June 2022

Science Jechnology REVIEW

ACES Project Boosts Nonproliferation Expertise





Also in this issue:

Transparent Ceramics Virtual Beam Line Code Extreme Ultraviolet Lithography





About the Cover

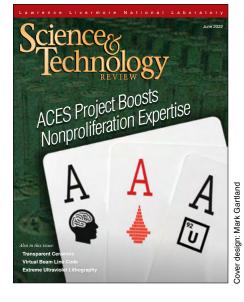
About S&TR

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As described in the feature article beginning on p. 4, the Adaptive Computing Environment and Simulations (ACES) project will develop new computer simulations of uranium enrichment, create a computational infrastructure to support and sustain these capabilities, and recruit and train an expert nonproliferation workforce. The cover illustrates ACES's three thrusts: brain trust, computer modeling, and uranium enrichment against an archive image from 1984 of gas centrifuges.



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June 2022

Lawrence Livermore National Laboratory

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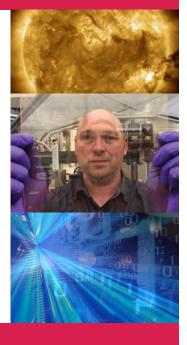
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Extreme ultraviolet research has resulted in stateof-the-art, multilayer-reflective optics for space exploration, microchips, and more.

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The latest generation of Livermore's workhorse laser physics code promises full integration across research and operations applications.





2 The Laboratory in the News

Commentary by Cindy Atkins-Duffin



W^{ITH} globalization and the spreading availability of technologies, nuclear proliferation challenges continue to grow and evolve. Lawrence Livermore National Laboratory works to stem proliferation by providing scientific and technological solutions and guidance to counter emerging threats. Working with the National Nuclear Security Administration (NNSA) and other government agencies, the Laboratory provides technical leadership to advance technologies that monitor and detect the proliferation of weapons of mass destruction worldwide, limit or prevent the spread of materials, and eliminate or secure inventories of nuclear materials and infrastructure usable for nuclear weapons.

In 2020, NNSA initiated the Nonproliferation Stewardship Program to ensure that foundational infrastructure, science, technology, and expertise in the Department of Energy (DOE) complex fully supports the U.S. government's mission to combat nuclear proliferation now and in the future. Some capabilities and expertise necessary for the nonproliferation mission originated from experience with materials processing and enrichment activities no longer utilized domestically at production scale. This initiative addresses the critical challege of technical knowledge transfer from experts to next-generation scientists and nonproliferation experts.

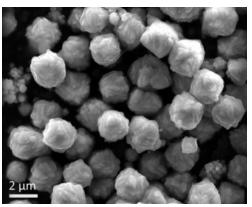
With its multidisciplinary teams of nuclear scientists, analysts, chemists, biologists, engineers, computer scientists, and technicians, Lawrence Livermore is an ideal place to develop the tools and solutions to address this challenge. The article beginning on p. 4 features the Laboratory's contributions to the Adaptive Computing Environment and Simulations (ACES) project. Funded by Congress and managed by NNSA's Office of Defense Nuclear Nonproliferation Research and Development (NA-22), ACES is the Laboratory's largest nonproliferation project.

ACES is developing the computational tools, infrastructure, and subject matter expertise necessary for proliferation detection and includes three thrusts: modeling uranium isotope separation centrifuge cascades, creating a corresponding computational infrastructure, and training and sustaining an expert nonproliferation workforce. The Laboratory has been the leader for the last two decades in the modeling and simulation

Clay-Based Antibiotics Kill Resistant Pathogens

Use of modern antibiotics has significantly reduced the number and severity of bacterial infections worldwide. Liberal or unrestrained use of antibiotics, however, allows some strains of bacteria to develop antibiotic resistance and become immune to traditional treatments. To tackle these especially resilient strains, Lawrence Livermore geochemists and biologists sought to rethink antibacterial formulation. Research published in the January 24, 2022, issue of *Scientific Reports*, points to the mineral components of naturally occurring clays as a promising antimicrobial source.

Clays rich in pyrite and smectite minerals have been known to express antimicrobial properties with the potential to kill antibiotic-



The Livermore team developed an artificial geochemical process using hydrothermal reactors to produce mineral substances that exhibit the same physical characteristics and reactivity

resistant bacteria.

absent the inconsistencies found in natural deposits. The synthetic clay formulations were tested on pathogens that have eluded conventional antibiotics and found to neutralize those pathogens in less than one hour of direct exposure.

The researchers then applied the minerals to mammalian fibroblast cells to assess whether the concocted alternative could safely eradicate pathogens in humans. Despite initial toxicity, the cells were able to safely regenerate once the antibiotic minerals were removed. Lead researcher Keith Morrison notes that the results "indicate that mammalian cells may experience minimal toxicity while invading pathogens are killed," raising hopes that the use of synthetic antimicrobial minerals to fight resistant strains may be imminent.

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Plasma-Based Lenses Show Potential

Powerful laser systems like those housed at the National Ignition Facility employ a wide array of optics made to redirect, amplify, and focus light beams to deliver a precise, intense shot at a target. These solid-state optical components are susceptible to physical damage from the extraordinary levels of energy they encounter. Despite constant design and resilience improvements, even the most robust optics will be unable withstand the relentless petawatt beam energies produced by an imminent generation of

ultrahigh-power laser systems. In an article published February 8, 2022, in *Physical Review Letters*, the research team, led by Livermore physicist Matthew Edwards, outlines the potential for diffractive plasma-based lenses to resist damage.

While plasma-based gratings, amplifiers, and mirrors have previously been demonstrated, focusing light by means of a plasma lens has proven challenging in high-repetition-rate experiments. The new lens design comes in two variations that make use of diffraction. The first relies on the precise excitation of a confined inert gas by two lasers; the resulting interference pattern produces concentric regions of plasma and gas. In the second design, lasers shape an existing plasma into the same configuration due to the plasma's tendency to be expelled from laser-excited regions. The result is a means of focusing the beam pulse that is exponentially smaller and more resistant to damage than even advanced solid-state optics.

The scientists tested both designs via computer simulation under a variety of conditions. The second method proved most effective in silico, capable of focusing beam intensities of up to 10^{17} watts per centimeter squared. With such high damage resistance, plasma lenses may be integrated into future ultrahigh-energy laser systems.

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New Methods Detect Effective Climate Mitigation Efforts

As researchers worldwide scramble for new technologies and policies to mitigate the effects of climate change, Lawrence Livermore climate scientist Mark Zelinka and international collaborators have devised statistical methods to more quickly detect changes in the global warming rate. In their study published March 24, 2022, in Nature Communications, the scientists' new methods filter out the noise of natural climate variability so that the signal—slowed warming from future emissions reductions-can shine through.

Trends in global temperature reflect not just the slow, steady rise associated with human emissions but also the short-term effects of natural fluctuations. For example, natural climate cycles like El Niño can make one year much warmer than prior years, obscuring whether emissions reductions are having a tangible effect on global climate. Drawing upon an approach pioneered by Zelinka and his Livermore colleagues, the team estimated and removed contributions from natural fluctuations on the global warming rate, allowing more easily detectable changes.

Previous methods could take up to 20 years to detect slowed global warming from emissions reductions. The new climate variability noise filter cuts this time in half. This means scientists and policymakers can gauge how emissions reductions alter the warming rate and whether nations are on track to meet their climate goals.

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Innovating and Delivering Solutions for Challenging Problems

of plant-level enrichment, and with ACES, the Laboratory will be integrating advanced data analytics and machine learning to answer new, complex questions and quantify uncertainties.

The research highlights in this issue also showcase Livermore's tool-building capabilities across a variety of fields to innovate and deliver solutions for challenging problems. As described in the article beginning on p. 12, the Laboratory has been a pioneer in optical lithography for decades. In the early 2000s, the extreme ultraviolet lithography team received two R&D 100 Awards for their work. Since that time, Lawrence Livermore researchers and their collaborators have made significant advancements in state-of-the-art, multilayer reflective optics for microchips and space exploration.

The Laboratory is one of the few places in the world that makes transparent ceramics more rugged and resistant to heat or corrosion than glass. These materials are ideal for scientific applications that require precision-particularly laser optics. The Livermore team also won an R&D 100 Award for their work on a gadolinium–lutetium–oxide transparent ceramic scintillator in 2016 and has continued to advance transparent ceramics. The research highlight on p. 16 details how the team recently leveraged additive manufacturing to control chemical composition and customize geometry-yielding transparent ceramics with unprecedented characteristics and enhancements.

The final research highlight beginning on p. 20 announces the launch of the next-generation of the Laboratory's Virtual Beam Line (VBL) laser simulation code: VBL++. This code utilizes physics models developed and prototyped by laser physicists from the National Ignition Facility and Photon Science (NIF & PS) Principal Directorate to understand beam propagation and diffraction, nonlinear frequency conversion, and other effects. VBL++ will also integrate the Laboratory's high-performance computing systems to generate highresolution simulations and unparalleled spatial resolution. VBL++ is a true testament to successful collaboration between the Laboratory's software engineers in the Computing Directorate and NIF & PS's physicists.

■ Cindy Atkins-Duffin is deputy principal associate director for Global Security.



The Adaptive Computing Environment and Simulations (ACES) project will advance fissile materials production models and reduce risk of nuclear proliferation.

RANIUM enrichment is central to providing fuel to nuclear reactors, even those intended only for power generation. With minor modifications, however, this process can be altered to yield highly enriched uranium (HEU) for use in nuclear weapons. The world's need for nuclear fuel coexists with an ever-present danger—that a nonnuclear weapons nation-state possessing enrichment technology could produce weapons-grade fissile material to develop a nuclear arsenal or supply radiological materials to others.

Nuclear nonproliferation—preventing the spread of nuclear weapons—is part of Livermore's national security mission. To this end, the Laboratory provides scientific and technological solutions and

advice to governing bodies—including the National Nuclear Security Administration (NNSA) and the International Atomic Energy Agency—to identify and counter emerging threats.

The Adaptive Computing Environment and Simulations (ACES) project will augment and modernize the Laboratory's ability to serve this mission through three thrusts. First, its researchers will develop new computer models and simulations of fissile materials enrichment using the gas centrifugebased method. "In nonproliferation work, analysts often integrate computational modeling into their assessments," says Stefan Hau-Riege, associate division leader in Applied Physics and leader of the ACES project. "The idea is to

provide them with a modern capability to model fuel enrichment integrating data science and machine learning." In the second thrust, researchers will create a new computational infrastructure to support and sustain this modeling capability. Finally, ACES will recruit and develop a trained workforce to carry out nonproliferation work that requires a detailed understanding of centrifuge enrichment technology. "ACES will capture knowledge from subject matter experts, improve the modeling and the computer environment to sustain the current expertise, and bring in new expertise," says Eddy Banks, deputy division leader for the Global Security **Computing Applications Division** (GS-CAD).

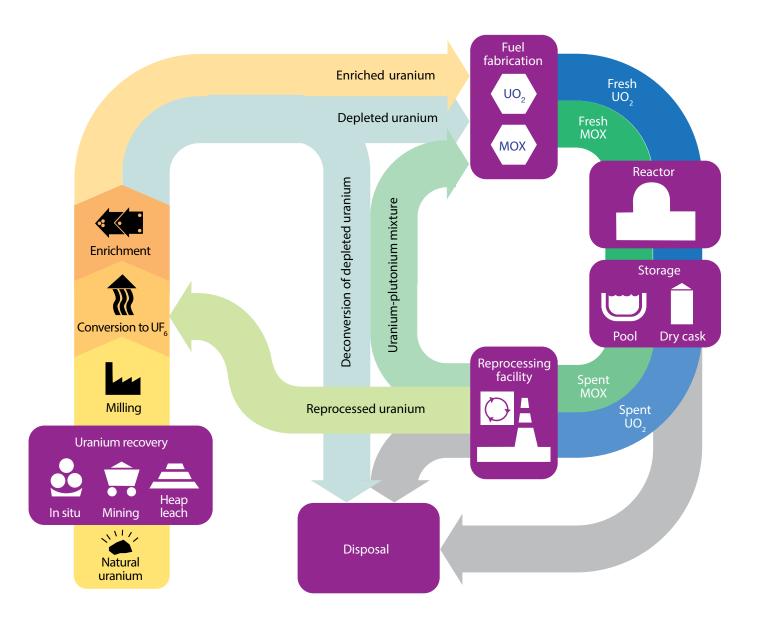
Improved Enrichment Simulations

The task of estimating enrichment yield derives from the fundamental chemical and physical properties of uranium isotopes. Two isotopes of the element uranium are commonly found on Earth, differing only in the number of neutrons in their nuclei. Each house 92 protons in its nucleus, but Uranium 235 (^{235}U) has 143 neutrons versus the 146 neutrons of Uranium 238 (²³⁸U). Nuclear fission—the release of energy from splitting atomic nuclei-provides heat to a nuclear reactor, transforming liquid water to steam that spins turbines to generate electricity. In theory, both isotopes can be split to release thermal energy, but in practice, only ²³⁵U can sustain a nuclear chain reaction in a reactor or a nuclear device. Naturally occurring uranium ore contains little 235 U, a mere 0.7 percent by mass. Because the dominant isotope, ²³⁸U, does not contribute to nuclear fission, natural uranium must be purified

or "enriched" to increase its percentage of ²³⁵U. Most nuclear power reactors utilize low-enriched uranium (LEU), which contains between 3 to 5 percent 235 U. HEU, the type of uranium used in weapons, can be obtained through multiple methods; however, gas centrifuges are overwhelmingly used to enrich uranium fuel. After mining and milling, uranium ore is eventually converted to a gaseous state, uranium hexafluoride (UF_6) , and passed through a cascade of rapidly spinning cylindrical centrifuges that separate the isotopes. The enriched UF_6 gas is eventually converted back into solid uranium for the next step in the nuclear fuel cycle—conversion to fuel rods for reactor use.

"Once a country has enrichment technology, how can we ensure that it performs only low-level enrichment and does not divert material to make weapons?" asks Kyle Chand, senior analyst in the Operations and Analytics group for GS-CAD. Most—but not all of the world's nations are signatories to the Treaty on the Non-Proliferation of Nuclear Weapons. Nonsignatories and extranational groups present areas of security concern. Through ACES, nonproliferation experts can simulate fissile materials enrichment at purported LEU enrichment facilities to understand how they might alter their processes to produce HEU.

Although the United States previously conducted research with centrifuge-based materials enrichment, which spurred small private-sector capacity, the nation did not rely on this technique to produce most of its fissile material stockpile. The lack of domestic experience with the process at industrial scale concerns nonproliferation experts, who assess the magnitude, efficiency, and effectiveness of other countries' enriched uranium production processes based on their technological configurations. "We



This nuclear fuel cycle infographic depicts the process of converting uranium ore concentrate into uranium hexafluoride (UF₆), enriching UF₆ concentrations of uranium 235 (235 U), and then fabricating uranium oxide (UO₂) or mixed-oxide (MOX) metal alloys for nuclear reactor fuel rods that are eventually reprocessed or disposed.

understand how the industrial processes work, but we have uncertainty over what goes into the models," says Chand. "We need to incorporate uncertainty quantification within software models and integrate them with data sciences. The ACES infrastructure will provide a modern, state-of-the-art infrastructure for data science not yet available within the NNSA complex."

Another major benefit of ACES is the experience its simulations will provide for increasing industrial capacity. "The U.S. doesn't have an enrichment industry now," says Chand. "We have a research and development program, but it's not

at the industrial level yet. ACES will allow us to gain experience if we bring up an industrial capacity." Computer modeling of enrichment cascades can provide nonproliferation analysts with signatures that characterize enrichment facility performance as well as system configuration and reconfiguration performance. At the Laboratory, ACES researchers will expand the capabilities of an existing set of models, applying data science and machine learning to model centrifuge enrichment at the cascade and facility scale. The models will also

be revamped to incorporate uncertainty quantification-methods that assess how accurately the models reflect known results in operating enrichment plants.

A second, complementary project at Oak Ridge National Laboratory (ORNL) focuses on modeling centrifuge enrichment at the component level and the gas dynamics of enrichment. Lawrence Livermore and ORNL will collaborate to develop an integrated modeling and simulation capability. To be effective, this integrated capability requires a computational environment that can handle diverse data and structures, function on a variety of computer systems, and adapt to the needs of projects with different objectives and users.

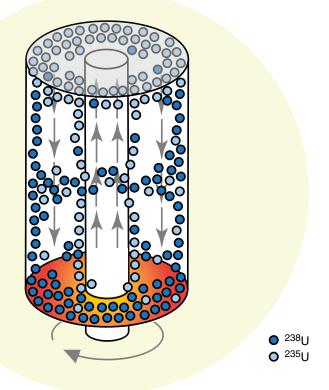
Advanced Computational Environment

Prior to ACES, nonproliferation analysts lacked a computing environment that efficiently modeled real-world uranium enrichment processes. Producing HEU requires a concert of material inputs, technologies, supplies, concentrations of experts at facilities, and other signatures that analysts can glean from public data. Analysts then generate models with a range of initial assumptions that can predict what they might later confirm. Previously, creating models was the task of programmers since analysts generally lacked the necessary coding skills. New functionality provided by ACES will circumvent the laborious process of changing model parameters and rerunning of simulations, yielding information the analysts need.

ACES pioneers a new type of computing environment that has been used in the private sector, but which has yet to be applied to NNSA's nuclear nonproliferation efforts. "Adaptive computing environments are unlike those in high-performance computing (HPC)," says Hau-Riege. "These adaptive environments consist of a variety of nodes,

and they lack the ultrafast networking used in HPC because they don't need them. For this application, we require nodes with different connected features." Node types can range from standalone desktops to cloud-based computers with different operating systems, and visualization and data-transfer capabilities. Porting a model—the translation of one programming language or protocol to another—is time-consuming, and usually necessitates rewriting code.

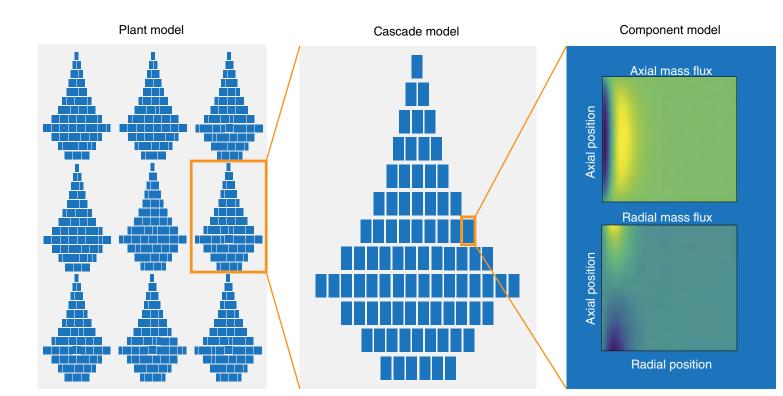
Prior to ACES, the Laboratory's efforts in computer modeling for nonproliferation were small scale and informal. "When I started at the Laboratory, we had servers and people running software that would affect other people's applications," says Livermore computer scientist Ted Stirm.



Inside a centrifuge or separator, centripetal force generated by rotation pushes heavier uranium 238 (²³⁸U)-containing gas outwards, leaving lighter gas molecules containing ²³⁵U closer to the centrifuge's center. Streams of gas slightly enriched with either ²³⁵U or ²³⁸U are then drawn out of opposite ends of the centrifuge. Passing UF₆ through one centrifuge only purifies the gas by a fraction of a percent, so this gas must travel through hundreds of centrifuges before it reaches a concentration high enough to be utilized for reactor fuel.

"We also lacked adequate personnel. Now we have funding and resources to architect a system that will provide stable support to multiple groups and projects."

The ACES computing infrastructure will leverage containers, which encapsulate software applications so that they can be deployed on a variety of systems, notebooks that allows users to create interactive documents, and Kubernetes, which maintains and manages ACES's containers. The nonproliferation world has a diverse digital workload utilizing web servers, machine learning with graphics processing units (GPUs), and web interfaces. HPC is not geared toward that kind of model. Traditional HPC systems are designed for performing tightly coupled, large-scale, and complex



The Adaptive Computing Environment and Simulations (ACES) project will allow users to simulate the centrifuge environment of fissile materials at different scales from an entire enrichment plant to cascades of centrifuges down to a single component

modeling tasks, but they are ill-suited for running services or providing the flexible compute options necessary for mixed workloads. A heterogeneous cluster with different node types allows the user to run whatever they need by leveraging containers, which package the code with the run-time environment. "We are not replacing HPC-we want to complement it by leveraging cloud-native, industrystandard technology so the applications developed for ACES can easily run on any cloud environment, with minimal porting. Kubernetes gives us that capability," says Stirm. The cloud environment makes software exchange possible. If the analysts need a different kind of computer system to solve a problem, they can move an application. "We can ship containers. We can build at Livermore,

ship to Oak Ridge and then run on their systems. Also, the containers talk to each other—the cascade simulation tool can talk to a facility simulation tool or call up a centrifuge tool," says Hau-Riege. ACES will also incorporate Jupyter Notebooks to help nonproliferation analysts run simulations themselves, analyze and document results, produce graphical plots, and share work with colleagues.

For those on the programming side, ACES provides a virtual test bed for comparing model results to real-world data from enrichment operations to validate that the models and simulations are providing reliable, explainable results. "We'll be coupling these models into a framework and collecting them into a virtual test bed capability," says Banks. Programmers can create a test

bed for a particular facility configuration, incorporating specific models and tools to simulate the configuration. Users can model processes at different scales, from individual centrifuges and cascades to entire facilities and even combinations of facilities. The test bed will fully manage simulations, provide information about its parameters and progressions, and capture the data generated by the simulations. Programmers will use test beds in the development environment, during the build-out of ACES infrastructure to test models and other software, as well as in the operational environment for nonproliferation projects.

Hiring and Sustaining Workforce

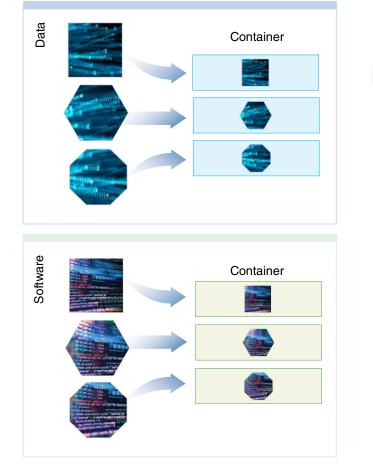
NNSA has committed to the ACES project to establish state-of-the-art computational solutions and grow and sustain an expert workforce. Prior to the Nonproliferation Stewardship Program (NSP), the federal government had no formal effort or dedicated funding to

maintain expertise in the nonproliferation modeling and simulation subfield. Expertise in uranium enrichment has been dwindling with the aging of prior generations, and has not been replacedformal university training in the field does not exist and a lack of awareness of the critical importance of this technology hampers recruitment.

ACES provides the opportunity for NSP to recruit and train dedicated new talent. "The project will bring a stable workforce and development environment," explains Chand. "We don't learn about uranium enrichment in college, so having a technical environment to train people is essential to developing new hires." This advanced computing hardware and

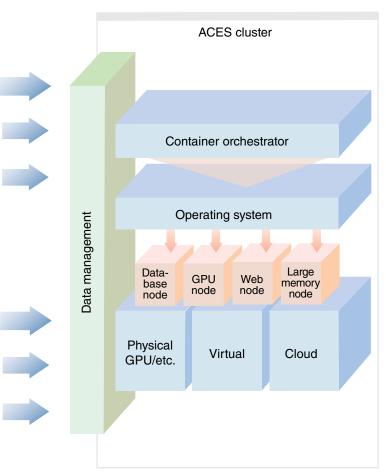
software environment provides the infrastructure necessary to attract and retain people. "ACES has a cuttingedge program integrating data science into nonproliferation. This is new, it's making inroads at the Laboratory, and will provide an interesting environment to address problems in nonproliferation requiring data science," says Chand. "ACES is an exciting project for computer scientists coming to the Laboratory," says Hau-Riege. "They can deploy software in Kubernetes and

As part of the ACES project, programmers will be able to containerize data and software (left). Containerized modules are independent of a computer's operating system, so the software can be plugged into different systems without rewriting the code. ACES will also allow different types of computer systems to connect within the ACES cluster (right).



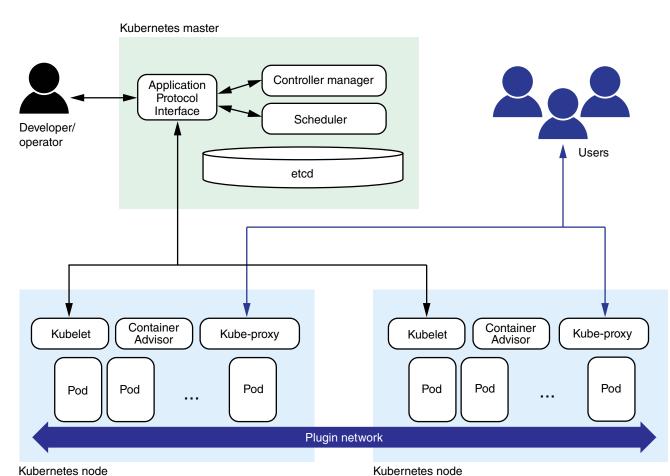
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containerize it without worrying about how to move it from one system to another." Beyond computer scientists, ACES is bringing in diverse specialties to support the next generation of nonproliferation analysis including physicists, computational modeling experts, data scientists with experience in machine learning and data-driven models, full-stack software developers, web developers, and nonproliferation analysts to interface with the Laboratory's customers in government agencies.





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Kubernetes node

A container-based, open-source software system used to deploy, maintain, scale up, and manage software, Kubernetes's architecture (above) allows users to "containerize" executable code so that it can be transferred from one operating system to another.

Support for R&D

S&TR June 2022

When complete, ACES will provide a set of modernized codes that incorporate better understanding of uncertainty quantification, a virtual enrichment test bed, a robust and portable computational environment that can be leveraged for other national security programs, and a revitalized workforce with the diverse expertise necessary to lead the next generation of nonproliferation stewardship. With this sustained computing infrastructure in the making, the Laboratory and NNSA are considering expanding ACES's range of applications. "This capability can be applied to other contexts

including energy security, cybersecurity, biosecurity, and other areas within Livermore's Global Security Principal Directorate," explains Scot Olivier, program leader for Nonproliferation Research and Development at the Laboratory. "Researchers in Global Security are also exploring ways to scale and implement this infrastructure for tackling a variety of national security problems. Through ACES, the nation will have a solid scientific and technical basis for understanding and assessing nuclear proliferation threats posed by fissile fuel enrichment in the nuclear fuel cycle and a capability to provide decision-makers

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with the knowledge necessary to meet those threats."

-Allan Chen

Key Words: Adaptive Computing Environment and Simulations (ACES) project, container, data science, fissile material, gas-centrifuge enrichment, highly enriched uranium (HEU), high-performance computing (HPC), International Atomic Energy Agency, Jupyter Notebook, Kubernetes, low-enriched uranium (LEU), machine learning, Nonproliferation Stewardship Program (NSP), Treaty on the Non-Proliferation of Nuclear Weapons.

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SHORT WAVELENGTHS YIELD BIG DIVIDENDS

In 2011, NASA's orbiting Solar Dynamics Observatory spacecraft captured this image of a filament eruption with extreme ultraviolet (EUV) multilayer mirrors Livermore developed for the mission. (Image courtesy of NASA.) **C**OLLABORATIVE research and development focused on the extreme ultraviolet (EUV) end of the spectrum has resulted in state-of-the-art, multilayer reflective optics used for space exploration, manufacturing microchips, and more.

Located on the high-energy end of the electromagnetic spectrum—just shy of x rays—EUV light claims the shortest wavelengths in the ultraviolet (UV) region: approximately 10 to 100 nanometers (nm). Emitted by the Sun and absorbed by the Earth's atmosphere, EUV's short wavelengths are created and utilized by many scientific and technical applications, including extreme ultraviolet lithography (EUVL), which etches nanometer-scale features onto computer chips, and for collecting images from space-based optical systems. Over the last few decades, the Laboratory has been at the forefront of developing multilayer optics and harnessing EUV's capabilities to benefit many mission-critical applications.

Pushing the Limits

The Laboratory's initial entry into EUV multilayer-coating technologies focused on creating coatings for laser-system optics and for some of the earliest space-borne solar physics telescopes, more than 30 years ago. (See S&TR, December 1999, pp. 11–13.) Laboratory physicist Regina Soufli, who has spent more than 20 years developing and characterizing EUV optics and advancing multilayer thin-film science, explains, "Livermore's Nova laser was one of the earliest laser systems that produced EUV and soft x-ray radiation—with waves that measure a few nanometers in length and are ideal for studying biological samples and nano structures. But we were faced with the challenge of how to make images from these x rays." Working with such short wavelengths is tricky: imaging must be performed in a vacuum environment and conventional refractive lenses will not work, because air and other materials absorb EUV. Reflective mirrors are needed to focus light, and yet, the EUV reflectivity of any single material at near-normal angles of incidence is nearly zero. To address this, scientists utilize multilayer interference coatings, which consist of alternating, thin-film layers with nanometer-scale thickness, of two or more materials, deposited onto an optical substrate. The constructive interference of EUV light bouncing between the layers results in high reflectance—a material's effectiveness in reflecting radiant energy. These multilayers enable operation at near-normal angles of incidence, resulting in imaging geometries with high effective areas, low aberrations, and exquisite resolution, using optics of modest size.

Over time, the Laboratory and its collaborators have made significant accomplishments, applying their know-how to evermore-challenging applications, including EUVL, which uses optical systems operating with light at 13.5 nm wavelengths to pattern microchips with the smallest achievable features. This technology was advanced at Livermore in collaboration with Lawrence Berkeley and Sandia national laboratories in a large Cooperative Research and Development Agreement (CRADA). The CRADA, initiated by Intel and funded by a consortium of semiconductor manufacturers, ran from 1997 to 2003 and garnered several R&D 100 awards. (See S&TR, November 1999, pp. 4–9; October 2002, pp. 10–11; and October 2003, pp. 8–11.) Due in part to the Laboratory's foundational contributions on multilayer optics and related metrology-the scientific study and realization of measurement-EUVL is now widely employed in manufacturing the microchips that power smartphones, tablets, and other digital devices. Eric Panning, Intel engineering manager, says, "Lawrence Livermore National Laboratory was a pioneer in addressing one of the biggest challenges of EUV—developing high-reflectivity, multilayer surfaces while simultaneously meeting figure and roughness requirements. The Laboratory figured this out, which propelled the program forward. Our efforts continue to push the boundaries of what is possible in this area and our collaborations have proved extremely valuable over the decades, with results that have benefited the entire microchip manufacturing industry."

As EUV-related technologies matured, Livermore's expertise in thin films—designing, depositing, and precisely characterizing thin layers from a few micrometers thick down to individual atomic layers onto various substrates—and in metrology grew as well. Accuracy tightened from the nanometer to picometer (one trillionth of a meter) range. Coating designs and functionality evolved from periodic—narrow band, equal thickness, and repeating pattern—to aperiodic—broad spectrum, unequal thicknesses, and nonrepeating patterns. These advances were motivated by the growing needs of various applications, including EUVL, solar and planetary physics, and astrophysics, as well as laboratory-based tabletop lasers, free-electron lasers, and attosecond $(10^{-18} \text{ or one quintilionth of a second) physics.}$

For these innovative technologies, the interfaces between coating layers that determine optical performance must be stable and have a smoothness at the atomistic level. But because no accurate theoretical models exist for these interfaces, researchers conduct detailed experimental studies focused on each layer and its thickness. Using these experimental data, Soufli and her team constructed models specific to each material layer in a system and studied how they interact. Armed with data from multiple studies, the team modifies the deposition process, refining and improving these complicated multilayer coatings. Reflectance measurements obtained at the exact EUV wavelengths of each coating are collected at the Advanced Light Source synchrotron beamline 6.3.2. at the Lawrence Berkeley National Laboratory (LBNL) Center for X-ray Optics (CXRO), led by Eric Gullikson, a key collaborator.

As applications become more dynamic and multifaceted, so do the requirements for these specialized optics and coatings.



The Geostationary Operational Environmental Satellites contain the first telescopes that image at six different EUV wavelengths using a single pair of mirrors. A close-up view of a test secondary mirror (above) with six segments, coated with molybdenum–silicon and molybdenum–yttrium multilayers. Each segment is designed to reflect at a different EUV wavelength. An aperture selector in the telescope allows illumination of the specific coating segment needed to pass the desired EUV wavelength. (Photo by Garry McLeod.)

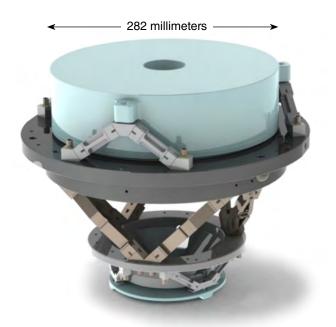
"The astrophysics community now needs broadband coatings with an extended wavelength range up to 90 nanometers to measure the EUV stellar flux or brightness of exoplanet host stars. Such measurements could help researchers understand how exoplanets lose their atmosphere to EUV ionization and heating. We don't, however, have accurate refractive index values for the corresponding multilayer coating materials, in the 30- to 90-nanometer range. So, we need to accurately measure these values and use them in our models to provide realistic coating performance expectations," says Soufli. Despite these challenges, Soufli and team members from LBNL and Institut d'Optique at Université Paris–Saclay, France, have recently developed new multilayer mirrors based on aluminum and scandium with record reflectance at wavelengths of 40 to 65 nm—a largely unexplored EUV wavelength range.

In 2010, NASA's Solar Dynamics Observatory (SDO) launched into orbit to capture the highest temporal and spatial resolution, full-disk images of the Sun. SDO contained four telescopes bearing multilayer mirrors co-developed and calibrated by Lawrence Livermore. (See *S&TR*, January 2011, pp. 16–18.) More recently, Laboratory scientists collaborated with their LBNL colleagues and others to develop multilayer mirrors for the Solar Ultraviolet Imager (SUVI) instrument onboard the National Oceanic and Atmospheric Administration's (NOAA) Geostationary Operational Environmental Satellites (GOES)-16, -17, -18, which launched in 2016, 2018, and 2022, respectively, as well as GOES-U, expected to launch in 2024. The coatings on the SDO and GOES mirrors facilitate the imaging of individual plasma lines emitted from the Sun's photosphere (surface) and atmosphere (corona). These images help scientists learn more about the impacts of the Sun's solar flares and coronal mass ejections on satellites, aircraft, radio communication systems, the electrical grid, and astronaut safety, as well as the climate.

Metrology Matters

A major challenge in making a multilayer mirror is successfully controlling the coating thickness on a large and often curved substrate to ensure that all points on the mirror have the correct reflective response in the prescribed waveband or group of wavelengths. When applying a coating to a largearea optic, performance must be measured and corrected, if needed, on every point of the surface. "To make it, you must measure it," says Soufli. Accurate, at-wavelength metrology provided during development and optimization and the final photometric calibration ensures the best possible performance of the optics. "Our collaboration with Berkeley Laboratory's CXRO has produced some of the world's most accurate EUV optics down to the picometer. We can measure coatings at the operational wavelength, whether for EUVL, space science, or any other application," says Soufli.

In another multilayer coating and metrological win, a collaborative effort among Livermore, LBNL, and optics manufacturer Zygo Corporation, funded by a consortium of semiconductor companies, achieved a breakthrough six years ago with the world's first high numerical aperture (NA)—the range of angles over which an optical system can accept or emit light—EUV optical lithography Micro-Exposure Tool 5 (MET5), now operational at LBNL's CXRO. For the MET5 project, the Laboratory developed the first diffraction-limited multilayer coatings for an EUV optical system with an NA of 0.5, a significant increase over commercially available systems that are limited to an NA of 0.33. This advance supports industry's drive to print continuously smaller features and accommodate higher resolution imaging. The coatings combined high reflectance with near-zero stress and thickness variation of a few picometers across a 250-millimeter diameter area, ensuring that the coating does not deform the optic shape. Zygo sponsored the project and developed the substrates, which also must conform to strict specifications. The project delivered eight mirrors for the four MET5 optical systems to Zygo, including the one integrated into CXRO's custom-developed EUV lithography tool. CXRO Director Patrick Naulleau explains, "High-quality optics are the heart of any lithography tool, but when dealing with EUV wavelengths, the requirements are incredibly challenging. To achieve perfect imaging optics as required for advanced lithography, the optical surfaces including the coatings must be controlled to the level of 0.1 nanometer." Since completion of the MET5 tool at CXRO in 2019, it has been a research and development workhorse accelerating the realization of commercial-scale high-NA EUVL manufacturing.



Continuing the march of computer microchips with ever-smaller features requires tools such as the Micro-Exposure Tool 5 (MET5). The result of a collaboration of Lawrence Livermore and Lawrence Berkeley national laboratories and Zygo Corporation, the MET5 is a micro-exposure tool with a numerical aperture of 0.5 that will enable the development of chips with nanometer resolution. This computer-generated image of an MET5 shows two aspherical EUV imaging mirrors (in light blue), which were multilayer-coated and characterized by Lawrence Livermore researchers, mounted in an adjustable optomechanical structure.

Making the Impossible Possible

Without EUV multilayer coatings, Soufli notes, producing smaller and denser computer chips with nanometer resolutions and examining the spectra of solar flares in detail would be impossible. "No avenue exists for addressing such technical and scientific challenges, except via EUV. The Laboratory understands that. By making substantial investments in this area, we maintain our role as pioneers," says Soufli.

-Ann Parker

Key Words: Center for X-ray Optics (CXRO), Cooperative Research and Development Agreement (CRADA), extreme ultraviolet (EUV), extreme ultraviolet lithography (EUVL), Geostationary Operational Environmental Satellite (GOES), Lawrence Berkeley National Laboratory (LBNL), metrology, microchip, Micro-Exposure Tool 5 (MET5), multilayer optics, Solar Ultraviolet Imager (SUVI), National Oceanic and Atmospheric Administration (NOAA), NASA, Solar Dynamics Observatory (SDO), solar physics telescope.

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S&TR June 2022 S&TR June 2022

ADDITIVE MANUFACTURING BRINGS NEW

Optician Colby McNamee holds a piece of the R&D 100 Award-winning gadolinium-lutetium-oxide transparent ceramic scintillator, developed at Lawrence Livermore, which converts x rays to visible light seven times more efficiently than glass.

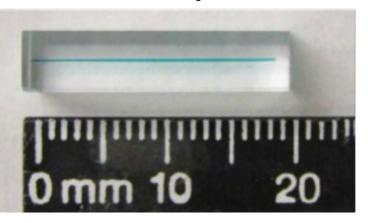
CONSIDER what makes a ceramic mug the perfect container U for a morning cup of coffee: the material is durable and resists heat and corrosion. Due to strong interatomic crystalline bonds created when clay, earthen elements, and water are heated to between 1,200 and 1,800°C, a ceramic mug will last a long time—as long as no one drops it. The material also keeps the coffee hot and does not chemically react with it. Transparent ceramics exhibit similar desirable characteristics and are used in streetlamps and bullet-proof windows. Having developed several transparent ceramics for radiation detection applications for the Department of Homeland Security and the Stockpile Stewardship Program, Lawrence Livermore recently leveraged its unique additive manufacturing resources and capabilities to develop transparent ceramics with properties not previously available for use as laser materials.

A Manufacturing Challenge

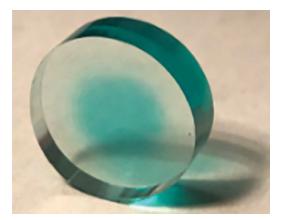
As Livermore researcher Zachary Seeley explains, the key difference between opaque and transparent ceramics is that transparent ceramics lack pores or holes. "In most common ceramics, microscopic pores or secondary structural crystal phases in the final product cause light to scatter, making them opaque," says Seeley. Transparent ceramics are formed by using extreme heat and pressure to consolidate raw material nanopowder, an inorganic, polycrystalline material, into an initial "green body" of weakly bound material. The green body is then heated in a vacuum or controlled atmosphere to just below the material's melting point in a process called sintering. To remove any remaining pores, the sintered ceramic is then subjected to very high temperatures and pressures in a process called hot isostatic pressing. The result is a fully dense nonporous ceramic object that is stronger and harder than glass and more resistant to corrosion, heat, or extreme environments than many other materials.

The ability to control the structure, composition, and properties of transparent ceramics makes them ideal for applications that demand a high degree of precision, particularly laser optics. (See S&TR, April 2006, pp. 10–17.) The Laboratory's early work on transparent ceramics that could replace glass in various applications led to several breakthroughs, including a gadolinium–lutetium–oxide (GLO) transparent ceramic scintillator developed by a team led by Nerine Cherepy, which won an R&D 100 Award in 2016. The GLO scintillator converts x rays to visible light more efficiently than glass, allowing advanced computed tomography systems to produce detailed, 3D images of large, complex objects in less time. (See S&TR, January 2017, pp. 12–13.) Currently, Ian Phillips and Josh Smith, materials scientists in the Laboratory's

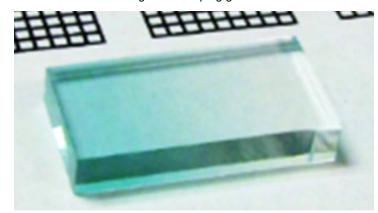
Planar waveguide



Thin disk



Longitudinal doping gradient



Custom-tailored yttrium-aluminum-garnet, laser-gain media—with ytterbium doping gradients and integral, undoped regions—provide laser-mode control, mitigate thermal nonuniformities, and improve laser system performance.

Materials Science division, are working with vendors to commercialize GLO plates in sizes up to 1,300 square centimeters. Research and development also continues into transparent ceramics for scintillators, which have applications in x- and gamma-ray detection. Cherepy and colleagues are currently developing transparent polycrystalline gadolinium– garnet ceramic scintillators doped with cerium for use in gamma spectroscopy and radiation portal monitors.

Still, challenges remained. Applications of transparent ceramics, particularly in the laser science arena, were limited by residual microstructural defects. "With its exceptional expertise in additive manufacturing, chemistry, and laser science, and its multidisciplinary approach," says Seeley, "the Laboratory was uniquely positioned to tackle this problem." Seeley notes that transparent ceramics offer an advantage over traditional crystalline optics materials-spatially controlled doping with ions that absorb and emit light. Doping entails introducing low concentrations of elements such as chromium, erbium, neodymium, and ytterbium into a ceramic's microstructure to absorb and emit light. While some transparent ceramics employ undoped endcaps or exterior cladding to maintain optical and thermal stability, others require separately doped cores or dopant gradients to improve laser beam propagation. Because doping concentrations must be carefully optimized and executed, additive manufacturing, with its flexibility and precision, presents an innovative method to produce doping gradients. "For most printed ceramics, you're not worried about smooth interfaces to 500-nanometers of precision," says Seeley. "It only comes into play when you're crafting materials to control laser beams that have to be optically perfect with extremely small refractive index fluctuations."

A team of Laboratory researchers, including Seeley, Cherepy, and Stephen Payne, have developed processes that use both direct ink write (DIW) and material jetting to create green bodies that yield transparent ceramics with precisely tailored properties. "Choosing the right process for an application depends on the desired geometry of the end product," says Cherepy. "The DIW process is best for thicker, three-dimensional applications, whereas the jetting process is best for creating structures that require more precise, finer granularity in material deposition." In the DIW additive manufacturing process, the team has worked with colleague Timothy Yee to develop methods to extrude a ceramic slurry in precise configurations, similar to piping frosting onto a cake. Dopants can be introduced into the slurry to produce the desired concentration gradient or to integrate variably doped regions. Material jetting, on the other hand, applies droplets of ceramic slurry to build up thin layers of doped and undoped ceramic. Another technique, composite pressing, can yield three-dimensionally controlled chemical composition. As additive manufacturing advances, the customizable geometry of transparent ceramics offers enhanced mode stability, thermal management, efficiency, and power in laser gain media.

New Challenges, Applications Ahead

Laboratory researchers continue to explore how additive manufacturing can contribute to transparent ceramics in areas as diverse as laser materials, scintillators, and light-emitting diode (LED)-based lighting.

In laser optics, researchers are focusing on the doping challenges involved with laser-gain media—optics used to amplify the power of laser beams. Such optics usually take the shape of rods, slabs, thin disks, or waveguides. When a laser beam travels through the gain medium, its shape and doping profile affects the laser beam's power and geometry. To achieve optimal performance for various applications, different laser systems require different gain media. As additive manufacturing methods improve and evolve, increasingly complex optical structures will be possible, opening doors to novel laser designs. A new Laboratory Directed Research and Development (LDRD) project led by Thomas Rudzik is developing additively manufactured strontium–fluoride ceramics with neodymium-doping gradients for the next generation of laser materials for a futuristic design of a possible successor to the National Ignition Facility.

As LED lighting becomes standard in homes, workplaces, and public spaces, improving the color temperature of the light they emit to more closely match natural sunlight is crucial. LED color temperature is controlled through a thin layer of phosphor, a substance that absorbs the blue LED light, converting it to green and red to produce white light in the fixture. The Laboratory's Ross Osborne recently consolidated the narrow-emitting red phosphor, KSF:Mn ($K_2SiF_6:Mn^{4+}$), into a transparent ceramic for the first time under funding by the Critical Materials Institute, which seeks to develop technologies that avoid using rare-earth elements. The KSF ceramic has an ideal red emission spectrum and offers superior thermal conductivity compared to traditional phosphor powders, allowing efficient warm-white lighting.

These advancements and more can be traced back to the Laboratory's early and continued investment in materials science, which established the foundation for transparent ceramics research and rewarded multidisciplinary collaboration. Cherepy notes that her team "works with every part of the Laboratory that could possibly utilize optical ceramics." Payne adds, "We collaborate across the Laboratory, applying transparent ceramics to state-of-the-art science and technology



A transparent phosphor ceramic KSF: Mn, developed and fabricated at Livermore, emits red light for solid-state, light-emitting diodes. The ceramic is not activated under normal room lights (left) but glows a brilliant pink-red when exposed to 450-nanometer-wavelength blue light (right).

in a variety of fields. We also collaborate with external partners, such as the United States Army, the Department of Homeland Security, and private industry. Internally, the LDRD program helps propel the transparent ceramics team to new heights with its focus on funding high-risk, potentially high-payoff projects." With so much going for it now, and the exciting challenges ahead, the future looks bright for transparent ceramics to find even more applications in the days ahead.

—Stephanie Turza

Key Words: Additive manufacturing, composite pressing, direct ink write (DIW), gadolinium–lutetium–oxide (GLO) transparent ceramic scintillator, KSF:Mn, Laboratory Directed Research and Development (LDRD), laser-gain media, laser optic, light-emitting diode (LED), scintillator, transparent ceramics.

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EXPANDED CAPABILITIES AND OPPORTUNITIES VIRTUAL BEAM LINE CODE

N the 25 years since breaking ground on the National Ignition Facility (NIF)—a cornerstone of the National Nuclear Security Administration's Stockpile Stewardship Program—Lawrence Livermore has steadily pushed the boundaries of laser physics, nonlinear optics, and photonics in service of inertial confinement fusion experiments and advanced photon sources development. Beyond the 192 beam lines of the primary laser facility with its world-record energy and fusion yields, the NIF & Photon Science Principal Directorate's capabilities have expanded to include chirped-pulse amplification, kilojoule petawatt-class short-pulse systems to generate hard x-ray radiographic probes, high-average power lasers for directed energy applications, and other scientific pursuits. (See *S&TR*, July/August 2017, pp. 4–11; September 2018, pp. 4–11; and, June 2019, pp. 4–11.)

One crucial capability that helps enable these activities is the Virtual Beam Line (VBL) laser simulation code, which launched in 2000. It can model all the major laser physics and technology involved in the design optimization, commissioning, and operations of tabletop to NIF-scale lasers. VBL provides scientists with high-fidelity models and high-resolution calculations of laser performance predictions for the entire NIF laser system, the Advanced Radiographic Capability, the Optical Science Laser, and parts of the High-Repetition-Rate Advanced Petawatt Laser System in the Czech Republic.

After more than two decades of experimentally verified physics and computing enhancements, a few years ago this unique code underwent a modernization effort to increase the scalability and expand the physics supporting a wider array of applications and customers. With funding from the Laboratory's Institutional Scientific Capability Portfolio (ISCP), VBL migrated from Java to C++ with a flurry of user interface and optimization features, as well as laser physics and high-resolution enhancements primed for parallel execution on Livermore's supercomputers. "VBL is key to laser scientists' ability to design architectures and experiments and to deliver results. It plays a critical role in ensuring machine safety and preventing damage during experiments. Our team is looking forward to deploying the new functionality into production," states software engineering manager Kathleen McCandless.

Rebuilding the Code Base

Like other mission-driven codes at the Laboratory, VBL's capabilities have changed over time to support additional users and new applications. It has grown to model lasers with

Inside the National Ignition Facility, 192 high-energy laser beams converge onto a tiny target. Livermore's Virtual Beam Line (VBL) code models the beam lines so users can fine-tune their experimental parameters before executing a shot. (Rendering by Jacob Long.)



Coupled with Laser Performance and Operations Model (LPOM) software, a robust user interface makes VBL++ more versatile than ever. Users like Livermore physicist Samuel Schrauth simulate the results before an experiment takes place. In the VBL++ interface (inset), users model their laser architecture by dragging-and-dropping adjustable components, parameters, and other variables affecting the laser's path toward the target. monochromatic to broadband spectra, various beam geometries, different gain media, and vastly different pulse durations from the femtosecond (10^{-15}) to nanosecond (10^{-9}) regime. For all these uses, VBL simulates laser amplification with wavelength-dependent emission cross section, nonlinear effects including Kerr self-focusing, and frequency conversion. Today, VBL is the physics engine used "under the hood" hundreds of times every day by the Laser Performance and Operations Model (LPOM) software as users set up their NIF experiments.

Over the years, increasing demands and scope prompted a thorough examination of VBL's original approach. McCandless explains, "Users need enhanced physics models that are more computationally intensive and require unprecedented resolutions, which means using the Laboratory's supercomputing capabilities. We could not run the original VBL in parallel on high-performance computing systems without rearchitecting it."

The VBL team decided to rewrite the mature Java code base in favor of a faster, more flexible programming paradigm. The C++ programming language minimizes memory movement while the code is running, improves performance, interfaces more directly with the computing hardware it runs on, and provides more control.

With many prior years invested in a Java code base, the team considered binding the two programming languages, but doing so could have made the code buggy and unstable. Ultimately, the stakes were too high to gamble with a patchwork solution. McCandless points out, "We must make sure performance is optimized and calculations are accurate. We don't want to hold up a NIF experiment or introduce errors when designing new advanced architectures."

Minor Name Change, Major Possibilities

The team has delivered multiple major releases of upgraded VBL code since 2017, and a new VBL++ (pronounced *vee-bee-ell-plus-plus*) is slated for LPOM production deployment. For portability to different types of computing systems—including classified computing systems and the forthcoming El Capitan exascale-class supercomputer—the code leverages Livermore's RAJA software abstraction framework. A wider array of physics calculations within VBL++ is now possible thanks to integration of another Laboratory-developed software library called SUNDIALS, which provides solvers for differential algebraic and ordinary differential equations.

Because VBL++ is optimized for parallel computing architectures, McCandless notes, "Our code can speed up the modeling time necessary for designing experiments, giving researchers more valuable time in the facility. Solutions are also higher fidelity because we can invoke more detailed physics models." VBL++ also has a robust interface that lets users optimize the parameters of their laser architecture; import external files from finite-element analysis codes to account for stresses and thermal effects inducing birefringence; resolve the impact of optical component imperfections; and perform an inverse solve to determine the input low-power pulse shape that will achieve the high-power request on target. Depending on an application's computational demands, laser physicists can run VBL++ using a graphical user interface on a laptop or submit batch processes on a Livermore supercomputer with thousands of cores.

All of these features are covered in user documentation, including video and live training sessions for Livermore scientists. "Our goal is to conduct broad training across the Laboratory to continue growing this expertise, incorporate more models for emerging needs, and engage more users and physicists in the project," says McCandless, noting Livermore's trusted

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reputation in laser physics modeling and high-performance computing among the scientific community.

The team is readying these advanced capabilities for new opportunities and collaborations. VBL++ project leader Jean-Michel Di Nicola points out that the ISCP investment demonstrates the importance of thinking broadly as laser science, nonlinear optics, and photonics enter a new era—one in which the code's engineering and computational capabilities can drastically reduce the risks, development cycle, and cost of new laser architectures. He explains, "We are building a multipurpose simulation code for customers with emerging and diverse laser designs, technologies, and applications."

Collaboration is Key

The VBL++ project is another success born from the longstanding partnership between NIF and Livermore's Computing Directorate, which encompasses numerous projects and technologies from diagnostic measurements and advanced control systems to data analysis, information technology infrastructure, and scientific simulation code development. To describe beam propagation and diffraction, frequency conversion, and other nonlinear effects, VBL++ leverages physics models developed and prototyped by Laboratory laser physicists. Software engineers incorporate the physicists' algorithms and code modules into the VBL++ code base to extend its physics modeling capabilities. Software developers work with physicists on test cases to evaluate these VBL++ extensions. "This strong collaboration across skill sets enables cutting-edge science, particularly with regard to physics-based modeling and simulation," says Di Nicola.

As the code's user base grows beyond NIF, the team is working to support other experimental laser systems and plans to support the designs for the Matter in Extreme Conditions laser facility at the SLAC National Accelerator Laboratory. According to McCandless, this expansion into new physics capabilities also serves as an attractive opportunity for recruiting talented scientists. She adds, "Our code has endured because no other product can handle everything that it can. Future laser systems will be very different from what we have today, and VBL++ will help Livermore meet those challenges."

-Holly Auten

Key Words: Institutional Scientific Capability Portfolio (ISCP), Laser Performance and Operations Model (LPOM), laser physics, National Ignition Facility (NIF), simulation, Virtual Beam Line (VBL) code.

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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

System and Method for Repeated Metal Deposition-Dewetting Steps to Form a Nano-Particle Etching Mask Producing Thicker Layer of **Engraved Metasurface**

Eyal Feigenbaum, Nathan James Ray, Jae Hyuck Yoo U.S. Patent 11,294,103 B2 April 5, 2022

Methods and Systems for Producing Nanolipoprotein Particles Matthew A. Coleman, Paul D. Hoeprich, Brent W. Seglke U.S. Patent 11,300,572 B2

April 12, 2022

Methods of Three-Dimensional Electrophoretic Deposition for Ceramic and Cermet Applications and Systems Thereof

Klint A. Rose, Joshua D. Kuntz, Marcus A. Worsley U.S. Patent 11,299,816 B2 April 12, 2022

Composite 3D-Printed Reactors for Gas Absorption, Purification, and Reaction

Du T. Nguyen, Sarah E. Baker, William L. Bourcier, Joshuah K. Stolaroff, Congwang Ye, Maxwell R. Murialdo, Maira R. Ceron Hernandez, Jennifer M. Knipe U.S. Patent 11,305,226 B2 April 19, 2022

System, Method, and Apparatus Relating to Colloidosomes Christine A. Orme, Sarah Baker, Yixuan Yu, Shelley L. Anna, **Charles Sharkey**

U.S. Patent 11,305,252 B2 April 19, 2022

System and Method for Compact Electro-Optical Interface Susant Petra, Razi-UI Muhammad Haque, Komal Kampasi

U.S. Patent 11.309.670 B2 April 19, 2022

Awards

The **Oppenheimer Science and Energy Leadership** Program (OSELP) named Livermore researchers Kathryn Mohror and T. Yong Han as Oppenheimer Fellows. The highly competitive program brings together exceptional leaders to explore the complexities, challenges, and opportunities facing national laboratories and the Department of Energy (DOE). Mohror, a computer scientist, leads the Parallel Systems group within Livermore's Center for Applied Scientific Computing (CASC) and focuses on data management performance in high-performance computing. Han, a materials scientist, leads the Functional Materials Synthesis and Integration group in the Laboratory's Materials Science division as well as the Production Enablement and Prototyping program working

System and Method for Engine Control with Pressure Reactive Device to Control Combustion Timing Nicholas Killingsworth, Daniel L. Flowers, Russell A. Whitesides

U.S. Patent 11,306,653 B2 April 19, 2022

Systems and Methodology for Electrical Energy Storage

Eric Duoss, Juergen Biener, Patrick Campbell, Julie A. Jackson, Geoffrey M. Oxberry, Christopher Spadaccini, Michael Stadermann, Cheng Zhu, Bradley Trembacki, Jayathi Murthy, Matthew Merrill U.S. Patent 11,309,574 B2 April 19, 2022

System and Method for Sub Micron Additive Manufacturing Sourabh Kumar Saha, Robert Matthew Panas, Shih-Chi Chen U.S. Patent 11,312,067 April 25, 2022

System with Buffer for Lateral Flow on a Porous Membrane

Jane P. Bearinger U.S. Patent 11.320.432 B2 May 3, 2022

Tunnel Drift Step Recovery Diode

Lars F. Voss, Adam M. Conway, Luis M. Hernandez, Mark S. Rader U.S. Patent 11,322,626 B2 May 3, 2022

Two-Color High Speed Thermal Imaging System for Laser-Based Additive Manufacturing Process Monitoring

Nicholas P. Calta, Gabe Guss, Manyalibo Joseph Matthews U.S. Patent 11,338,390 B2 May 24, 2022

Systems and Methods for Additive Manufacturing to Encapsulate **Transformative Colloidal Suspensions**

Julie A. Mancini, Eric Duoss, Alexandra Golobic,

Mark Christian Messner, Christopher Spadaccini, Kenneth J. Lob U.S. Patent 11,339,847 B2 May 24, 2022

to accelerate integration of new materials into defense technologies. Mohror and Han will join OSELP awardees from each of the national laboratories for leadership mentoring from senior DOE professionals.

The Society for Industrial and Applied Mathematics (SIAM) named Livermore computational mathematician **Rob Falgout** recipient of the 2022 SIAM Activity Group on Supercomputing **Career Prize**. The award recognizes his contributions to theory, algorithms, and open-source software in parallel scientific computing. A Distinguished Member of Technical Staff at the Laboratory, Falgout leads the hypre linear solvers project and XBraid parallel time integration project.

S&TR June 2022

The ACES in Our Hand

Abstract

A new Livermore project provides nonproliferation experts with a computing toolkit to simulate the dominant nuclear fuel enrichment process in the world, gas centrifuge enrichment, to better understand how the process might be subverted to make materials for nuclear weapons. The Adaptive Computing Environment and Simulations (ACES) project has three thrusts: developing new computer models and simulations of gas centrifuge-based fissile materials enrichment that incorporate data science and machine learning; creating a computational infrastructure to support and sustain these new capabilities; and recruiting and training an expert nonproliferation workforce that understands centrifuge enrichment technology. Contact: Stefan Hau-Riege (925) 422-5892 (hauriege1@llnl.gov).

Rewarding Technology Innovation



Lawrence Livermore received three 2021 R&D 100 Awards as part of *R&D World* magazine's international competition to identify the top 100 innovations of the year.

Also in the next issue:

- A Laboratory-developed training program for nuclear emergency responders simulates any radiological training scenario in real-time.
- New infrastructure supporting the 2023 introduction of exascale computing to the Laboratory has been completed ahead of schedule.
- Livermore scientists advance the nanofabrication of flexible, implantable probes to study and treat conditions of the eyes, ears, and brain.

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