Lawrence Livermore National Laboratory

January/February 2017

Science & Technology REVIEW

Supercomputers Bolster Manufacturing Efficiency

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About the Cover

Manufacturing industries create a vast array of products, from steel I-beams to paperback books. Ensuring the long-term vitality and economic competitiveness of U.S. manufacturing industries in an increasingly globalized marketplace will require more energy-efficient processes and better material conservation. As the article beginning on p. 4 describes, the Department of Energy's High Performance Computing for Manufacturing (HPC4Mfg) Program combines the expertise and high-performance computing capabilities at Lawrence Livermore, Lawrence Berkeley, and Oak Ridge national laboratories with industry partners to realize process efficiencies, improve product quality, and accelerate technology development. Depicted on the cover is an artist's representation of a manufacturing facility.

Cover design: Alexandria Holmberg

About *S&TR*

At Lawrence Livermore National Laboratory, we focus on science and technology research to ensure our nation's security. We also apply that expertise to solve other important national problems in energy, bioscience, and the environment. *Science & Technology Review* is published eight times a year to communicate, to a broad audience, the Laboratory's scientific and technological accomplishments in fulfilling its primary missions. The publication's goal is to help readers understand these accomplishments and appreciate their value to the individual citizen, the nation, and the world.

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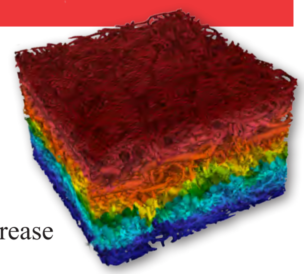

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Additive Manufacturing Promotes Material "Origami"

A team of Livermore researchers has demonstrated three-dimensional (3D) printing of shape-shifting structures that can fold or unfold to reshape themselves when exposed to heat or electricity. An article published in the June 15, 2016, issue of *Scientific Reports* describes the fabrication of micro-architected structures—boxes, spirals, and spheres—from a conductive, environmentally responsive polymer ink developed at the Laboratory. Although using responsive materials in 3D printing, often known as four-dimensional (4D) printing, is not new, Livermore researchers are the first to combine 3D printing and subsequent origami folding with conductive smart composite materials to build complex structures.

In the paper, the researchers describe creating primary shapes from an ink made from soybean oil, additional copolymers, and carbon nanofibers, and "programming" a temporary shape at a specific temperature. Next, shape-morphing was induced with ambient heat or an electrical current, which reverts the part from its temporary shape back to its original shape.

Lead author and Livermore postdoctoral reasearcher Jennifer Rodriguez explains, "We take the part out of the oven before it's done and set the permanent structure of the part by folding or twisting after an initial gelling of the polymer." Ultimately, Rodriguez says, researchers can use the materials to create extremely complex parts. "If we printed a part out of multiple versions of these formulations, with different transition temperatures, and ran it through a heating ramp, they would expand in a segmented fashion and unpack into something much more complex."

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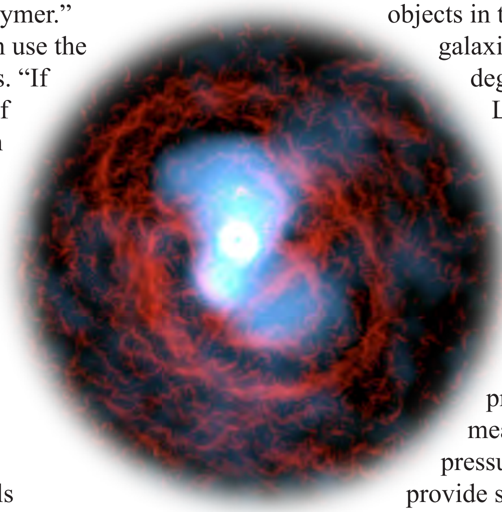

Platform Measures Cell Response

For the first time, Lawrence Livermore researchers have successfully incorporated adult human peripheral nervous system cells on a microelectrode platform for long-term testing of chemical and toxic effects on cell health and function. The study, part of a project known as iCHIP (in vitro chip-based human investigational platform), was recently published in the June 28, 2016, online issue of the journal *Analyst*. The paper describes the integration of primary human dorsal root ganglia (DRG) cells and glial cells onto a microfluidics chip with embedded electrodes and the successful testing of several chemicals on the living cells over a period of up to 23 days.

Ultimately, scientists say the research will provide a noninvasive testing platform outside the human body that will predict human exposure to drugs and toxins more accurately than animal studies. "It's a platform for testing low-level chronic exposure to chemicals and for therapeutic drug screening and testing of environmental contaminants in cases where we can't test directly in humans," says the paper's lead author, Livermore scientist Heather Enright. "iChip provides a way to get human-relevant data without using animals, especially since those results don't always extrapolate to humans."

During the study, the team repeatedly exposed human DRG neurons and glial cells to capsaicin, a chemical found in chili peppers, ATP (a neuron receptor activator), and potassium chloride. The neural responses to the chemicals were recorded and compared to other reports of similar interactions found in the scientific literature. iCHIP principal investigator Elizabeth Wheeler said the team will continue to recapitulate different tissues of the body to better understand pain mechanisms and other cell–chemical interactions.

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Team Tracks Core of Massive Object in Universe

The Perseus cluster is a group of galaxies in the constellation Perseus (see image at left) and is one of the most massive objects in the known universe, containing thousands of galaxies immersed in a vast cloud of multimillion-degree gas. The Hitomi collaboration, in which Lawrence Livermore scientist Greg Brown is a member, found that the turbulent motion of the intracluster gas in the Perseus cluster is only a small fraction of the mechanism responsible for heating the gas to 50 million kelvins.

This finding, published in the July 6, 2016, edition of *Nature*, demonstrates that an accurate mass of a cluster can be inferred almost exclusively from its thermal hydrostatic pressure without having to rely on low-accuracy measurements and estimates of the turbulent pressure of the system. Accurate cluster masses provide strong constraints on cluster cosmology and dark matter.

This recent discovery is the result of measurements taken with the Soft X-ray Spectrometer (SXS), which was flown on the Hitomi X-ray Observatory and designed and built at NASA's Goddard Space Flight Center. The high-energy resolution of the SXS made it possible, for the first time, to measure a high-resolution, high-throughput spectrum of a cluster of galaxies. Brown says, "The high-resolution of the SXS has revolutionized our view of some of the largest, most energetic objects in the universe."

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(continued on p. 24)

Commentary by Bruce E. Warner

Breakthroughs Advance U.S. Competitiveness

AT Lawrence Livermore, we foster an environment where mission and national needs combine with state-of-the-art science, technology, and computational capabilities to deliver innovative solutions to a wide range of problems. In this issue of *Science & Technology Review (S&TR)*, we focus on innovation and its importance to U.S. industry and our mission sponsors.

As the article beginning on p. 4 describes, we are applying our expertise in high-performance computing (HPC) and materials science to improve manufacturing capabilities, and in doing so, advance the nation's economic competitiveness. Through the Department of Energy's (DOE's) High Performance Computing for Manufacturing (HPC4Mfg) Program, the Laboratory applies modeling, simulation, and data analysis to manufacturing challenges. The goal is to help the industry optimize processes, improve efficiency, enhance quality, reduce waste, and shorten the time needed to adopt new more energy-efficient technologies.

Since its inception in 2015, the HPC4Mfg Program has expanded from 5 seedling projects to 28. Our industrial partners propose which manufacturing issues to target, a formal selection process follows, and the selected projects and companies team with experts at Lawrence Livermore, Lawrence Berkeley, and Oak Ridge national laboratories to address longstanding technical energy and manufacturing challenges using HPC. This program demonstrates how the synergy of the national laboratories' world-recognized expertise in materials science, additive manufacturing, and computational codes and simulations is helping us predict materials performance and enhance manufacturing processes.

This issue also includes highlights on innovative ways Laboratory researchers conduct research at the intersection of basic and applied science. In 2016, the Laboratory garnered three R&D 100 Awards from *R&D Magazine* in its annual competition to honor top scientific and engineering technologies with commercial potential. The gadolinium–lutetium–oxide (GLO) transparent ceramic scintillator dramatically increases high-energy radiography throughput, enhancing the ability to look inside large, high-density metal parts such as turbines, jet engines, and ship welds. GLO provides seven times faster imaging than glass scintillators and decreases the x-ray dose required to obtain detailed imagery. The polyelectrolyte enabled liftoff (PEEL) technology allows freestanding polymer films to be fabricated that are larger, stronger, and thinner than conventional methods can produce. PEEL can fabricate membranes as thin as 30 nanometers daily, and because the process is easily scalable in size and manufacturing quantity, it could eventually be applied for sensing, catalysis, filtration, and wound-healing applications. The Carbon Capture Simulation Initiative (CCSI) toolset is a suite of computational tools and models for accelerating the development of carbon-capture technologies. CCSI is a partnership between national laboratories, industry, and academic institutions. In addition to the three winners, a Livermore team was also nominated as a finalist in the 2016 competition for developing a technique for growing large-scale, economical stilbene crystals that can accurately distinguish neutrons from gamma rays to identify and distinguish nuclear materials.

The final highlight explains how we are using resonance ionization mass spectrometry (RIMS) to rapidly identify interdicted nuclear and radiological materials. Livermore's laser ionization of neutrals (LION) laboratory uses RIMS to analyze materials and provide answers about their origins and intended use. Because sample materials are laser vaporized and then immediately probed with resonant ionizing lasers, this process can be completed in hours. We can measure isotope ratios of elements such as uranium and plutonium and determine the level of threat they pose. Although the RIMS technique is typically used in cosmochemistry research for identifying isotope concentrations in cosmic dust, LION is one of a few laboratories that has a dedicated RIMS capability for nuclear forensics.

The scientific and technological breakthroughs discussed herein are a testament to the exceptional staff and technical capabilities of the Laboratory and demonstrate the diversity of challenges we endeavor to overcome through innovative thinking. Furthermore, as seen by these examples, partnerships with industry, academia, and other laboratories are an essential component to advancing solutions that address pressing national needs and boosting U.S. competitiveness.

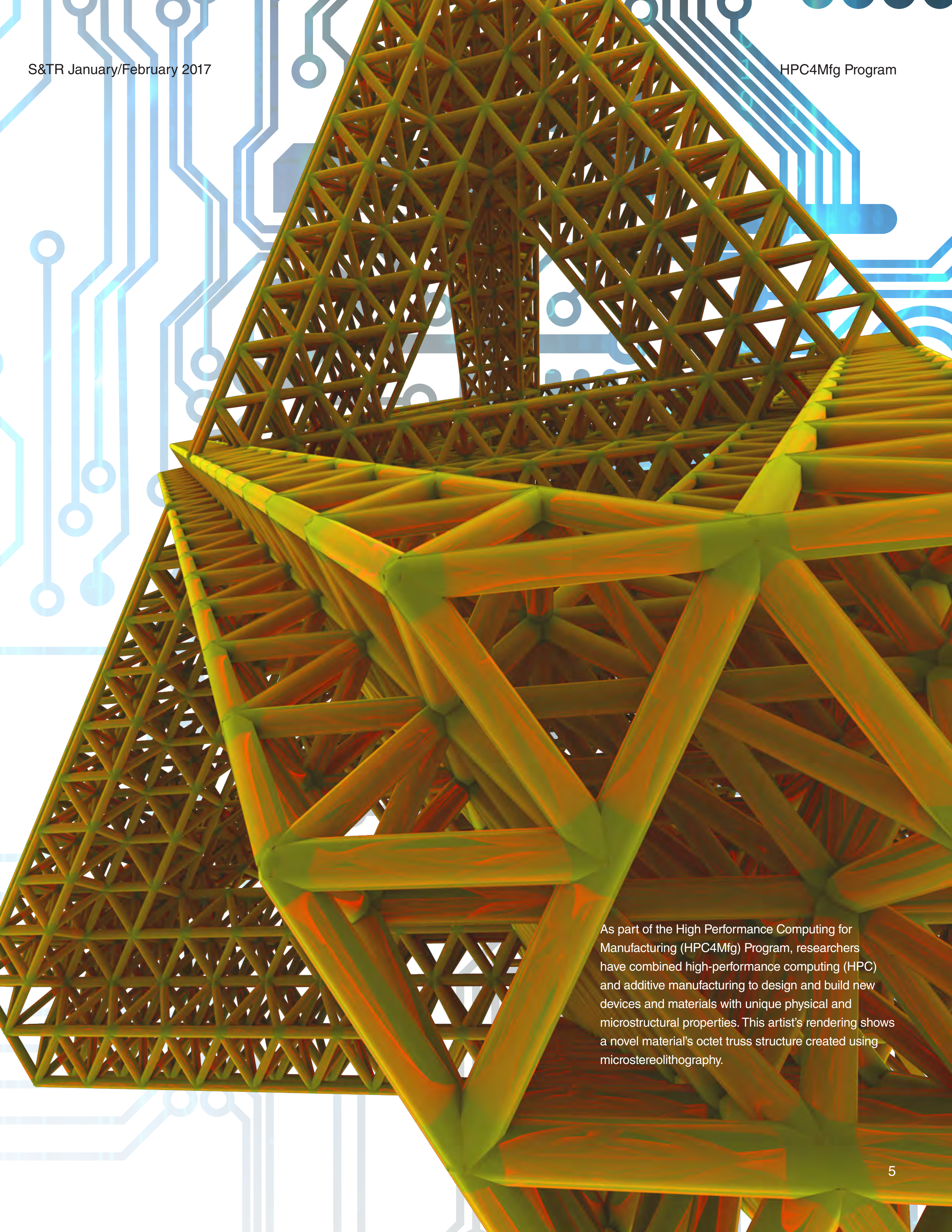
■ Bruce E. Warner is principal associate director for Global Security.

COMPUTATIONAL Innovation Boosts MANUFACTURING

High-performance computing solutions provided by Lawrence Livermore and other national laboratories help U.S. manufacturers accelerate innovation and increase efficiencies.

MANUFACTURING industries create a vast array of products, from steel I-beams to Blu-ray™ players to paperback books. However, ensuring the long-term vitality and economic competitiveness of U.S. industries in an increasingly globalized marketplace will require more energy-efficient processes and better material conservation. In 2015, the Advanced Manufacturing Office, within the Department of Energy's Office of Energy Efficiency and Renewable Energy (EERE), and Lawrence Livermore instituted the High Performance Computing for Manufacturing (HPC4Mfg) Program to advance clean-energy technologies, increase the efficiency of manufacturing processes, accelerate innovation, reduce the time it takes to bring new technologies to market, and improve the quality of products.

The program unites the world-class high-performance computing (HPC) resources and expertise of Lawrence Livermore, Lawrence Berkeley, and Oak Ridge national laboratories with U.S. manufacturers to deliver solutions that could revolutionize the manufacturing industry. Jeff Roberts, Livermore's deputy director for Energy and Climate Security, who oversees EERE projects at the Laboratory, says, "We are showing



As part of the High Performance Computing for Manufacturing (HPC4Mfg) Program, researchers have combined high-performance computing (HPC) and additive manufacturing to design and build new devices and materials with unique physical and microstructural properties. This artist's rendering shows a novel material's octet truss structure created using microstereolithography.

companies how they can use high-performance computing and national laboratory expertise to become more competitive and bring new products to market faster by reducing energy, waste, and rejected parts." Peg Folta, a deputy program manager in the Laboratory's Global Security Principal Directorate and founding director of the HPC4Mfg Program, adds, "The national laboratories have experts in advanced modeling, simulation, and data analysis. We match our people with industry partners to address technical challenges targeted by the manufacturers."

Under the guidance of Folta and her successor, Lori Diachin, the department head for Information Technology in Livermore's Computation Directorate, the HPC4Mfg Program solicits proposals on manufacturing challenges twice a year. Once concept papers are selected, principal investigators (PIs) from within the three partner laboratories team up with the industry partners to produce full proposals. This year the program will add to its list of participating laboratories, making more PIs available to help execute individual projects. Each $3 million solicitation provides up to $300,000 for a funded project. Folta notes, "Through extensive outreach, we encourage manufacturers during the submittal and re-submittal process, identifying projects that best utilize high-performance computing to address issues with high impact." She adds the proposals provide insight into the challenges facing these companies. "We found a surprising number of unique materials projects were being proposed, as well as ones related to unusual welding issues." Roberts explains, "The Laboratory is world recognized for its expertise in materials science, additive manufacturing, and HPC codes and simulations. The ability to help predict materials performance is becoming increasingly important, and the Laboratory shines in this area."

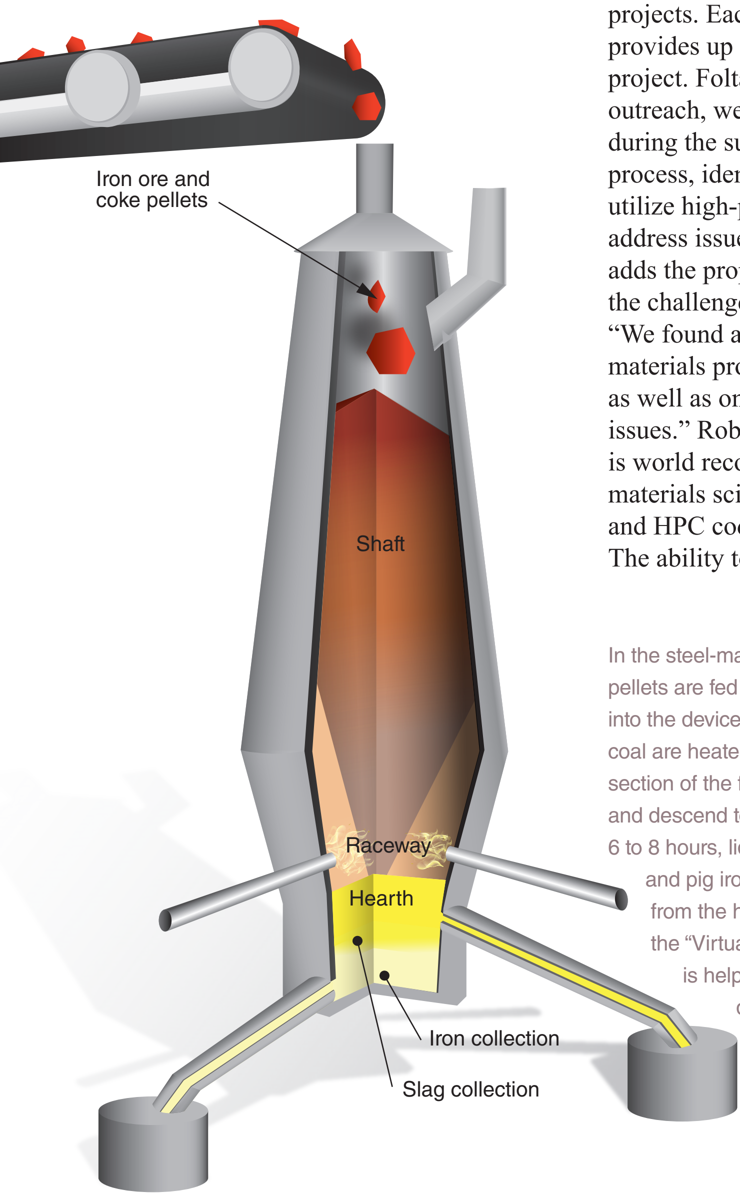
Yearlong demonstration projects based on the funded proposals are aimed at showing industry partners how HPC can address their manufacturing challenges and provide a high return on investment. Solutions developed through these projects can then be fully implemented through industry, consortium, government funding, or a combination thereof. The entire process has been designed to streamline private–public partnership and provide a means for sharing what has been learned to the broader industry, while protecting intellectual property. Three of the program's initial five seedling projects serve as prominent examples of what can be achieved through the HPC4Mfg collaborative model. (See the box on p. 8.)

It's a Blast (Furnace, That Is)

Steel is used in many industry sectors, including transportation, home goods, energy, and construction. The steel industry is also the fourth largest energy-consuming industry in the nation. Thus, decreasing its energy consumption by even a small percentage could yield big cost savings and reduce environmental impacts.

Livermore computational physicist Aaron Fisher is working with Purdue University Northwest's Center for Innovation through Visualization and Simulation (CIVS) and a steel manufacturing consortium on the HPC4Mfg "Virtual Blast Furnace" project. One goal is to help reduce steel manufacturers' reliance on coke—a coal-based fuel with high carbon content. To manufacture steel, iron ore is combined with coke in a blast furnace then heated and melted, creating molten pig iron.

"If we could optimize the smelting process to reduce the average amount of coke used to produce a ton of hot metal by 5 percent, the industry could



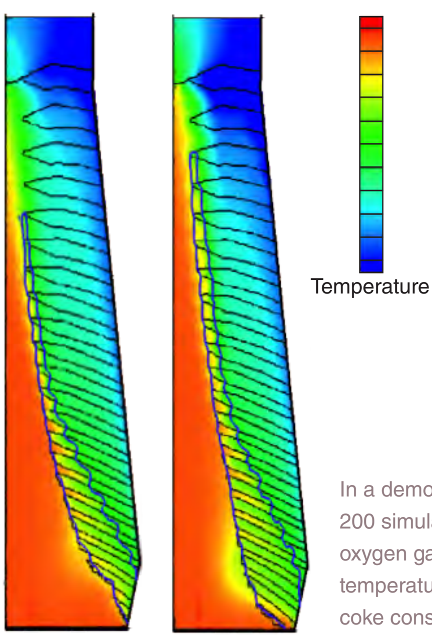
In the steel-making process, iron ore and coke pellets are fed through the top of a blast furnace into the device's main body, or shaft. Oxygen and coal are heated and injected into the raceway section of the furnace. The raw materials ignite and descend to the bottom of the furnace over 6 to 8 hours, liquefying into slag (waste material) and pig iron. The slag and iron are drained from the hearth at regular intervals. As part of the "Virtual Blast Furnace" project, Livermore is helping parallelize a series of Purdue-developed simulation codes to model furnace processes.

save $80 million a year," says Fisher. Another aspect of their research focuses on increasing the energy efficiency of the centuries-old furnace process. Fisher notes, "Twenty furnaces in the U.S. produce all the country's steel, and those furnaces consume about 65 percent of the energy in the steel-making process."

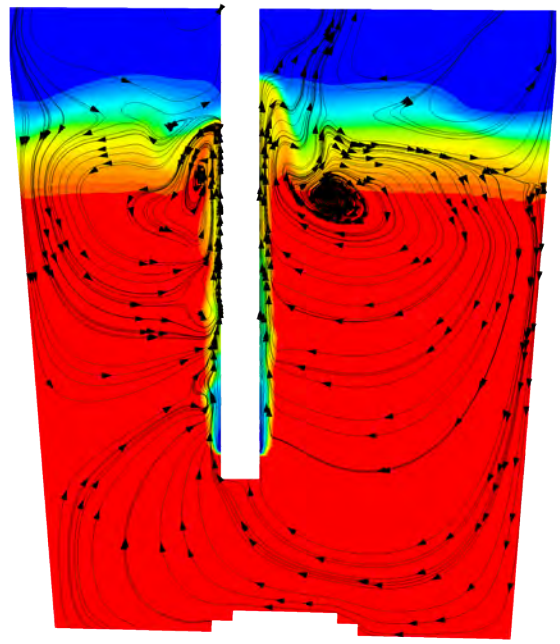
Much of steel manufacturing is still an art, dependent on the experience of skilled workers to understand the conditions inside the furnace. "We can't place sensors inside the furnace to gather data because the furnace temperatures are too high," says Fisher. To help operators and manufacturers better understand this heat-intensive environment, CIVS created a series of simulation codes to model three independent sections of the furnace. The Shaft code models gas flow and reactions through alternating layers of iron ore and coke. The Raceway code models the fuel injection flow and combustion occurring below the shaft. The Hearth code models the behavior of the bottom part of the furnace where the liquid iron and the slag (waste material) flow out of tapholes. These codes run serially on a dedicated desktop computer at Purdue. It takes one week of 24/7 operations for the codes to complete a two-dimensional (2D) simulation, and 1 to 2 months to run a three-dimensional (3D) simulation—and that's without a crash or power outage.

The lack of serious computational power means the models are limited. For instance, they cannot describe dynamic processes, such as those occurring during startup, shutdown, and periods of instability. Also, the three models must be connected manually, in sequence, to simulate the whole furnace. Fisher explains, "We proposed integrating the individual codes into a single one that can run on Livermore's HPC clusters. By using a thousand processors in parallel, we could run the code nearly a thousand times faster and reduce the run time of a 3D simulation to less than one day."

The team conducted two demonstration studies. In the first study, Livermore developed the capability to launch multiple instances of the Shaft code in parallel. Each 2D simulation had different input parameters for the amount of oxygen enrichment, the natural gas-injection rate, and the hot blast temperature. The study showed that with Livermore's HPC clusters, potentially hundreds of simulations could be run for analyzing coke consumption rates and furnace stabilities in significantly less time than with CIVS current computing resources. In the second demonstration, the team focused on the steel industry's "ladle" operation, in which molten iron and alloying materials are poured into a huge cup and stirred to make steel. Foundries are interested in shortening the stirring time while increasing how much molten steel can be produced. One stirring method involves injecting neutral gases to facilitate the mixing of iron and alloy materials. Using the CIVS computing cluster and desktop and an off-the-shelf engineering code, it took CIVS two weeks to model the gas process at low resolution. Livermore proposed using 2,000 processors and adding zones to achieve more detail. A scaling study with these simulations showed that the Livermore clusters could run problems of this type (and larger) 35 times faster than the CIVS



In a demonstration study, Livermore researchers ran more than 200 simulations of critical blast furnace parameters, such as oxygen gas enrichment, natural gas injection rate, and hot blast temperature. Simulation outputs (shown here) were analyzed for coke consumption rate and furnace stability.



Livermore researchers established the versatility and speed of using a commercial, off-the-shelf code running on the Laboratory's supercomputing clusters to simulate the steel industry's ladle operation. The simulation was run using a range of mesh sizes and different numbers of central processing units. The color scale represents the percentage of alloyed steel in the fluid. Red is fully mixed steel, and blue is the slag layer.

cluster and 1,400 times faster than the dedicated desktop.

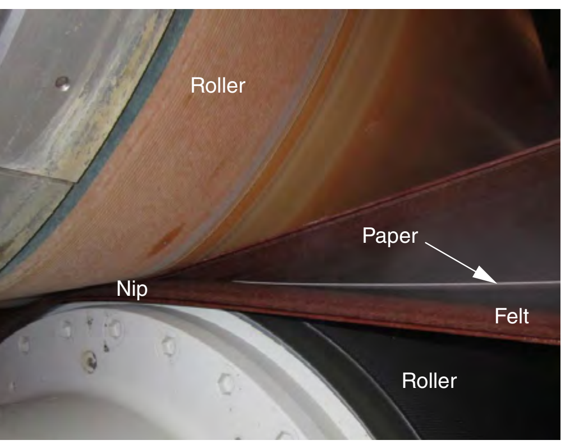
The project team is now merging the three CIVS codes and redesigning them to run in parallel on Livermore's machines. Fisher says, "Our long-term vision is to use HPC and advanced numerical and computational methods to develop an interactive, virtual blast furnace that combines a comprehensive, integrated, high-fidelity, dynamic, multiphysics model with fast data visualization." Once the codes are running as one, the team plans to partner with members of the steel consortium to study ways to improve furnace operation.

Paper's Pressing Problem

Turning wood pulp into paper is the third largest energy-consuming process in manufacturing. The Agenda 2020 Technology Alliance, a nonprofit organization that aims to identify and solve challenges in the pulp and paper industry, turned to HPC4Mfg to explore ways to cut costs and save energy. Livermore's Yue Hao and Wei Wang partnered with Lawrence Berkeley's David Trebotich and Agenda 2020's Jun Xu and David Turpin to improve the industry's energy efficiency.

In the paper-pressing process, wet, porous paper pulp is fed onto a moving belt of fine-mesh screening that holds a felt layer. The felt–pulp layers are squeezed through rollers and passed over steam-heated cylinders to remove the remaining water. Hao explains, "Reducing the amount of energy required in the drying process by 20 percent could save the industry $250 million annually."

One way to save considerable energy might be to reduce the "re-wetting" of the pulp that occurs during the pressing process. The rollers squeeze water out of the paper at the pinch point (called the nip), and the felt soaks up the water. However, as the layers leave the rollers and the pressure eases, the pulp sucks up some of the residual moisture from the felt, re-wetting the paper. Hao says, "The industry determined it needed an accurate numerical model to understand the physics of re-wetting, so it could take steps to design more energy-efficient equipment."



In paper processing, wet paper pulp and felt layers are pressed between rollers at high speed to remove water from the paper. "Re-wetting" occurs after the paper and felt leave the high-pressure area of the nip. In collaboration with the Agenda 2020 Technology Alliance, Lawrence Livermore and Lawrence Berkeley national laboratories are exploring the re-wetting process with the goal of maximizing water removal and minimizing power consumption.

HPC4energy: Precursor to HPC4Mfg

Started in 2015, the High Performance Computing for Manufacturing (HPC4Mfg) Program is fairly new, but it had its genesis in previous Laboratory efforts. Four years earlier, Lawrence Livermore hosted a meeting on high-performance computing (HPC) for the Council on Competitiveness Technology Leadership and Strategy Initiative advisory committee. The Council on Competitiveness is a nonprofit, nonpartisan, nongovernmental organization made up of corporate chief executive officers (CEOs), university presidents, and labor leaders. During that meeting, the council's president and CEO called HPC an "innovation accelerator," adding it offered an extraordinary opportunity for the United States to design products faster and to minimize the time needed for creating and testing prototypes. Soon after, Livermore created the HPC4energy incubator, a one-year pilot program for accelerating energy technology development and boosting U.S. competitiveness in the global marketplace by bringing together industry and the Laboratory's scientific and computing resources. The pilot concluded in 2013 to praise from the Laboratory and industry participants alike (see *S&TR*, June 2013, pp. 4–12; and June 2012, pp. 24–25).

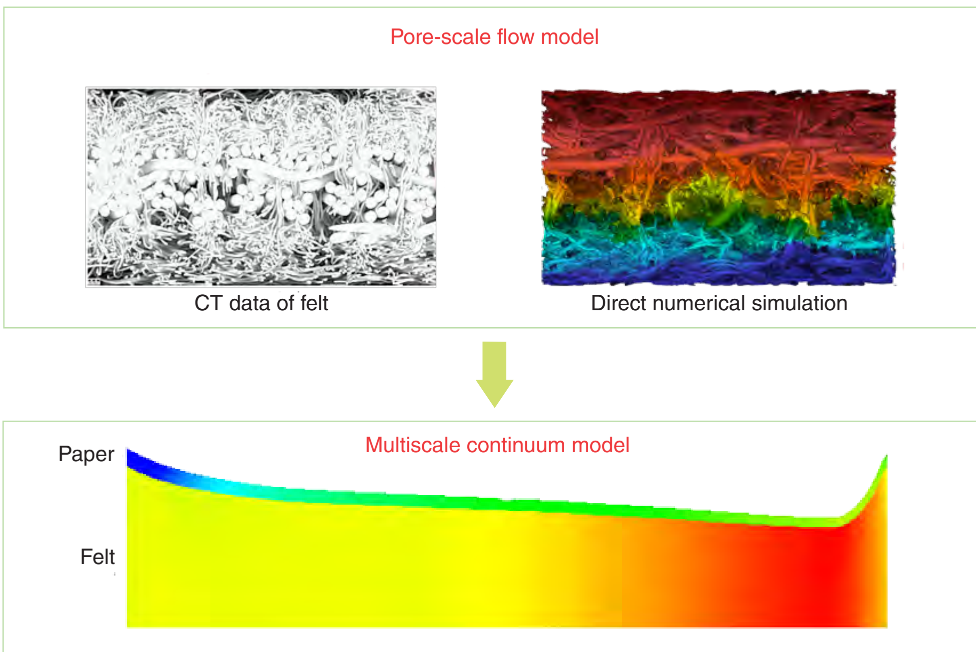
The exact mechanism for re-wetting is not well understood. Thus, Agenda 2020 turned to the simulation experts at Livermore and Berkeley to create a multiphysics modeling framework. Using existing industry data, including felt measurements, computerized tomography (CT) images of the felt, and paper-machine press data, the two national laboratories developed a coupled-physics simulation framework to determine how water flows through porous paper pulp during and after the pressing process. Berkeley developed a 3D model to look at pore-scale flow behaviors in the felt, running the model on up to 50,000 central processing units at the National Energy Research Scientific Computing Center. Livermore then used the results of Berkeley's pore-scale simulation to constrain its continuum model, which integrates all multiscale data into a single model.

Hao notes that the problem was complicated, involving a very narrow physical space and short timeframes. The results from the initial continuum model clearly showed the deformation and dryness of the paper as it traverses rollers and provided a detailed numerical view of the process—an essential first step to optimizing paper drying. Next, industry must be encouraged to continue support for model development, which will require obtaining better CT images of the paper for improving model fidelity. A CT machine with much higher resolution than what the industry currently has available will be needed since the paper is only 400 micrometers thick. "As new information and data are added," says Hao, "the model can be modified to more closely reflect the reality of the process."

Growing High-Quality Crystals

Gallium nitride (GaN) is an emerging semiconductor material making inroads in many technological areas, such as solid-state lighting and power electronics. One application that most people are familiar with is the Blu-ray player, which uses a violet laser diode on a GaN substrate to read Blu-ray DVDs. For GaN-based light-emitting diodes, GaN layers are typically deposited on a nonnative substrate such as sapphire or silicon carbide, leading to lattice strain—displacement of atoms—between the two materials and reducing device reliability and performance. GaN-based devices that use a GaN substrate (known as GaN-on-GaN technology) have higher power operation and higher efficiencies than those made with traditional semiconductor materials. As a result, they also have the potential to drastically cut energy consumption in consumer applications.

The challenge to making GaN-on-GaN devices a widespread reality is finding scalable ways to grow high-quality crystals of the material quickly and inexpensively. Semiconducting materials are typically grown using melt techniques. However, GaN crystals cannot be grown using such methods because the material's melting temperature is exceedingly high (2,500 degrees Celsius), and high pressures are needed to keep the material from decomposing into its two elemental constituents. The most common GaN-production process is hydride vapor-phase epitaxy (HVPE), which involves reacting ammonia with gallium chloride at about 1,100 degrees Celsius. Although this process has high growth rates, it is also expensive and usually results



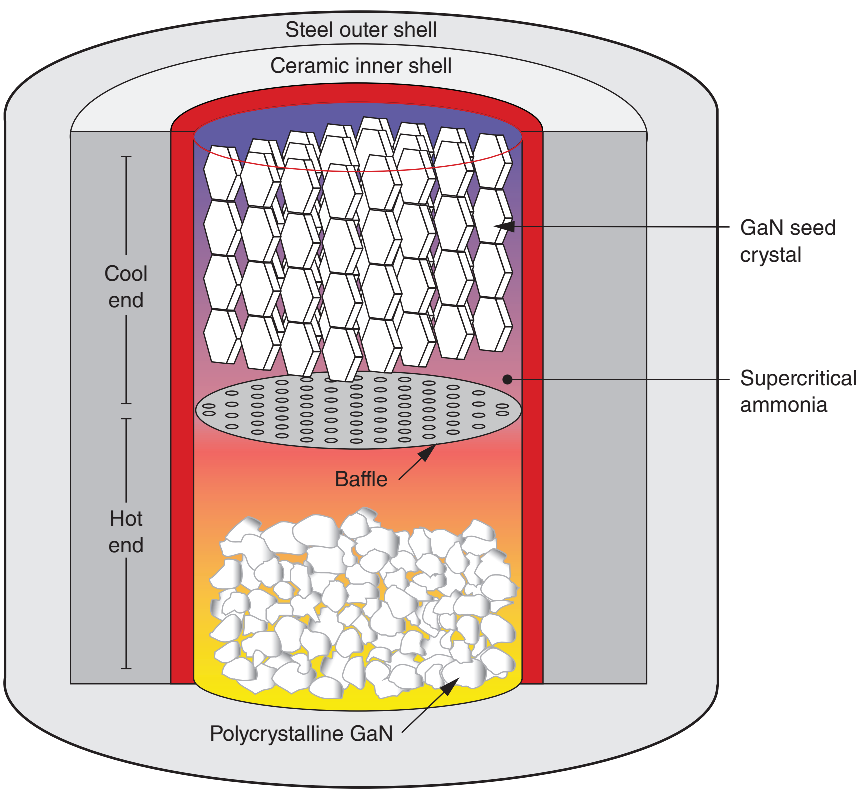
Lawrence Berkeley used industry-derived data and measurements collected from scanning electron microscopy and computerized tomography (CT) to create a pore-scale model of water flow behaviors in the felt. Results were then fed into a multiscale continuum model developed by Livermore. The model shows the deformation and dryness of the compressed paper and felt. Red represents higher dryness and blue represents lower dryness.

in crystals with too many defects for many applications.

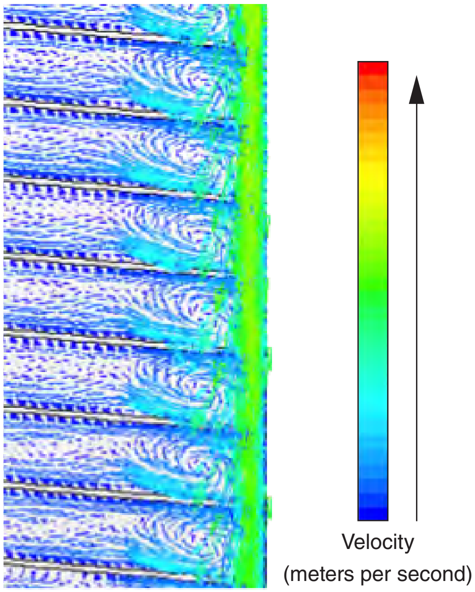
The SORAA company, the world's leading developer of solid-state lighting based on GaN substrates, is working on a promising GaN crystal-growth technology that could reduce production costs of high-quality GaN-on-GaN light-emitting diodes by 20 percent and enable the development of next-generation power electronics, such as controllers for motors in hybrid cars. The company is developing a small, high-pressure autoclave or reactor for ammonothermal growth, where ammonia (a solvent) helps reduce the required growth temperature. (The process is similar to a highly successful technique wherein water is used as a solvent to grow quartz crystals.) However, with the current reactor setup, the productivity is still rather low. In addition, the autoclave can operate at pressures exceeding 700 megapascals (7,000 atmospheres) and at temperatures as high as 750 degrees Celsius. Given the corrosive nature of ammonia and various chemicals used, the reactor must be made of high-strength steels or corrosion-resistant alloys and metals. These conditions, combined with the infeasibility of measuring the environment within the reactor, make it extremely difficult to understand what is happening inside the autoclave.

SORAA teamed with Livermore through HPC4Mfg to better understand the growth process using multiphysics simulations run on the Laboratory's HPC systems. Livermore computer scientist Nick Killingsworth, the PI for the project, turned to the licensed code StarCCM+ to simulate the reactor, improve throughput, and run higher fidelity models. "SORAA has the experience, but they just needed some simulation power to help them understand the dynamics inside the reactor," he explains. Using the Laboratory's SYRAH supercomputer and StarCCM+, the team ran simulations incorporating more mesh points to better understand the flow within the ammonothermal reactor, completing each simulation in two to three days. Previous simulations run on SORAA's 12-processor workstation took an entire week to complete.

Results from the higher fidelity simulations revealed a much more complicated flow structure in the autoclave than anticipated. Modeling the flow and temperature profile along the walls of the reactor showed a flow that was transient—changing over time—and turbulent. The results improved predictions of local temperatures and flow velocities within the reactor,



The SORAA reactor for growing high-quality gallium-nitride (GaN) crystals is filled with supercritical ammonia and is hotter at the bottom than at the top. The polycrystalline GaN "nutrient" is placed on the bottom, where the temperature and solubility is highest. Dissolved GaN is transported by free convection up through a baffle to the cool end of the system. As it cools, the material's solubility decreases and it deposits on seed crystals. The GaN-depleted solvent then sinks to the bottom of the reactor and the cycle is repeated. The crystals grow larger with each loop through the system.



High-fidelity simulations of the flow within the GaN reactor, developed as part of the collaboration between Livermore and SORAA, show more complicated, turbulent flow structures compared to previous work. Color gradient indicates magnitude and direction of velocity vectors within the reactor. Complicated vertical structures near the reactor walls were found to vary with time.

providing valuable insight. As a result, SORAA is now in a better position to optimize the uniform growth of GaN crystals. Killingsworth says, “This new high-fidelity model could save years of trial-and-error experimentation that are typically needed to bring a process into large-scale commercial production.” Once large crystals can be grown quickly and with fewer defects, the door will be open for wider use of GaN in high-power electronics and other applications.

HPC4Mfg Running at Steady State

Since its inception, the HPC4Mfg Program has expanded from the first five seedling projects to more than 28 projects involving three national laboratories. As the program continues to solicit proposals twice a year, it aims to build an HPC–manufacturing community through industry outreach and academic involvement. The first annual “Industry Engagement Day,” to be held in March 2017, will bring together companies, laboratories, academia, consortia, and state and local government officials to learn about the benefits of HPC adoption in manufacturing and how HPC capabilities at the national laboratories can support manufacturing companies. Participants will also be able to discuss current manufacturing challenges. In addition, the event provides a venue for HPC4Mfg Program managers to receive feedback on work done thus far for refining and improving collaborations.

Long-term, the HPC4Mfg Program will also play a role in fostering future talent for the manufacturing industry. The program has been successful in recruiting postdoctoral researchers and students to the Laboratory, and has provided input on ways to improve engineering curriculums at universities. Expanded programs are being planned to encourage students, professors, and industry professionals to train the next-generation manufacturing workforce.

Already, the partnerships achieved through the HPC4Mfg Program are proving fruitful. “Our projects address diverse challenges,” says Folta, “helping with process optimization, design improvement, and introduction of new computational tools where they can benefit most. We continue to reach out to companies and are working to ensure that after each project is completed, HPC is being woven into the fabric of manufacturing.” The program strives to make connections and help the nation’s most energy-intensive industries become more energy-efficient and globally competitive, culminating in a win–win for U.S. manufacturing, the national laboratories, and the nation.

—Ann Parker

Key Words: ammonothermal growth, Blu-ray player, crystal growth, economic competitiveness, energy efficiency, gallium nitride (GaN), GaN-on-GaN technology, high-performance computing (HPC), HPC4energy, High Performance Computing for Manufacturing (HPC4Mfg) Program, light-emitting diode, paper manufacturing, semiconductor, steel industry.

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Novel Scintillator **Improves X-Ray Imaging**

MEDICAL doctors began using x rays as an imaging technology not long after Wilhelm Röntgen discovered their penetrating effects in 1895. Since that time, x rays have become a powerful diagnostic tool in many fields, from medicine to manufacturing. In fact, over the last few decades, advanced computed tomography (CT) systems have enabled detailed three-dimensional (3D) images of inanimate objects. Such technology allows manufacturers to improve an object's design and fabrication by quickly revealing interior defects that would otherwise remain undetected. Now, a Livermore team led by Nerine Cherepy has developed a first-of-its kind transparent ceramic scintillator that significantly improves throughput for CT-based 3D imaging for manufacturing and other applications.

Simply put, a scintillator is a substance that lights up when excited by ionizing radiation. Inside CT scanners, scintillators convert x rays to visible light. The gadolinium–lutetium–oxide (GLO) transparent ceramic scintillator, an R&D 100 Award–winning technology, substantially reduces data acquisition time and enhances the spatial resolution of images from CT systems, capturing highly detailed views of objects in real time. With this capability, scientists and engineers can improve the assessment and quality control of high-density parts, such as those used in power plant turbines and jet engines. To Livermore, the technology is a great boon for the Stockpile Stewardship Program, allowing researchers to obtain imagery of stockpile components more quickly. More broadly, archaeologists could use the technology to look inside ancient artifacts, and industry could apply it to evaluate complex machinery, including rocket engines.

2016 R&D 100 WINNER

Defects Reduce Desired Properties

The road to GLO began more than 10 years ago, when Jim Trebes, currently the division leader for Physics within the Laboratory's Physical and Life Sciences Directorate, asked Cherepy if her team could create a material that would provide better spatial resolution for an x-ray system than what was currently being used. In particular, Trebes was interested in the scintillator for the confined large optical scintillator screen imaging system (CoLOSSIS), an advanced 3D imaging system his team had developed for nondestructive evaluation of the nuclear stockpile. (See *S&TR*, July/August 2009, pp. 12–17.)

For imaging a component, CoLOSSIS passes a high-energy beam of x rays through the object, which is placed on a rotating platform. The emerging pattern of radiation then passes through a glass scintillator screen, where it is converted to visible light that is then focused and captured by a sensitive charged-coupled-device camera. Although the screen, made from specially formulated glass, was effective, a more sensitive material could provide even better detail. "Glass has an amorphous structure, which does not provide efficient scintillation," says Cherepy. "A crystalline material such as a transparent ceramic can provide higher light yield."

Originally developed in the 1990s in Japan, transparent ceramics have demonstrated their usefulness as transparent armor in military applications, and as lenses and laser amplifiers in optical applications. "In 2006, Livermore made a strategic internal investment in several specialized furnaces needed for fabricating transparent ceramics. Without this investment, our success in research and development of these materials would not have been possible," says Steve Payne of the Laboratory's Materials Science Division. Cherepy adds, "Livermore's R&D capability for transparent ceramics is unique."

The team's original formulation for the transparent ceramic scintillator used lutetium oxide doped with a small amount of europium—a material that has high x-ray stopping power and high light yield (a measure of the material's ability to convert

Zachary Seeley holds a gadolinium–lutetium–oxide (GLO) transparent ceramic scintillator plate. GLO scintillators convert x rays to visible light seven times more efficiently than existing ones made from glass. As a result, advanced computed tomography systems can produce three-dimensional images of large, complex objects in less time.

x rays to visible light). However, this initial "recipe" generated small defects in the material, causing it to be translucent rather than transparent. With further research, the group discovered that adding gadolinium into the mix produced a perfectly transparent polycrystalline material—the basis for Livermore's GLO patent.

Scaling Up GLO Manufacture

The fabrication process for the GLO scintillator begins with a powder that consists of almost perfectly round nanoparticles. A graphite die presses the powder, which is heated to 1,200 degrees Celsius, into a 60-percent-dense solid. Through a series of steps, the material is progressively heated and pressed to exact specifications. Livermore worked with several industrial partners to make the materials and scale up the manufacturing process to produce full-sized GLO optics. Nanocerox, Inc., synthesized the powder feedstock; Technology Assessment and Transfer, Inc., provided the hot pressing services needed to convert the powder to its initial solid state; and American Isostatic Presses, Inc., provided the hot isostatic press to render the final transparent material. "We began by manufacturing small millimeter-sized samples and worked up to larger sizes, eventually graduating to full-sized plates," says ceramist Zachary Seeley. The team has successfully made a 30-by-30-centimeter plate for the CoLOSSIS system.

The team's new transparent ceramic has an effective light yield seven times better than its glass predecessor—a rare and significant jump in performance in a field that usually sees incremental improvements. In addition, the testing performed by Livermore scientists Daniel Schneberk and Gary Stone revealed that the GLO scintillator allows a CT system to capture images in about two hours instead of eight. Now, industrial partners are working with Livermore to commercialize GLO so that it can find its place in tomographic applications for industry and scientific research alike.

—Allan Chen

Key Words: confined large optical scintillator screen imaging system (CoLOSSIS), computed tomography (CT), europium, gadolinium-lutetium-oxide (GLO), glass, polycrystalline, R&D 100 Award, scintillator, three-dimensional (3D) imaging, transparent ceramic, x ray.

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Development team for the GLO transparent ceramic scintillator: (from left) Zachary Seeley, Scott Fisher, Nerine Cherepy, Gary Stone, Stephen Payne, and Daniel Schneberk. (Not shown: Peter Thelin.) (Photo by Randy Wong.)

Toolset Promotes **Carbon-Capture Solution**

CARBON dioxide (CO_2)—a greenhouse gas that traps heat and makes the planet warmer—is emitted in large quantities from fossil fuel use in power generation and other industries. To reduce environmental impacts of CO_2 by preventing its emission into the atmosphere, scientists are working to develop efficient carbon-capture technologies. Unfortunately, commercially viable carbon-capture processes of sufficient size and sophistication are slow to reach fruition because of the high cost of pilot projects and the lack of computational models to simulate new, potentially promising technologies prior to development.

To help accelerate design, research, and maturation of carbon-capture technologies, a Livermore team, in partnership with colleagues participating in the National Energy Technology Laboratory's (NETL's) Carbon Capture Simulation Initiative (CCSI), helped develop the CCSI toolset. A 2016 R&D 100 Award–winning technology, the CCSI toolset is the only fully integrated suite of computational tools and validated models specifically designed to support the development and scale-up of various innovative technologies into carbon-capture solutions.

The CCSI toolset addresses key industry challenges such as gaining a better understanding of sources of error (or uncertainty) in process-simulation results, quantifiying and reducing that uncertainty, and assessing the risks of scaling up a particular technology. "This capability is critically important since pilot projects represent an expensive, limited opportunity to collect the data necessary to move a technology to commercial-scale production," says NETL's David Miller, the CCSI project's technical director. "Thus, the CCSI toolset represents a significant advance in the state-of-the-art computational tools and models available for bringing these technologies to market."

2016 R&D 100 WINNER

A Versatile Computational Tool

The CCSI toolset has interconnected modules for integrating multiscale, multiphysics models with advanced optimization, uncertainty quantification (UQ), and other modeling techniques. As a result, it offers a range of capabilities across the technology development cycle, from identifying the most promising carbon-capture concepts and determining which experiments to conduct, to scaling up the technology to pilot and demonstration studies, and eventually enabling full-scale commercial deployment.

The toolset's computationally efficient and accurate dynamic models incorporate the physical properties, kinetics, and thermodynamics of a potential carbon-capture technology at three primary scales: laboratory and pilot scales (experiments and resulting data), process system scales (design and optimization metrics), and device scale (validated three-dimensional models and computational fluid dynamics simulations). The CCSI toolset is a hierarchically integrated modeling package wherein data are applied across all submodels so that information generated at one scale is preserved at all other scales. The computational suite includes a seamless verification-and-validation hierarchy that ensures model fidelity and can be used to identify data requirements. The computational suite can also provide fast and accurate nonlinear models.

The toolset also has an advanced machine-learning tool that determines simple algebraic parameters for an array of data types, which are applicable to various chemical processes. It also exploits parallel computing platforms, supports multiple simulation tools and software applications, and automatically manages thousands of simulations in parallel on cloud-based computers.

Livermore Ensures FOQUS

Lawrence Livermore was instrumental in providing software-development support and building the CCSI toolset's UQ and risk-analysis capabilities. Specifically, as part of the toolset's buildout, Livermore helped establish the UQ capabilities of

Carbon dioxide, a greenhouse gas, is emitted in large quantities from fossil fuel use in power generation and other industries. The Carbon Capture Simulation Initiative (CCSI) toolset is a fully integrated software suite developed specifically to support the rapid, cost-effective development and scale up of carbon-capture technologies.

the carbon-capture models, the application user interface, and the data-management architecture. The Laboratory utilized its expertise in high-performance computing and UQ software to create the framework for optimization and quantification of uncertainty and sensitivity (FOQUS) computational platform, one of the CCSI toolset's critical products. FOQUS integrates multiscale models with advanced systems optimization and UQ techniques to rapidly synthesize and identify the best potential carbon-capture processes and determine the level of uncertainty associated with them.

One of the key applications that powers FOQUS is the problem solving environment for uncertainty analysis and design exploration (PSUADE). This software toolkit includes applications for performing UQ tasks such as uncertainty analysis, global sensitivity analysis, design optimization, and model calibration. Livermore researcher Charles Tong, the developer of PSUADE, says, "The flourishing of simulation-based scientific discovery has fueled rapid advances in model validation and UQ disciplines. The goal of these emerging disciplines is to enable scientists to make more precise statements about the degree of confidence they have in their simulation-based predictions."

Accelerating Technology Innovation

Carbon-capture technologies are an important approach for significantly reducing domestic and global CO_2 emissions. Informed and enabled by cutting-edge, high-speed, and efficient computational power, CCSI is dedicated to developing, demonstrating, and deploying its advanced computational tools to reduce the risk and time required to bring new technologies to bear on this worldwide problem. Miller says, "The CCSI toolset will lead to more thorough vetting of options, complete understanding of how processes will operate at scale under field conditions, and increased understanding of how uncertainty affects risk."

With the CCSI toolset, analyses of new energy technologies can be completed at rates much faster than in the past. It is also highly versatile, filling general technology gaps to increase speed and effectiveness of most commercialization efforts. As a result, the capabilities of the CCSI toolset are also applicable to complex process analysis in many markets, enabling other industries to reduce the time, risk, and expense of developing and scaling up technologies for commercialization.

—Mike Garrison

Key Words: carbon capture, Carbon Capture Simulation Initiative (CCSI) toolset, carbon dioxide (CO_2), climate change, framework for optimization and quantification of uncertainty and sensitivity (FOQUS), problem solving environment for uncertainty analysis and design exploration (PSUADE), uncertainty quantification (UQ).

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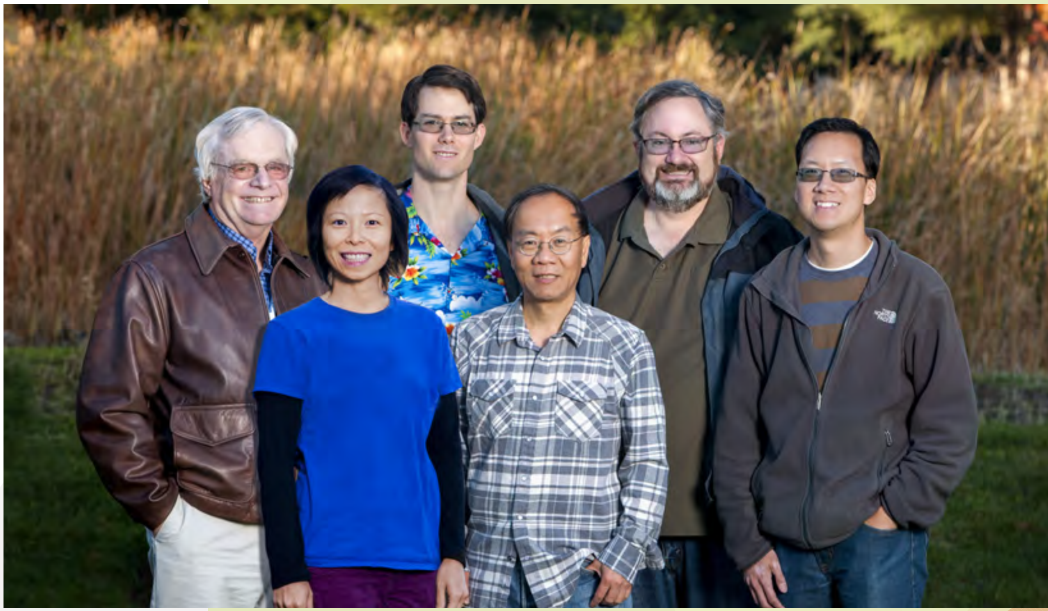
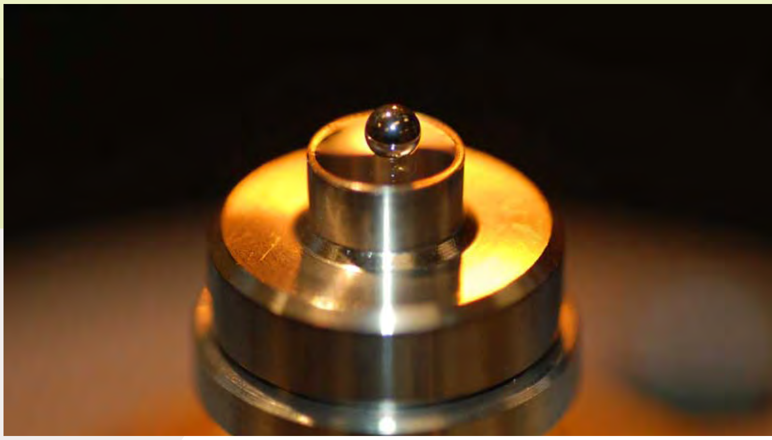


Development team for the CCSI toolset: (from left) Greg Pope, Brenda Ng, Jim Leek, Charles Tong, Tom Epperly, and Jeremy Ou. (Not shown: Natalia Kitch). (Photo by Randy Wong.)

Fabricating the **World's Thinnest Plastic Wrap**



THIN polymer films are important for various applications, including optics, microelectronics, and micromechanics. At Lawrence Livermore, these films are crucial to experiments conducted at the National Ignition Facility (NIF), where they are used in targets to suspend deuterium–tritium fuel capsules inside tiny gold-plated cylinders called hohlraums. However, even extremely thin films have the potential to negatively affect target implosions during an experiment. "This freestanding film is similar to a 'barely there' plastic wrap, which must also be pliable enough to stretch over a container without breaking," explains Salmaan Baxamusa, a materials scientist at Lawrence Livermore.

In industry, freestanding films are typically created by dissolving a polymer material into a solvent and then depositing that mixture onto a substrate. Lifting the film from its deposition substrate—a process known as liftoff—is perhaps the most critical step in fabrication, and several techniques have been developed to help facilitate this operation. One method uses a sacrificial interlayer between the film and the substrate to create a physical separation between them. The film and the substrate separate once a suitable solvent, typically water, dissolves the sacrificial layer. However, this approach has its limitations. First, the sacrificial layer must be deposited smoothly and uniformly, which becomes more challenging over large areas and difficult to accomplish consistently. Second, interactions between the sacrificial layer and the polymer can create imperfections in the film. Finally, film deposition must be compatible with the properties of the interlayer—if the interlayer is dissolved in water, then the film itself must be deposited using nonaqueous techniques.

Livermore scientists have used another separation method in which household glass cleaner is applied to the substrate as a surfactant. The glass cleaner can help the film release more easily, but the film can sometimes stick or stretch during liftoff. In addition, since household glass cleaner is a commercial product, the manufacturer could change the cleaner's formulation, reducing its efficacy. To combat these problems, Livermore scientists, including principal investigators Baxamusa and Michael Stadermann, along with colleagues from General Atomics, have developed an R&D 100 Award–winning liftoff technique called polyelectrolyte enabled liftoff (PEEL). The method enables the creation of ultrathin films without the need for glass cleaner or a sacrificial material between the film and the substrate.

Discovering Direct Delamination

The new PEEL technique was discovered while the team was using a sacrificial material that happened to be positively charged. "I was going to reuse the wafer [substrate], but all the previously applied material had not washed off. When I dipped the substrate into water, the film lifted off beautifully," says Baxamusa. More serious experimentation with this technique led the scientists to ultimately develop PEEL, which works via direct delamination of the film from the substrate.

Direct delamination requires the strain energy in the film to exceed the interfacial energy resisting separation, which is usually not possible for very thin films (those less than 45 nanometers thick). However, with the PEEL technique, scientists achieve direct delamination by pretreating the substrate with a layer of an electrically charged polymer known as polyelectrolyte. Scientists then rinse the substrate thoroughly with water, leaving behind a single layer of the polyelectrolyte that sticks tightly to the substrate. The chemistry of the modified surface decreases the interfacial energy resisting separation enough to easily delaminate films—even ones less than 10 nanometers thick.

PEEL technology provides a host of advantages over previous liftoff approaches. Namely, the method is self-optimizing, A thin sheet of plastic approximately 200 atoms thick produced using the polyelectrolyte enabled liftoff (PEEL) technique supports a stainless steel ball. Developed by researchers at Livermore and General Atomics, PEEL received an R&D 100 Award in 2016.

reproducible, and scalable to large areas; works reliably over numerous batches; and does not contaminate the water used to delaminate the film. In comparison to the use of sacrificial material, Stadermann says, "Normally, you add something to the substrate and then spread it out somehow, which results in a bumpy surface. PEEL always produces a smooth surface with no spreading required."

The thin plastic films can support loads from milligrams to grams, and the method also allows a wider range of materials to be used in the process. "The PEEL technique can be used to dispense various materials at new, ultrathin thicknesses," says Baxamusa. "The condition," adds Stadermann, "is that you have to be able to dissolve the material in a solvent and cast it." In addition, the substrate must have a positive or negative charge—a minor caveat considering that the most common substrates, glass and silicon, have negative charges.

Film Technique Has Possibilities

Currently, PEEL is used to create compliant load-bearing polyvinyl-formal membranes for NIF targets. This capability is important to NIF because it can produce films less than 45 nanometers thick, which has allowed experimentalists to verify that film thickness directly affects the performance of imploding fuel capsules.

The new technological innovation could have other potential applications, including for wound healing, filtration, sensing, and catalysis. "The produced films could even be used as substrates for other processes, allowing us to deposit something on essentially nothing," says Stadermann. The team aspires to further promote PEEL so that the technique may find additional uses. "We have developed a manufacturing method for creating ultrathin films that enables manufacturers to choose which polymers to use, with confidence that the materials will be compatible with the PEEL process," says Baxamusa. Thanks to Livermore ingenuity, a technique for creating the world's thinnest plastic wrap could have countless possibilities.

—Lauren Casonhua

Key Words: direct delamination, freestanding polymer films, polyelectrolyte, polyelectrolyte enabled liftoff (PEEL), polyvinyl-formal membranes, R&D 100 Award, sacrificial layer, strain energy.

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Development team for PEEL: (from left) Tayyab Suratwala, Salmaan Baxamusa, Michael Stadermann, Chantel Aracne-Ruddle, and Phil Miller. (Not shown: Art Nelson.) (Photo by Randy Wong.)

Revealing the Presence of **Hidden Nuclear Materials**

Development team for solution-grown crystals for high-energy neutron detection: (from left) Stephen Payne, Natalia Zaitseva, Scott Fisher, Leslie Carman, and Andy Glenn.

ILLICIT trade in highly enriched uranium and plutonium poses a significant threat, especially if those materials are used in a weapon of mass destruction. Moved clandestinely in small quantities, these special nuclear materials (SNMs) are easy to hide. A Livermore team, led by Natalia Zaitseva, has developed a novel method for growing solid organic crystals from stilbene—an aromatic hydrocarbon known to effectively detect the fast, high-energy neutrons emitted by SNMs. The technique enables larger crystals to be grown more quickly than with conventional crystal growth processes for developing stilbene-based radiation detectors. The development team was an R&D 100 Award finalist in 2016.

When neutrons pass through stilbene crystal, its molecules absorb some of the neutrons and emit photons, a process called scintillation, producing a unique, measurable spectrum of light. Uranium and plutonium yield spectra particular to each isotope, and stilbene is the most effective scintillator for capturing neutrons and reliably discriminating them from other kinds of radiation. However, stilbene crystals large and inexpensive enough to use in radiation detectors have been difficult to grow. Consequently, today's scintillation-based detectors typically use cheaper, more easily obtained organic liquids, which are also less sensitive, somewhat toxic, flammable, and challenging to use in the field. Thus, they are not ideal for quickly and definitively detecting the presence of high-energy neutrons from SNMs that may be hidden in cargo ships, trucks, and other transport.

Larger Crystals in Less Time

Industrial manufacturers typically use the high-temperature, melt-growth process to produce many solid crystalline materials. With this method, crystallization is conducted by cooling an initial liquid melt until it becomes a solid. Unfortunately, the melt–growth process for stilbene is very slow and produces only small crystals.

Zaitseva's team developed a faster way to grow larger crystals (greater than 10 centimeters long) by first dissolving the hydrocarbon in an organic solvent. Inside a crystallization tank, the solution gradually crystallizes onto a tiny stilbene seed crystal as the environment within the tank undergoes controlled temperature reduction. Whereas conventional methods of growing stilbene result in crystal growth rates of a few millimeters per day, the solution-grown technique produces crystals at a rate as high as 20 millimeters per day.

The final product of the team's novel crystal-growth technique is a pure single crystal of stilbene that offers much higher performance than the team's previously designed plastic scintillators (see *S&TR*, October/November 2012, pp. 10–11)—technology that garnered an R&D 100 Award in 2012. In addition, tests of the stilbene crystals have shown that the material has greater light output and superior high-energy neutron discrimination compared to liquid scintillators. "These crystals work much better than anything else at detecting high-energy neutrons," says Zaitseva. "We developed the commercial production process to make them available in the marketplace."

From Laboratory to Industry

Livermore's commercial partner INRAD Optics licensed the technology and has ramped up the solution-growth method to make much more stilbene commercially available. Zaitseva's team is continuing to work with INRAD to develop methods to further increase production rate, reduce cost, and meet the growing demand for these materials. Zaitseva foresees the solution-growth method could also be used to develop functional crystals from other organic solutions.

At sufficiently low cost, crystalline stilbene-based radiation detectors could protect sea- and airports, stadiums, power plants, and other large facilities, as well as help authorities interdict the smuggling of SNM. Accurate neutron detectors also have application in research settings including studies of particle and nuclear physics.

—Allan Chen

Key Words: aromatic organic crystal, high-energy neutrons, R&D 100 Award finalist, scintillation, solution-growth, special nuclear materials, stilbene.

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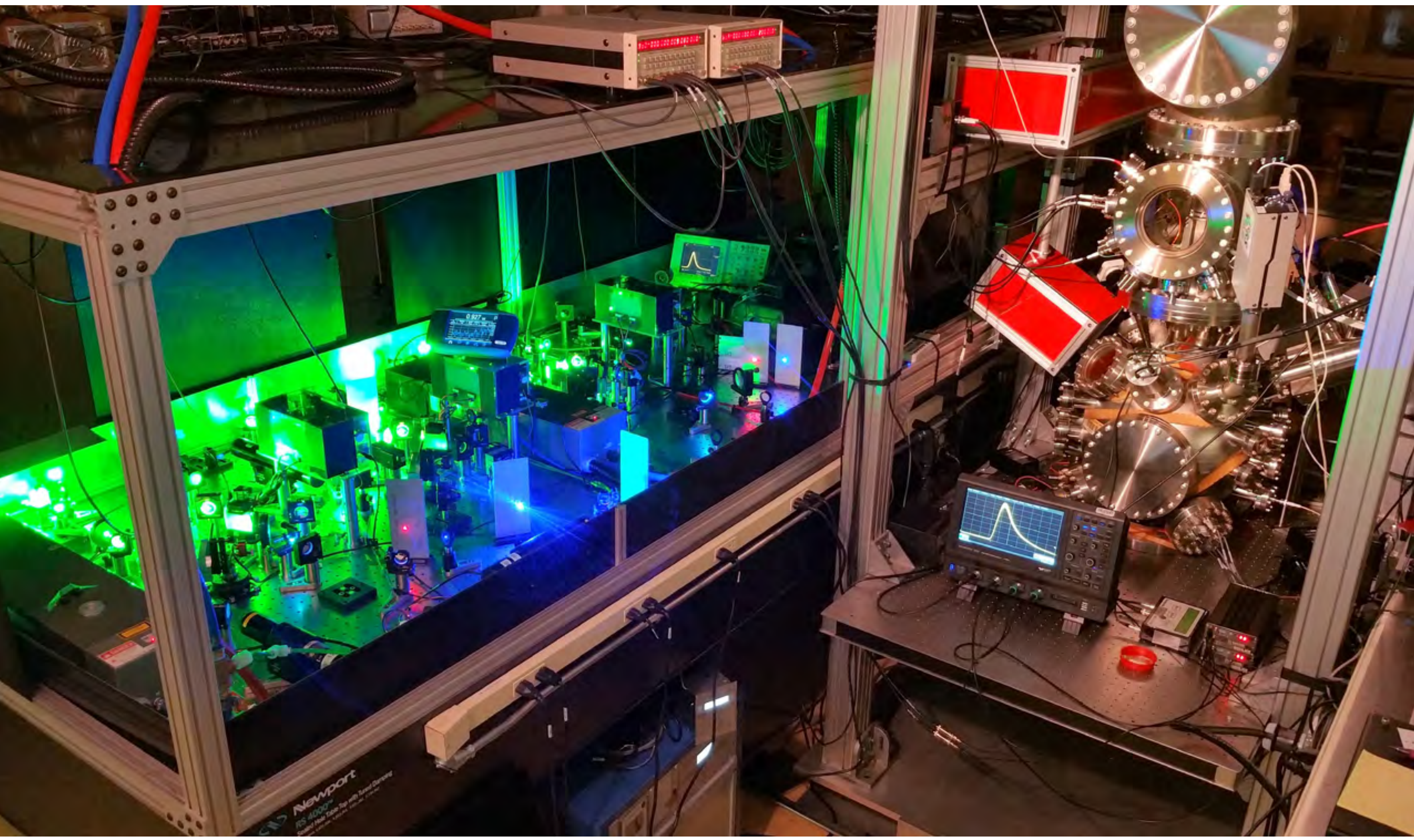
LION Hunts for Nuclear Forensics Clues

In the event illicit nuclear material is intercepted by authorities, Lawrence Livermore scientists are prepared to help officials find the culprit. Using nuclear forensics, a science that Livermore played a prominent role in creating, the Laboratory's experts will analyze the material to enable authorities in determining its source, the pathway it took from its source to the perpetrator, and its intended use.

The new laser ionization of neutrals (LION) laboratory at Livermore can quickly analyze nuclear material and provide critical information to help investigators determine the material's possible origin and intended use. It uses a technology called resonance ionization mass spectrometry (RIMS) to measure isotope ratios of elements such as uranium and plutonium. Within hours, RIMS can provide authorities with a read of whether a material was manufactured for use in a nuclear reactor or a weapon, or repurposed for weapons from reactor fuel—details that can provide the first clues to its origin.

Nuclear forensics scientists use various techniques and technologies to trace nuclear materials, and RIMS has a particular role to play within their bag of tricks. RIMS can identify the specific isotope a scientist wants to quantify using lasers tuned to unique resonant frequencies that ionize only the atoms of that particular element. Measurements can be obtained using just a small sample, and little sample preparation is needed so the results arrive quickly. The RIMS technique also does an excellent job of distinguishing between isotopes of different elements that have the same atomic weight, such as uranium-238 (^{238}U) and plutonium-238 (^{238}Pu). This feature is particularly important for identifying stages in the nuclear-fuel processing cycle. In fact, preliminary analysis by RIMS could well become one of the initial steps in the material characterization process. The technique has also shown the ability to measure uranium and plutonium isotopes in fallout debris from nuclear tests.

"About half a dozen facilities for RIMS analysis exist in the world," says Brett Isselhardt, a Livermore nuclear engineer. "LION is the only one we know of that is focusing on nuclear forensics." Isselhardt, colleague Michael Savina, and their team have built the RIMS instrument from their own custom design. They are now testing the equipment's ability to accurately measure relevant isotope ratios and determine with



The LION (Laser Ionization of Neutrals) laboratory at Livermore uses resonance ionization mass spectrometry (RIMS) for nuclear forensics. Tunable lasers (left) are used to excite isotopes of a particular element. An electric field accelerates the ions into the time-of-flight mass spectrometer (right) for measuring their masses. A tunable femtosecond laser (not shown) provides ultrafast laser pulses for added flexibility.

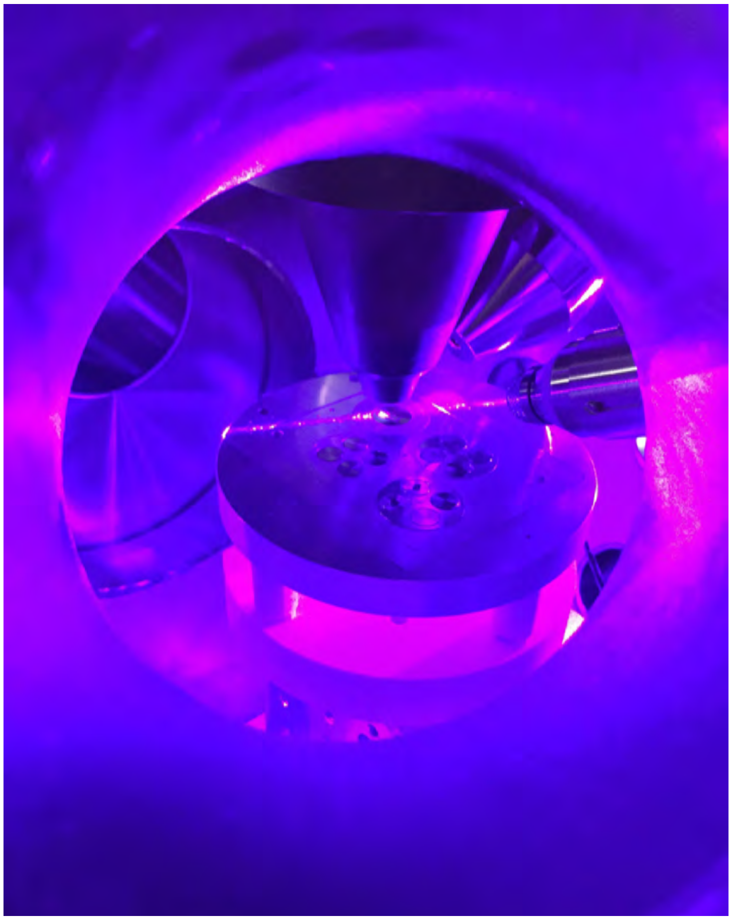
sufficient confidence the instrument's usefulness for forensics applications.

RIMS' Realm of Possibilities

The RIMS technique uses a laser beam to shake loose atoms and molecules from a solid sample, forming a rapidly expanding cloud. A voltage pulse removes the ions in the cloud, leaving the neutral atoms behind. Subsequently, lasers tuned to a particular element hit the cloud with two or three pulses that selectively excite then ionize resonant electrons in the atoms of the target element. Using an electric field, the now-charged ions are accelerated into a time-of-flight mass spectrometer, which identifies and measures the quantity of the various isotopes of that element. (See *S&TR*, April/May 2012, pp. 11–13.)

The late Livermore scientist Ian Hutcheon, who was instrumental in advancing the science of nuclear forensics and founded the Laboratory's forensics team, saw RIMS' potential when it proved quick and accurate at measuring isotopes in dust particles relevant to cosmochemistry. He approached Savina—an expert on laser-based spectroscopic methods—to begin assessing RIMS' application in forensics. Savina, then at Argonne National Laboratory, was applying RIMS to study actinides, the elements of the periodic table that include uranium and plutonium, in cosmic dust. He says, "Ian's interest in RIMS really piqued once he saw our plutonium measurements from the dust samples because the instrument was so much more capable than other methods."

Over the years, Livermore has received growing funding for this work from the Laboratory Directed Research and Development Program, the Department of Homeland Security's National Technical Nuclear Forensics Center, the Defense Threat Reduction Agency, and the Department of Energy's Office of Nonproliferation Research and Development. During that time, Isselhardt, who began studying RIMS as part of his Ph.D. dissertation in 2006, Savina, and colleagues at Livermore and Argonne led an in-depth study of RIMS for nuclear forensics applications. "It was slow going at first. The instrument at Argonne was often fully booked," says Isselhardt. But the team's perseverance paid off, and in 2011, Isselhardt, Savina, and colleagues published their research, which suggested that RIMS could measure uranium isotope ratios with the necessary precision. Four years later, they demonstrated precise RIMS measurements of the ratio of ^{240}Pu to ^{239}Pu, another measurement essential to nuclear forensics. They also showed that RIMS could measure ^{238}Pu accurately even when the sample had significant amounts of ^{238}U. This isobaric interference (caused by an isotope of a different element with the same atomic



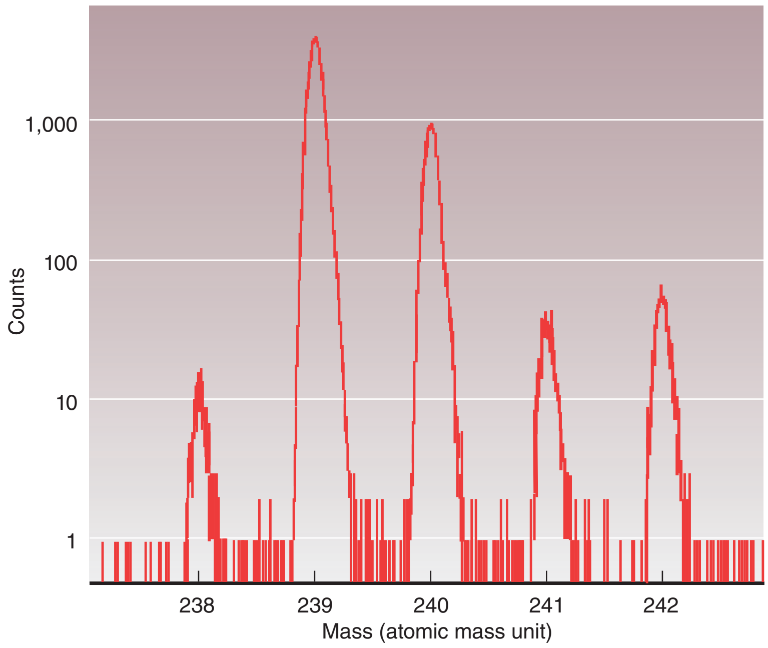
A laser beam (produced from three individual lasers) ionizes a sample of uranium (center) within the RIMS instrument. The lasers are tuned to the precise resonant frequencies of a particular element, or pair of elements simultaneously, such as uranium and plutonium. The isotopic compositions of various elements provide indicators of whether the nuclear material was enriched as nuclear reactor or weapons-grade material. Trace impurities can help pin the sample to a particular enrichment process.

weight as the target isotope) has confounded many other mass spectrometry techniques.

RIMS measurements are now capable of quantifying uranium isotope ratios with accuracy as high as 0.5 percent. Minimizing error is important because "the isotope ratios in nuclear materials tell you about its irradiation history, what sort of environment it was in, and what the purpose of the material was—whether it was for weapons or for nuclear reactors," says Isselhardt. Ultimately, inaccurate measurements can lead to incorrect conclusions about the material's origin.

The Emergence of LION

In 2015, when Savina joined Livermore, he and Isselhardt, in collaboration with mechanical technician Dave Ruddle, postdoctoral researcher Andrew Kucher, programmer Raja Gopal, and visiting scientist Bruce King from the University of Newcastle in Australia, finished building the Laboratory's LION facility. Within a few months, the team produced its first result, and the researchers are continuing to put LION through its paces. "The facility is operational and functional. We are improving the instrument's automation and integration," says Isselhardt. Their current task is to ensure its accuracy by reproducing and improving on the results they achieved for uranium and plutonium while using the Argonne instrument. "Our goal is to make these measurements rapid, robust, and routine," says Savina. "We want to be able to deliver meaningful measurements within four hours of receiving a sample."



A measurement of plutonium using the RIMS instrument at Livermore's LION laboratory demonstrates the instrument's ability to accurately measure five plutonium isotopes (238, 239, 240, 241, and 242) despite the presence of a 10-times higher concentration of uranium-238 in the sample. The logarithmic scale on the y-axis shows the number of ions detected for each isotope.

The team is also beginning to take measurements of other isotope ratios. "Having made accurate uranium and plutonium measurements, we're moving toward studying isotope ratios of americium, curium, neptunium, and trace fission products, especially those from the nuclear fuel cycle because they can give additional information about the age and enrichment history of nuclear materials," says Isselhardt.

Although LION's focus will be nuclear forensics, the researchers expect to put their facility to use in basic science studies as well. Cosmic dust carries evidence of how some stars evolve into supernovae. Savina is planning to take measurements of plutonium in lunar dust from the Apollo mission in search of particles that may have been produced in supernovae explosions and later drifted onto the lunar surface. With the LION facility fully operational, Livermore provides the nation with an important capability for cosmochemistry, and most importantly, for nuclear forensics as LION hunts for clues to the origins of nuclear materials.

—Allan Chen

Key Words: americium, cosmochemistry, curium, isotope ratio, Laboratory Directed Research and Development Program, laser, laser ionization of neutrals (LION) laboratory, neptunium, nuclear forensics, nuclear fuel cycle, plutonium, resonance ionization mass spectroscopy (RIMS), trace fission products, uranium.

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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-digit number in the search box at the U.S. Patent and Trademark Office's website (http://www.uspto.gov).

Patents

Method of Securing Filter Elements
Erik P. Brown, Jeffery L. Haslam, Mark A. Mitchell
U.S. Patent 9,457,297 B2
October 4, 2016

Mechanically Robust, Electrically Conductive Ultralow-Density Carbon Nanotube–based Aerogels
Marcus A. Worsley, Sergei O. Kucheyev, Theodore F. Baumann, Joe H. Satcher, Jr.
U.S. Patent 9,460,865 B2
October 4, 2016

Electrostatic Stabilizer for a Passive Magnetic Bearing System
Richard F. Post
U.S. Patent 9,464,670 B2
October 11, 2016

Resistively Heated Shape Memory Polymer Device
John E. Marion, III, Jane P. Bearinger, Thomas S. Wilson, Duncan J. Maitland
U.S. Patent 9,476,412 B2
October 25, 2016

Awards

Experimental physicist **Tammy Ma,** National Ignition Facility (NIF) division leader **Lisa Belk**, and research engineer **Monica Moya** were highlighted in ***Diablo Magazine's*** 2016 "**Forty Under Forty**" issue. The annual list recognizes young professionals in California's San Francisco East Bay area who are leaders in their fields.

Ma was recognized for her work developing and executing experiments aimed at creating sustained fusion at NIF. Belk was honored for heading a team of more than 80 people who provide computation support to national security, discovery science, and energy security missions at NIF. Moya received acknowledgement for her work using three-dimensional printing to create tubes made from human cells and biomaterial that guide small blood vessel development. Her research is part of a larger effort to develop a way of predicting the body's response to chemical agents without human or animal testing.

Retired Air Force General **Larry Welch** became the second recipient of the **John S. Foster Jr. Medal**. Established by **Lawrence Livermore National Security, LLC**, and bestowed annually by the director of Lawrence Livermore National Laboratory, the medal recognizes an individual for exceptional leadership in scientific, technical, and engineering development and policy formulation in support of U.S. nuclear security objectives.

Welch has been dedicated to serving the nation since 1951 and remains active in service, even in retirement. His distinguished career is highlighted by four years of service as the 12th Chief of Staff of the Unites States Air Force. As a member of the Joint Chiefs of Staff from 1986 to 1990, he served as one of the principal military advisers to the secretary of defense, the National Security Council, and the U.S. president. Welch also served as commander in chief of the Strategic Air Command from 1985 to 1986, responsible for operational planning for all U.S. strategic nuclear systems.

Now retired, Welch continues to serve the nation as a senior fellow of the Institute for Defense Analyses, a federally chartered research center providing operations and technical analysis for the Department of Defense and other U.S. government agencies. He led the institute as president and CEO from 1991 to 2003 and again from 2006 to 2009.

The **Meteoritical Society** honored Livermore researchers **Carolyn Crow** and **Greg Brennecka** during their annual meeting in Berlin, Germany. Crow, a postdoctoral researcher in the Nuclear and Chemical Sciences Division who studies impact signatures recorded in lunar and terrestrial zircons, won the **Gordon A. McKay Award** for her presentation on methods of using lunar zircon crystals to measure the magmatic and impact histories of the Moon, especially the formation histories of large basins. The award is given to the society member who is a full-time student and gives the best oral presentation at the Meteoritic Society's annual meeting.

Brennecka, now at the Institute for Planetology at the University of Munster, studies the importance of supernovae in the early solar system. He was awarded the **Nier Prize** for his research on isotopic variations in meteorites and the chronology of the solar system. The Nier Prize recognizes outstanding research in meteoritics for scientists under 35 years old. His work with fellow Livermore scientists Lars Borg and the late Ian Hutcheon led to an understanding of why uranium isotopes vary on Earth and also to the discovery of variations in uranium isotopes in meteorites, which was previously thought to not exist. This discovery changed the way the solar system's age is calculated.

(continued from p. 2)

Ultralightweight and Flexible Metallic Materials

Livermore engineers, scientists, and academic partners, which include Virginia Polytechnic Insititute and State University (Virginia Tech) and the Massachussetts Institute of Technology (MIT), have achieved unprecedented scalability in printing three-dimensional (3D) architectures of arbitrary geometry, opening the door to super-strong, ultralightweight, and flexible metallic materials for aerospace, military, and automotive applications. In a study published in the July 18, 2016, online issue of *Nature Materials* (and susequently featured on the cover of the journal's October issue) the team reported fabricating multiple layers of fractal-like lattices with features ranging from the nanometer to centimeter scale. This work resulted in a nickel-plated mechanical metamaterial with a higher than expected tensile elasticity.

According to lead author Xiaoyu "Rayne" Zheng, a former Livermore technical staff member who is now professor of mechanical engineering at Virginia Tech, "These nanoscale 3D features have some really interesting properties, but people have never been able to scale them up and see how they behave. We've figured out a strategy of hierarchically building them to take advantage of the nanoscale features at a large scale."

The lattices were initially printed out of polymer, using a one-of-a-kind large-area projection microstereolithography printer invented by Livermore engineer Bryan Moran, who won an R&D 100 Award in 2015 for the design. The lattice structure was then coated with a nickel–phosphorus alloy and put through postprocessing to remove the polymer core, leaving extremely lightweight, hollow tube structures. Chris Spadaccini, director of the Laboratory's Center for Engineered Materials and Manufacturing, says, "Using the structural concept of unit cells and lattices, combined with nanoscale features, we can achieve high strength at a very light weight, as well as a ductile-like behavior in materials that are normally brittle."

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Pulsed Ion Beams Probe Radiation Defects

Materials scientists at Lawrence Livermore, along with colleagues at Texas A&M University, have developed a novel experimental method to access the dynamic regime of radiation damage that occurs in nuclear and electronic materials. The new approach uses pulsed ion beams to measure defect lifetimes, interaction rates, and diffusion lengths. Because of the complexity involved, a full predictive capability of radiation damage still does not exist even for the simplest and best studied materials, and understanding mechanisms of dynamic radiation damage formation in solids remains a major materials physics challenge.

In a paper published in the August 3, 2016, edition of *Scientific Reports*, the team describes how they addressed this challenge using pulsed-ion-beam measurements of the dynamics of defect interaction in silicon carbide, a prototypical nuclear ceramic and wide-band-gap semiconductor. The team found that in the material, the dominant defect relaxation processes occur on millisecond timescales, and that the defect lifetime exhibits a non-monotonic temperature dependence.

"The pulsed-beam method allowed us to access the dynamic regime of radiation damage formation, which is essential for predicting the material behavior in different radiation environments," says Livermore materials scientist L. Bimo Bayu Aji, the lead author of the paper. Laboratory scientist Joseph Wallace summarizes, "The understanding of radiation defect dynamics may suggest new paths to designing radiation-resistant materials." Livermore project lead Sergei Kucheyev adds, "The understanding of defect interaction dynamics, probed in our pulsed-beam experiments, also is essential for using laboratory findings for predicting the material behavior under irradiation over timescale relevant to nuclear material service."

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De-icing Agent Remains Stable Under Extreme Pressure

Lawrence Livermore scientists have overturned established assumptions about the high-pressure structural behavior of magnesium chloride ($MgCl_2$), an effective de-icing agent used in aviation. The Livermore team observed $MgCl_2$ to be extensively stable under pressure, in contradiction to previously well-established structural systematics. The work, published in the August 12, 2016, edition of *Scientific Reports*, sought to provide equations of state (EOS) and structural phase diagrams to improve the confidence of semi-empirical thermochemical calculations predicting the products and performance of detonated chemical formulations.

"To determine accurate EOS data, we first conducted high-pressure x-ray diffraction measurements up to 40 gigapascals (GPa), or 400,000 times atmospheric pressure," says Joe Zaug, a Livermore physical chemist and the project leader. "According to previous theoretical studies and the well-established phase diagram of high-pressure compounds," adds lead author and Livermore physicist Elissaios Stavrou, "$MgCl_2$ should have transformed to a higher coordination number [more dense] and a three-dimensionally connectivity structure well below 40 GPa." However, $MgCl_2$ remained in a low-coordination layered structure, even after crossing the 1-megabar (1 million atmospheres) pressure limit.

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Abstract

Computational Innovation Boosts Manufacturing

The High Performance Computing for Manufacturing (HPC4Mfg) Program, funded by the Department of Energy's Advanced Manufacturing Office, aims to unite the world-class computing resources and expertise of national laboratories with U.S. manufacturers to increase manufacturing's energy efficiency and advance clean-energy technology. The program solicits proposals on manufacturing challenges twice a year from U.S. companies. High-performance computing (HPC) experts from Lawrence Livermore, Lawrence Berkeley, or Oak Ridge national laboratories are paired with the selected manufacturers. This article highlights three of the program's initial "seedling" projects. In one, Livermore computer scientist Aaron Fisher worked with Purdue University Northwest's Center for Innovation through Visualization and Simulation to improve models of the blast furnace processes used in making steel, with the goal of reducing the industry's use of coke—a coal-based fuel with high carbon content. Yue Hao from Livermore teamed with Lawrence Berkeley's David Trebotich and the Agenda 2020 Technology Alliance to determine how to reduce re-wetting in papermaking, which could save approximately $250 million annually. Finally, Nick Killingsworth and the SORAA company, a developer of solid-state lighting based on gallium-nitride (GaN) substrates, explored ways to scale up GaN crystal growth technology to significantly reduce production costs and improve crystal growth rates and quality, potentially ushering in a new generation of power electronics.

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Coming Next Issue

Center of Excellence Prepares for Sierra

Lawrence Livermore computational scientists adapt Laboratory-developed codes in anticipation of the institution's next-generation supercomputing platform.

Also in March

• Three-dimensional measurements of granular media under stress reveal new information about material properties and energy dissipation.

• Livermore scientists have developed a highly effective payload material for destroying chemical and biological weapons facilities.

• A novel, extremely accurate laser tracker speeds alignment of critical diagnostics for experiments at the National Ignition Facility.

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