’d have to watch the entire video, and with hundreds of hours of new video being added to the internet every minute, that’s just not practical. It gives us the ability to process more data than we ever could before."

The team plans to further develop partnerships to improve the system by advancing the video spoke and adding an audio spoke, as well as other types of data such as patent schematics. "We will always love to customize the system to meet the needs of individual analysts. Having more analysts in the loop to provide feedback on retrieval results will help the system learn from its mistakes and improve performance," says Chen.

A new multimodal effort funded by the NNSA’s Defense Nuclear Nonproliferation R&D called Advanced Data Analytics for Proliferation Detection (ADAPD) is also looking to leverage the system to help with its own mission. ADAPD brings together Livermore, Los Alamos, Oak Ridge, Pacific Northwest, and Sandia national laboratories to develop a global-scale, real-time capability to detect, locate, and characterize low-profile proliferation. Eddy Banks, ADAPD’s principal investigator at Livermore, says, "We need a predictive capability to detect the steps that a nation might take as it moves toward weapons development."

Detecting seismic signals from a nuclear test is too late—by then, the proliferator already has a weapon. ADAPD is looking to detect signals from earlier activities like hiring people with particular nuclear weapons engineering expertise, orders of relevant equipment, or an increase in traffic around a targeted facility. Detecting these signs provides the nonproliferation community with the evidence it needs to mobilize international efforts to intercede.

"This is where the work of Barry Chen’s group is important to ADAPD," says Banks. This partnership between human minds and deep neural networks to find and interpret evidence promises to help the international community reduce the dangers of the spread of nuclear weapons.

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**Key Words:** Advanced Data Analytics for Proliferation Detection, ADAPD, Artificial Neural Network (ANN), information retrieval, bidirectional quadruplet loss, Deep Neural Network (DNN), semantic embeddings, joint loss weight optimization, Laboratory Directed Research and Development (LDRD) Program, Livermore Big Artificial Neural Network (LBANN), machine learning, multimodal deep learning, natural language processing, nuclear fuel cycle (NFC), nuclear proliferation, nonproliferation, open-source information, Semantic Wheel.

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Computing is in Livermore’s DNA. From its founding in 1952, Livermore has depended on computers to help answer extremely difficult technical questions. As physicist George Mauchen said early in Lawrence Livermore’s history, “We are not like Thomas Edison. We don’t test a thousand light bulbs to figure out what is the best filament. Here we model everything first on a computer, then we do a test to confirm what we already know from our modeling.”

Fast forward to 2020. Lawrence Livermore is leading a new research center responsible for creating high-performance computing (HPC) software to aid the development of groundbreaking functional materials. These materials respond to stimuli such as voltages, light, or magnetic fields and could be used in quantum computers, photovoltaic solar cells, or solid-state data storage devices.

Funded by the Department of Energy’s (DOE’s) Basic Energy Science (BES) Program, the Center for Non-Perturbative Studies of Functional Materials under Non-Equilibrium Conditions (NPNEQ) is working to develop software that can simulate movements of electrons and ions at the quantum mechanical level. Based on a method called real-time time-dependent density functional theory (RT-TDDFT), the software allows researchers to simulate the response of quantum mechanical electrons and ions in a material in response to strong external stimuli such as a high-intensity laser. This might trigger an instantaneous change of crystal structures, leading to a dramatic change of electronic properties. Such nonequilibrium phenomena taking place in a billionth of a second have long been sought to make new types of materials.
opto-electronic devices that source, detect, and control invisible light such as gamma rays, x rays, ultraviolet, and infrared.

For functional materials—such as the ones used in transistors and diodes—the static picture of the state of electrons calculated by DFT was good enough for explaining their functionalities. Now, the RT-TDDFT software developed at the NPNEQ Center, combined with the DOE leadership-class HPC systems, opens the possibility of simulating nonequilibrium states of materials in the nonperturbative limit where standard approaches that rely on small corrections to exact model systems no longer apply. The software developed by the Center is expected to open up a new era of ab-initio material design, meaning it will allow researchers to go beyond material modeling to building custom compounds from the ground up with specifically designed properties.

The NPNEQ Center brings together three national laboratories with complementary resources and expertise. Lawrence Livermore, an internationally recognized leader in HPC architecture and software design, is contributing its supercomputing facilities and expertise in software development for exascale HPC. Researchers from SLAC National Accelerator Laboratory are using their cutting-edge experimental and theory programs in advanced materials science to conduct ultrafast experiments and simulations. SLAC also assists in the implementation and testing of additional software functionalities. Researchers from Lawrence Berkeley National Laboratory (LBNL) are expert in spectroscopy simulations and assisting with software validation through interpretation of experimental results.

Tadashi Ogitsu, the NPNEQ Center director and a physicist specializing in computational physics in Livermore’s Physical and Life Sciences Directorate, says, “Now that we have the computing power we need, our vision is to develop a first-principles, nonperturbative simulation framework that provides material-specific predictions and guidance for experimental efforts. We are using an experiment-theory approach. Our goal isn’t to develop the materials themselves, although that is an exciting prospect. Our goal is to help many industries, educational institutions, and other organizations working to design, synthesize, and characterize new materials by providing easy-to-use tools to handle the complex, convoluted data that comes from material experiments.”

### Powerful Computers Matched to New Software

The software developed by the NPNEQ Center is specifically designed to take advantage of the ongoing transition to exascale computing. This powerful combination of software and exascale supercomputers will allow researchers to perform theoretical modeling at extreme scales and complexity, and to use these models to guide and interpret corresponding experimental efforts. Data from experiments will be fed back into the software to refine and validate the simulation approaches to continually improve the software.

The Center researchers are currently tapping into the power of Lawrence Livermore’s Lassen HPC system for this effort. Most recently ranked number 17 on the November 2020 Top500 list of most powerful computers, Lassen has a peak performance of 23 petaflops (23 quadrillion calculations per second). The Laboratory is also home to the Sierra HPC system, ranked number 3 with a peak performance of 125 petaflops, and will continue to dominate the Top500 list when El Capitan starts up in 2023, with an anticipated performance of 1.5 exaflops (1.5 quintillion calculations per second).

Livermore’s most current HPC systems use a combination of central processing units (CPUs) and graphics processing units (GPUs). HPC designers looked at earlier systems, optimized by Lawrence Livermore’s experts in software development for exascale, Xavier Andrade and Alfredo Correa, bring unique expertise in code optimization and RT-TDDFT software development. While RT-TDDFT software was available in the past, it was not commonly used in part because it took more time and expense than DFT. But now the NPNEQ Center is working to broaden the use of TDDFT software, making it faster and easier to use.

### Supporting BES Goals in Tandem with Other Centers

The NPNEQ Center supports BES interest in fundamental investigations in the fields of material and chemical sciences by creating software that will work for a variety of applications on a range of potential materials that optimize the full power of HPC systems. With code that is easier to run, users will be able to prepare simulations and make predictions about complex systems for a number of applications. The Laboratory’s BES Lab Coordinator, Eric Schwager, says, “The BES Computational Materials and Chemical Sciences program was established with the goal of developing user-friendly, open-source software that can benefit many researchers. The NPNEQ Center is directly contributing to this goal by enabling the use of sophisticated TDDFT codes that take full advantage of the latest HPC platforms.”

The NPNEQ Center is one of several BES centers that complement one another. Livermore Laboratory also participates in the Center for Predicitive Simulation of Fundamental Materials, led by Oak Ridge National Laboratory, which is focused on the development of quantum Monte Carlo-based approaches. The Laboratory also participates in the SPARC-X Center, led by Georgia Institute of Technology, which focuses on a computational framework for performing highly scalable DFT calculations.

With easy-to-use software tools, the power of HPC will become more accessible to researchers, paving the way to transformative technologies such as novel quantum materials and the design of materials with specific functionality. Software designed by these centers can be expanded to support new investigations in nanomaterials, photovoltaics, hydrogen production, and condensed matter physics.

—Karen Rath

Key Words: Center for Non-Perturbative Studies of Functional Materials under Non-Equilibrium Conditions (NPNEQ), time-dependent-density functional theory (TDDFT), quantum materials.
Scorpius, a 125-meter-long linear induction accelerator diagnostic tool, is designed to generate high-speed, high-fidelity radiographic images of contained subcritical experiments with fissionable nuclear material, specifically plutonium. Once deployed underground at the Nevada National Security Site (NNSS), Scorpius’s multipulse flash x rays will offer researchers a view of the late stages of a nuclear weapon implosion. As a diagnostic, Scorpius will help identify the effects of aging and manufacturing methods on stockpile performance and inform future stockpile changes, including modernization programs and incorporation of enhanced security features. As a type of scientific classroom, Scorpius will offer training and knowledge for the next generation of experimentalists and weapon designers in the way underground testing experience and data enlightened designers decades ago.

“Scorpius represents a significant step forward in the diagnostics supporting the nation’s nuclear stockpile modernization,” says Mike Zika, deputy for Transformational Weapon Science in the Weapon Physics and Design Program of the Laboratory’s Weapons and Complex Infrastructure Principal Directorate. “The use of plutonium rather than non-fissile surrogate material will set Scorpius apart in enabling modern certification and assessment of the current and future nuclear stockpile.”

A Powerful Partnership
Scorpius will be delivered by the Advanced Sources and Detectors (ASD) project within the National Nuclear Security Administration’s Enhanced Capabilities for Subcritical Experiments portfolio. Los Alamos National Laboratory leads the joint effort to design and build Scorpius, leveraging expertise from NNSS and Lawrence Livermore and Sandia national laboratories.

The advanced diagnostic tool will consist of four main components. Its injector will generate high-energy electron beam pulses, and accelerator cells will boost the injected electron beam energy to over 20 mega electron volts. In the downstream transport region, the high-energy electron beam will collide with a metal target generating x rays that penetrate test objects. Finally, a detector will convert the x rays into images recorded by a sensitive, high-speed camera. Because plutonium is very dense and moves very fast during the experiment, a short burst of intense x rays is required for the best image resolution.

Livermore’s innovative solid-state pulsed-power technology will drive the Scorpius accelerator and energize the injected electron beam. With pulsed power, energy gradually accumulates into capacitors and is quickly released, maximizing energy over time to reach exceptionally high power levels. The difference offered by the Livermore technology is its reliance on solid-state integrated circuits to create an electrical pulse rather than the separate generator bank used in older technologies. The Livermore pulsers are designed to make at least four 25,000-volt pulses, providing Scorpius unique flexibility to program pulse width and spacing and optimize the number of x rays imaging an object as a function of time.

“Scorpius will provide an unprecedented ability to tailor the radiographs to individual experiments,” says Zika. Dave Funk, the Los Alamos lead for the project, adds, “We’ve made...
a bold choice by choosing solid-state pulsed power. The Livermore technology gives us the opportunity to develop a machine like no other. This will enable transformational experiments, gathering the data many of us have long desired to see.” Livermore has already built prototype pulsers to perform integrated testing of the accelerator and injector cells designed by partners at both Los Alamos and Sandia national laboratories. Once the pulsers are tested with prototype accelerator and injector cells, Livermore will build all 984 pulsers specified for Scorpius. Flash x-ray (FXR), a Livermore radiographic tool with all 984 pulsers specified for Scorpius. Flash accelerator and injector cells, Livermore will once the pulsers are tested with prototype Los Alamos and Sandia national laboratories.

Livermore has already built prototype pulsers for Scorpius. Flash x-ray (FXR), a Livermore radiographic tool with double-pulse capability for high-speed imaging (See S&TR July 2018, pp. 12-15), will evaluate selected components of the accelerator’s hardware and diagnostics during the design and build process.

Now that the prototype pulsers have been delivered to partner laboratories and support Livermore’s integrated testing of the Los Alamos accelerator cell prototype, the team is looking ahead to equipment purchases and fabrication steps that will bring Scorpius to life. Commissioning of the injector at the Integrated Test Stand, planned for 2023–2024, will help establish and train an operations team of NNSS employees while providing a first systems-level demonstration of the technology. The multi-lab team expects Scorpius will be commissioned at full energy in U1a by 2025. “Anticipating national needs is our mission, and drives our timeline,” says Zika.

One of the first experiments planned will confirm the viability of Livermore’s modernization programs to lengthen the service life of an existing warhead while enhancing its safety, security, and reliability. Scorpius will also serve as a training tool for pulse-pulse engineering—a technology with a limited pipeline of researchers, particularly in terms of understanding an all-solid-state machine, according to Zika. “Scorpius is the first of its kind in the world,” he says. As deputy for Transformational Weapon Science, Zika, who serves in a newly created role and is responsible for the development of capabilities and partnerships to transform the nuclear security enterprise. Scorpius falls squarely in the categories of both capability and partnership development. “The technology is remarkable, and the Scorpius team never loses sight of its mission to fill a critical capability gap,” says Zika.

Key Words: accelerator, Cygnus, Nevada National Security Site (NNSS), nuclear weapons, plutonium, pulsed power, radiography, Scorpius, solid-state pulsed power, stockpile stewardship, subcritical experiment, U1a.

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Yucca Flat, Nevada. The devices weren’t working. Two high-profile tests of Livermore’s first nuclear weapon designs fizzled. Based on an idea promoted by pioneering physicist Edward Teller that was, among other things, supposed to reduce the required critical mass of uranium, the Ruth and Rae hydride devices were meant to revolutionize fission weapons design with their small size and impressive punch. The Cold War was heating up and the goal was to construct a powerful, versatile, and compact weapon that could be deployed in combat, require less nuclear material, and counter the perceived Soviet advantage of larger nuclear payloads. Instead, Ruth didn’t even vaporize the tower supporting it. And Rae didn’t do much better. All eyes were on the Livermore team, especially those in Los Alamos and Washington, D.C.

A Remarkable Approach

After helping Allied B-24 bomber pilots evade Nazi radar during World War II, John S. Foster Jr., aka “Johnny” Foster, arrived in Berkeley, California in 1949 on a motorcycle to join Ernest Lawrence’s Rad Lab in a group led by experimental physicist Luis Alvarez. Before long, Foster was responsible for developing a massive ion-pump vacuum system for a new accelerator invented by Lawrence. The Mass Test Accelerator (MTA) was crucial for producing tritium and plutonium for...
Johnny Foster

Foster and Brown had other ideas. They decided to pursue a hydride device despite Ruth and Rae's lackluster performance. The Radiation Lab's Berkeley site. Teller wanted to try yet another approach: every new hectoton warhead had to survive a “pre-mortem” review where an external group of physicists not involved in the design process examined the warhead assuming it would fail and left it up to Foster’s team to convince them otherwise. The time-consuming pre-mortems frustrated group leaders like Foster, yet they worked. While Teller initially insisted on continuing with a hydride device, he eventually came around to supporting Foster’s design. Then, after 20 months and several weeks of York’s pre-mortems, Cloe was packed into two suitcases in the back of a “woody” station wagon and driven to the Nevada Test Site under the protection of a summer intern carrying a .45-caliber pistol.

Foster couldn’t be sure what would ultimately happen. His intent was to build a small atomic warhead that worked, and his team had designed a weapon that pushed the very boundaries of science. The Livermore Laboratory (then still an adjunct of Lawrence’s Rad Lab in Berkeley) was meant to augment Los Alamos with thermonuclear research, but there was not much need for another laboratory if its weapons did not work. The stakes could not be higher: Early on the morning of Tuesday, March 1, 1955, an extremely bright atomic flash filled the Nevada desert skyline. This time, Foster’s warhead worked with an even greater yield than predicted. Cloe was Livermore’s first successful nuclear detonation, and Foster, thrilled by success, called Lawrence in a rush to deliver the good news, then realizing he had gone over by his boss’s head, found York, told him what he had done and apologized for breaching protocol. Within the next two years, Foster led his team to develop the Robin, a prototype atomic device for the future. The successes of the Hecoton Group meant an effective, smaller weapon could be deployed in a variety of situations: atop missiles, aboard submarines, and inside artillery shells. The versatility demonstrated by these successive designs led to the development of the miniaturized Polaris warhead, and nuclear deterrence became a viable strategy.

Legacy of a Legend

Foster and his colleagues in California laid the groundwork to keep the Cold War cold, earning them a personal visit from President John F. Kennedy in 1962, where he thanked Livermore’s scientists for helping the United States avoid a nuclear war. With his track record for innovative team science, Foster was asked to be the Laboratory director in 1961 where he expanded the Lab’s national security responsibilities to meet existing and emergent national needs. After time in Washington, D.C. as director of Defense Research and Engineering at the Department of Defense, and then at TRW Inc. where he worked as Officer for Science and Technology, Foster retired in 1988. Over the following years, Foster continued to advise Laboratory leadership on pursuing game-changing innovations in science and technology to make the nation more secure and won many prestigious awards for his service.

In 2015, Lawrence Livermore National Laboratory bestowed its inaugural John S. Foster Award to John S. Foster, Jr. himself at the Center for Strategic and International Studies in Washington, D.C. The Laboratory now gives the award annually (except for the pandemic year of 2020) in recognition of demonstrated exceptional leadership in science, technology, and engineering or policy formulation in support of U.S. nuclear security. Medal recipients receive a citation, a gold medal bearing the likeness of John S. Foster, Jr., and a $25,000 cash award.

The early years of Lawrence Livermore National Laboratory were guided by a variety of legendary names: Ernest Lawrence, Edward Teller, John von Neumann, John Wheeler, Herb York, and others. John Foster, Jr. led a life that was influenced by all of them but took a course of its very own. Foster’s biographer, Tom Ramos, a physicist and longtime Laboratory employee, has written Call Me Johnny, a book about Foster’s early years at Livermore. To Ramos, it’s difficult to overstate the influence of Foster’s work on the fate of the American nuclear deterrent. “This one man made difference after difference in service to the United States,” says Ramos.

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In November 2019, Linton Brooks was awarded the John S. Foster, Jr. Medal at a ceremony at Lawrence Livermore. A former head of the National Nuclear Security Administration, Brooks was instrumental in the establishment of both Strategic Arms Reduction Treaties, credited with removing 80 percent of the world’s nuclear weapons then in existence. During the ceremony, the 97-year-old Foster, touted by Brooks as a “living legend,” surprised the attendees and rose to the podium. Off the cuff, he remarked on the approach taken by the award’s winners, its namesake, and the Laboratory that pioneered so much over the last 67 years: “Great wisdom, wisely applied.”

Key Words: Johnny Stuart Foster, Jr., Ernest O. Lawrence, Lawrence Radiation Laboratory, Los Alamos National Laboratory, nuclear deterrence, thermonuclear weapons, University of California (UC) Radiation Laboratory.

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Neural Networks Search for the Nuclear Needle in a Haystack

Sometimes evidence of nuclear proliferation is not locked in a vault but hiding in plain sight on the Internet: images, video, job listings, and patent applications. To find these needles in the Internet haystack, nuclear proliferation analysts need tools to sift through hundreds of billions of bytes of extraneous information. Livermore researchers have developed an information retrieval system built on neural networks that have been trained to find nuclear fuel cycle-related text, images, and video. The product of a landmark collaboration of the Laboratory’s proliferation analysts and computing experts, the system makes image-to-image and image-to-video searches of proliferation technology possible—a powerful new tool to help analysts find evidence of nuclear development.

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