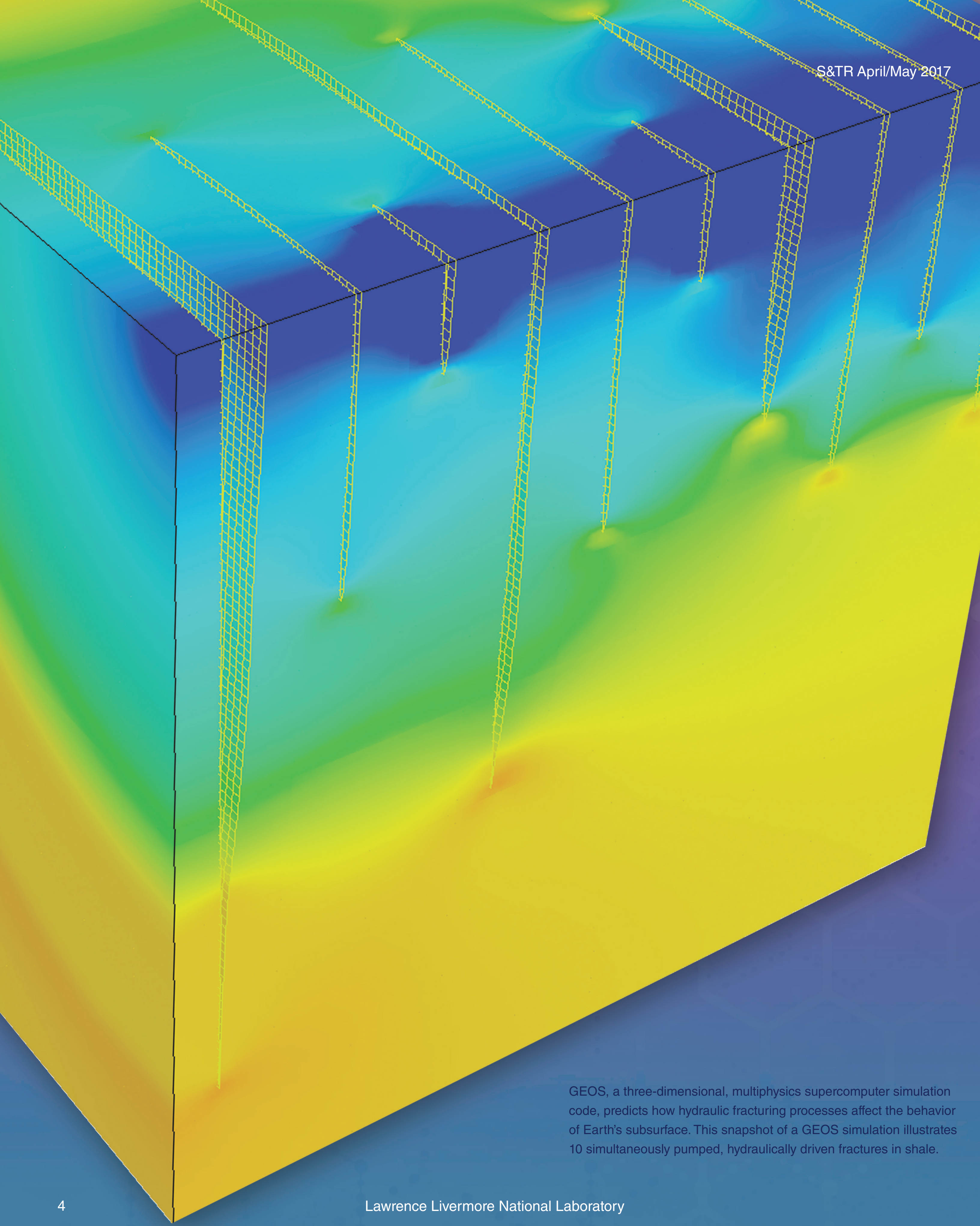


GEOS, a three-dimensional, multiphysics supercomputer simulation code, predicts how hydraulic fracturing processes affect the behavior of Earth's subsurface. This snapshot of a GEOS simulation illustrates 10 simultaneously pumped, hydraulically driven fractures in shale.

INVESTING IN THE NATION'S FUTURE

The Laboratory Directed Research and Development Program has been a significant engine of scientific discovery for 25 years.

FOR more than a quarter century, the Department of Energy's (DOE's) Laboratory Directed Research and Development (LDRD) Program has yielded an exceptional return on a relatively small investment. Through LDRD funding, Livermore researchers make possible transformative scientific and technological solutions to ever-changing national security challenges.

"LDRD is vital to maintaining the long-term health of Lawrence Livermore's national security mission and its core competencies," says Rokaya Al-Ayat, who is senior advisor to the Laboratory director and also oversees the institution's LDRD Program. Under LDRD, the Laboratory invests 6 percent of its operating budget (about $87 million in fiscal year 2017) in areas beyond the scope of programmatic research and where high-risk endeavors could lead to big payoffs. As the Laboratory's primary source of discretionary research and development funding, the program helps maintain the vitality of science and technology disciplines relevant to national security and explores ways to meet future mission needs.

The most innovative science and engineering programs at Livermore often have roots in LDRD. Livermore physicist Peter Amendt says, "LDRD projects offer the possibility of transformative advances." He adds that these efforts have been effective mechanisms for overcoming difficult physics challenges whose solutions require more time to fully discover the underlying science or technology.

Projects sponsored by LDRD contribute significantly to Lawrence Livermore's intellectual property, publications, and collaborations. The technical output of LDRD researchers—patent disclosures, peer-reviewed publications, and publications cited by other authors—typically accounts for one-quarter of the Laboratory's total. About half of Lawrence Livermore's patents and 20 percent of published journal articles result from LDRD investments. In the last 10 years, some 60 percent of Livermore's R&D 100 awards have also been attributed to LDRD funding. In addition, many technologies that come out of the LDRD Program have commercial value. The Laboratory's Industrial Partnerships Office licenses these technologies to the private sector to strengthen U.S. industry.

Attracting New Talent

Among the most valuable aspects of the LDRD Program is its role as an outstanding tool for professional growth and recruitment. Projects funded through LDRD are at the forefront of science, helping to attract promising young scientists and engineers. LDRD historically supports more than half of Livermore's postdoctoral researchers, and the projects they work on often influence their career paths. For example, the Laboratory has 15 DOE Early Career Research Program award winners, 14 of whom were supported by LDRD. In addition, 15 of the Laboratory's 23 Presidential Early Career Awards for Scientists and Engineers recipients have been LDRD principal investigators or co-investigators.

LDRD initiatives have proven transformative in all aspects of national security. Four research areas help illustrate the rapid advances possible when a modest investment is made in a talented team of scientists and engineers focused on a new idea. These examples are additive manufacturing (AM), which is revolutionizing the science of how structures are made; new designs, materials, and manufacturing methods for targets used at the National Ignition Facility (NIF); advanced software for improving the efficiency of hydraulic fracturing operations; and the transfer of pathogen-detection technology to industry.

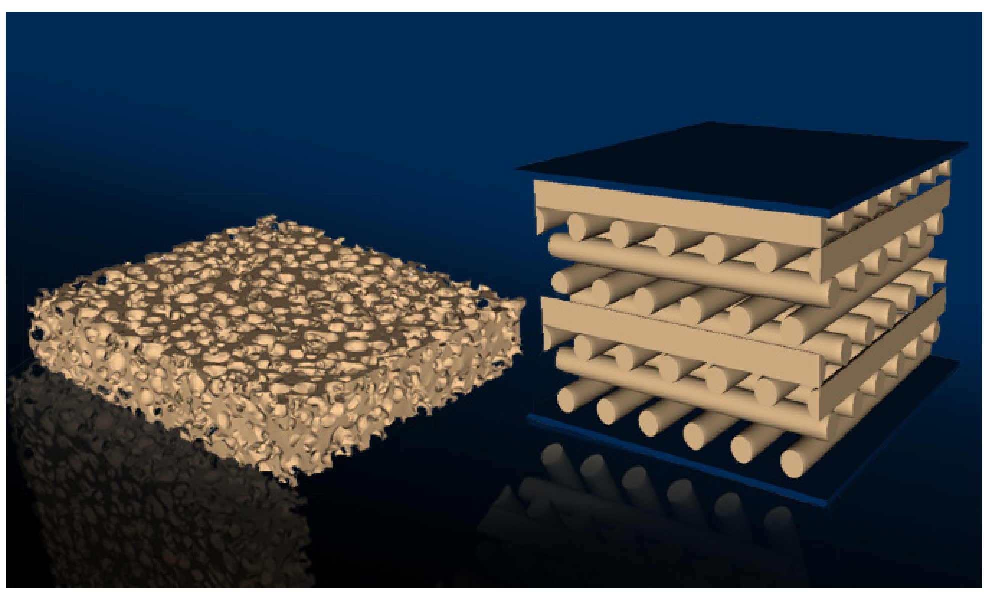
A Manufacturing Revolution

Numerous LDRD projects have supported research and development of radically new methods to make materials and parts faster, cheaper, lighter, and with entirely novel properties. "Many of Livermore's manufacturing and materials solutions have resulted from its LDRD portfolio," says Chris Spadaccini, director of the Laboratory's Center for Engineered Materials and Manufacturing.

AM, often in the form of three-dimensional (3D) printing, typically adds successive layers of material to precisely fabricate 3D objects that may have accompanying complex geometries. Livermore-developed AM technologies, which are revolutionizing manufacturing by producing materials with unprecedented structural, thermal, electrical, chemical, and photonic properties, are rooted in LDRD. Livermore's focus is to advance those technologies that are not commercially available by integrating manufacturing expertise, precision engineering, materials science, and high-performance computing. The result is innovative multifunctional materials for stockpile stewardship, global security, and energy security.

LDRD-funded projects have led to the manufacture of components incorporating polymers, metals, and ceramics. These parts are produced with reduced cost, less waste, and often remarkably fast turnaround, all of which have greatly accelerated the design–build–test cycle. A materials designer can often produce a prototype part in a few hours, immediately assess its viability, and, if necessary, change a design for improved performance. Indeed, LDRD efforts have demonstrated how components for national security purposes can be produced in weeks to months instead of the several years required using conventional approaches.

In all, LDRD initiatives have resulted in more than 40 AM projects spanning



Three-dimensional (3D) printing allows researchers to create materials with custom structures, shapes, and mechanical properties while saving time and expense. The microstructures of two different foam materials show (left) a traditional open cell form and (right) a 3D-printed foam with a tetragonal lattice structure.

a broad range of missions. For example, LDRD-driven investments have supported the creation of novel tools such as “optical tweezers” (see *S&TR*, March 2010, pp. 11–13) that use a highly focused laser beam to move microscopic objects, and 3D multibeam lithography, which projects holographic light patterns into photo-curable liquid resins to create 3D structures. Among several new AM processes invented under the auspices of LDRD is laser diode AM (DiAM). A key component of DiAM—now patented and licensed—is the optically addressable light valve. The technology was originally invented by Livermore researchers to shadow defects in valuable NIF optics and prevent further damage.

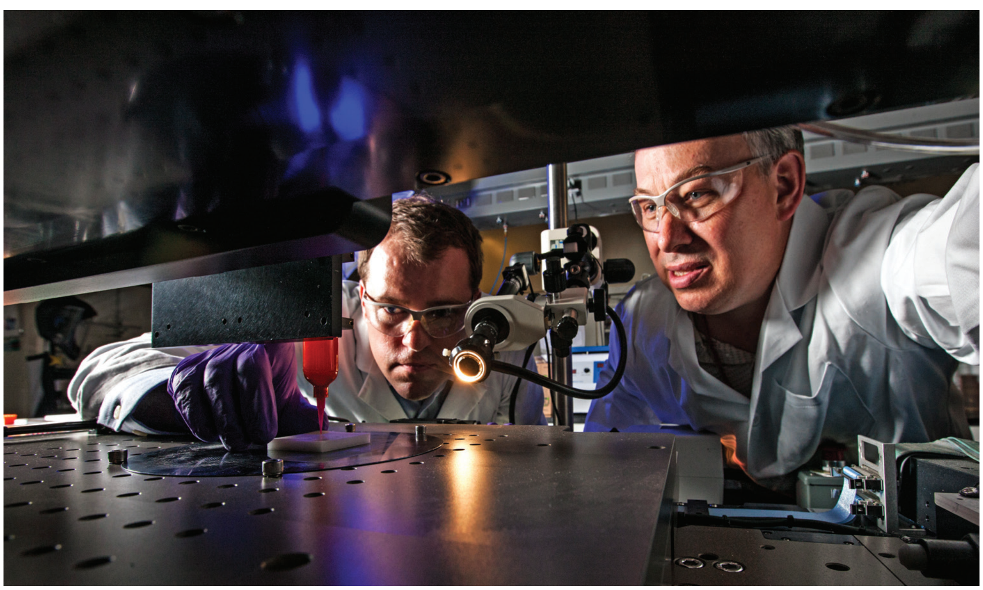
Innovative modeling and simulation methods for AM have potential for use in stockpile stewardship applications including qualification and certification. An LDRD project headed by Wayne King, leader of the Laboratory’s Accelerated Certification of Additively Manufactured Metals project, is advancing the fundamental understanding of the complex physics behind AM and 3D metal printing. “We want to accelerate qualification and certification of these new materials and components to take advantage of the flexibility of metal additive manufacturing,” says King.

A stellar example of an AM advance is direct ink writing (DIW), a technique based upon filamentary extrusion of polymer-based “inks.” In 2010, researchers at Livermore collaborated with then University of Illinois Urbana-Champaign professor Jennifer Lewis (now at Harvard University) on an LDRD Strategic Initiative (SI) to adapt the DIW technique. Only two years later, Livermore partnered with the National Nuclear Security Administration’s (NNSA’s) Kansas City National Security Campus to work on manufacturing technologies using DIW.

By 2013, Livermore had designed and procured a unique printing system for making parts with DIW. The following year, Livermore advances were being heralded in international forums and technical journals. The team received an NNSA Award of Excellence in 2015 for exceptional creativity in developing a process for cushions and pads. (See *S&TR*, September 2014, pp. 20–23.) These energy absorbers have tailored mechanical responses and are made with significantly reduced production time, production footprint, and enhanced production yield combined with improved aging characteristics. Livermore researchers have also used DIW to make engineered graphene aerogel microlattices. This work combines the structural properties of the lattice with the electrochemical functionality of the graphene to form, in one instance, a strong, lightweight, yet compressible high-performance supercapacitor. (See *S&TR*, April/May 2015, pp. 14–18.)

The most visible result of the impressively rapid rise of LDRD-supported AM science is the 13,000-square-foot, $9.4 million Advanced Manufacturing Laboratory at the Livermore Valley Open Campus. (See *S&TR*, March 2011, pp. 22–25.) This facility, now under construction, will provide a space for Livermore employees to collaborate with industry and academic partners on AM technologies. Spadaccini says that initial LDRD support of AM research helped expand the method’s possibilities, which has led to support for such a facility.

The growing AM effort has attracted talented scientists and engineers to Livermore, including more than 40 postdoctoral researchers and 60 summer interns over the past 6 years. Livermore researchers have also been collaborating with graduate students at universities across the nation on related efforts. In this area, more than 80 invention disclosures and 50 patents have been filed. Moreover, upwards of 10 Cooperative Research and Development Agreements (CRADAs) and industry-related projects are under way.

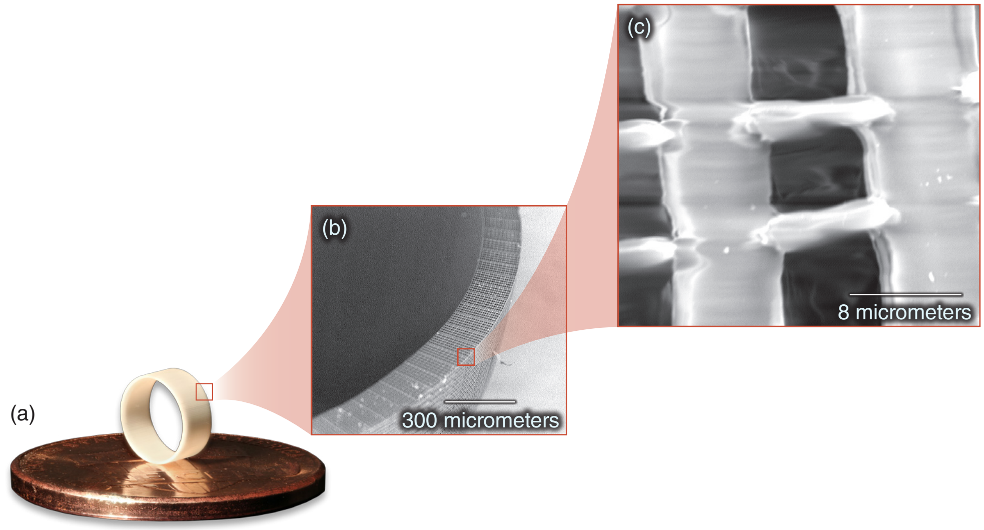


Livermore engineers Eric Duoss (left) and Tom Wilson use an additive manufacturing process called direct ink writing to develop an engineered porous cushion. (Photo by George A. Kitrinos.)

Improved Target Fabrication

NIF experimental targets, typically no larger than a few millimeters in diameter, include two broad categories: high-energy-density (HED) physics targets that test materials at nuclear weapons–related extreme temperatures and inertial confinement fusion (ICF) targets aimed at furthering the understanding of laser fusion. LDRD investments in fabricating both types of targets have resulted in substantial contributions to both materials science and national security.

Before NIF began operation in 2009, two three-year-long LDRD SIs, one begun in 2005 and the other in 2008, were highly successful in establishing new designs and manufacturing capabilities for advanced laser targets. These two efforts were conducted under the auspices of Livermore's Nanoscale Synthesis and Characterization Laboratory (NSCL). Under the SIs, researchers greatly advanced the science and engineering needed to produce nanocrystalline grains, nanoporous foams, high-strength aerogels, atomic-layer deposition techniques, advanced lithography, and joining techniques for precision microassembly. Alex Hamza, former NIF target fabrication manager and now director of the NSCL, says, "The impact on the materials science community was enormous. The two SIs resulted in technical papers that have been cited more than 8,000 times."



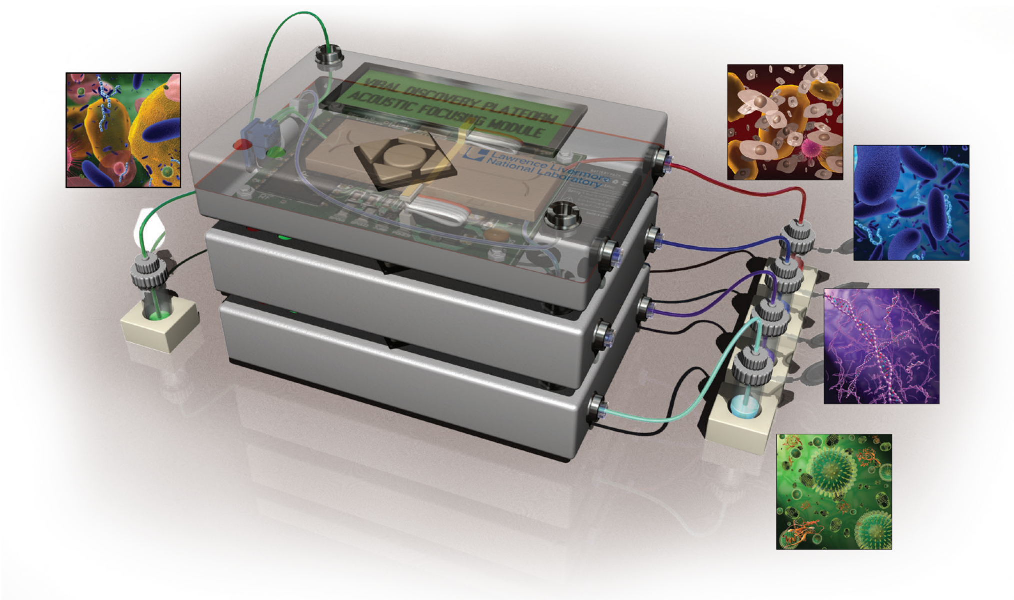
Using the two-photon polymerization direct laser writing technique, a Livermore research team manufactured (a) a hohlraum foam liner template. Scanning electron microscopy images show the liner magnified (b) 230 and (c) 10,000 times. The liner's thickness, density, and composition were specifically "tuned" by the on-demand fabrication process.

Amendt notes that the contributions from the first SI alone continue to yield dividends. Many advancements have been adopted by Livermore programs, while other efforts are being pursued in subsequent LDRD efforts. For example, scientists devised a prototype double-shell ICF target as a test bed for integrating new materials and methods. The double-shell design is a complementary approach to the traditional single-shell target. Early experimental results have been encouraging.

An SI breakthrough, accomplished with the collaboration of Diamond Materials and General Atomics, was a high-strength diamond capsule to replace plastic ablator shells. A key advantage of diamond over plastic is its roughly three times higher density, permitting diamond ablator shells to be only one-third the thickness of plastic ones. Diamond shells can also be fabricated with extremely smooth surfaces. Together, these advantages result in better confinement of deuterium–tritium (DT) fuel. Hamza says, "Diamond capsules for both ICF and HED targets are now regularly used at NIF."

Other LDRD-fostered ideas have included changing the design of the hohlraum, a tiny metal casing open at both ends that encloses the NIF target. A candidate design is a rugby hohlraum, which resembles a cylinder with the corners rounded off to minimize surface area. The hohlraum's oblong shape helps

Rugby hohlraums (one-half of a prototype is shown here) resemble a traditional cylinder-shaped hohlraum, but with the corners of the cylinder rounded off. Laser light enters the casing through both ends, and the rugby design reduces energy loss in the walls because of their smaller surface area.



An artist's concept shows the viral discovery platform Livermore researchers developed to separate viruses from other sample materials, such as bacteria, mammalian cells, free DNA, and proteins. The work was done as part of a Laboratory Directed Research and Development project to more rapidly identify and characterize pathogens. (Renderings by Kwei-Yu Chu and Sabrina Fletcher.)

reduce energy losses that typically occur through a holhraum's wall surface.

One of the biggest payoffs from LDRD investments in target designs, fabrication methods, and materials was new techniques to produce nanoporous foams—extremely lightweight porous structures made from different materials with uniformly sized holes at the nanoscale. Researchers have created an entire suite of low- to high-*Z* (atomic number) foams, including those with graded densities. A DT-saturated polymer foam developed over the last decade is designed to replace the thin layer of DT "ice" typically used in ICF experiments.

LDRD funding also led to the development of the polyelectrolyte enabled liftoff (PEEL) technology, which can fabricate polymer films that are larger, stronger, and thinner than those produced with conventional methods. The extremely thin (about 6 nanometers or 30 atoms thick) PEEL-produced membranes serve as "tents" for suspending ICF fuel capsules inside hohlraums. PEEL was named one of the top 100 industrial inventions worldwide for 2016 by *R&D Magazine*. (See *S&TR*, January/February 2017, pp. 16–17.)

Advances in AM developed through LDRD investments are further empowering target fabricators. An LDRD-funded team led by Livermore's Juergen Biener is accelerating fabrication time from weeks to hours for polymer foam and aerogel components used in targets. The "on demand" capability allows researchers to easily change a material's properties, such as density, elasticity, and brittleness, and parts can be 3D printed with specified properties, structure, and shapes. Biener says, "With AM technology, we are independently controlling the surface area, pore size, and pore volume of our aerogels."

Another idea borne out of LDRD investments is incorporating a foam liner into a hohlraum to improve implosion symmetry. Through an AM process called two-photon polymerization direct laser writing, Biener's team fabricated the first millimeter-sized, low-density foam parts with nanoscale features for material strength tests and as hohlraum liner templates. The breakthrough production methods can also be applied to sustainable energy applications such as hydrogen and electrical energy storage. In another example, LDRD funding laid the foundation for creating an on-chip material library of nanoporous gold structures for studying the relationships of structures and properties, such as those of neural interfaces. "We're still reaping the benefits of LDRD investments that ended seven to ten years ago," says Hamza.

New Ways to Identify Pathogens

LDRD investments have long supported the development of new approaches for rapid and accurate detection of biological agents that could be unleashed by rogue nations and terrorist groups. Half of Lawrence Livermore's royalties from licensing agreements are from novel technologies developed within its biotechnology program, and LDRD has been the seedbed for many of these commercial successes. A particularly notable technology transfer success was the formation of QuantaLife, Inc., which converted an LDRD-developed technology aimed at detecting dangerous pathogens to commercial medical applications.

Two long-term Livermore employees, Bill Colston and Fred Milanovich, left the Laboratory in 2008 to found QuantaLife and develop sensitive and accurate commercial genetic-testing products based on Livermore-developed pathogen-detection technology. Specifically, QuantaLife licensed digital polymerase chain reaction (PCR), a refinement of real-time PCR, which allows researchers to quickly identify extremely low concentrations of pathogens contained within a sample.

The key technology was what QuantaLife called droplet digital PCR (ddPCR). For years, scientists had solely used traditional PCR to identify the genetic composition of a specimen. However, this technique can miss extremely small amounts of DNA or RNA that signal the presence of a pathogen. With ddPCR, the sample is split into a large number of equivalent droplets, and then traditional PCR is carried out in each partition. In this way, ddPCR detects rare DNA that might typically be lost in the background.

The ddPCR technique had its origins in an LDRD project called the viral discovery platform. The project, led by Chris Bailey, focused on development of a new approach for rapidly identifying and characterizing viruses in liquid samples. Bailey's team leveraged Livermore advances in microfluidics (manipulation of liquids in tiny channels) and demonstrated microfluidic isolation of virus particles in complex biological samples. The team also developed the first-ever bioinformatics (software to analyze biological data) system that optimized pathogen signatures (regions of DNA unique to a species) for rapid identification. Another advancement was the team's creation of the first comprehensive, automated sample-preparation system for sorting all components in clinical samples. Furthermore, the LDRD effort advanced the technology of microarrays, where gene sequences are placed onto a chip to detect pathogens.

"Biological samples are messy and complicated. Our aim was to develop a platform where we could isolate low concentrations of pathogens and identify them," says Bailey. "Typically, scientists are looking for only one pathogen, but we developed a technique that could test for many different pathogens. We brought together various technologies to get a deeper view of what a biological sample contained. We were successful because we had such diverse capabilities at the Laboratory, especially bioinformatics, which is critical to analyzing complex samples and generating unique signatures."

The third generation of the microbial discovery platform contained bacterial and fungal signatures in addition to those for viruses, making it the most accurate and sensitive genetic analysis platform for pathogens developed at the time. The system was tested on various samples, including those from paralyzed children in Pakistan and sick sea lions living on the California coast. The system was also used to check the purity of a commercially available rotavirus vaccine. The platform detected contamination from a porcine virus. Subsequently, sales of the vaccine were suspended until it could be proven safe.

With the help of Livermore's Industrial Partnerships Office, QuantaLife gained the rights to commercialize the Livermore technology and apply a breakthrough originally developed for national security to clinical medicine. Colston helped grow QuantaLife into a company of more than 60 employees by 2011. During his Livermore career, Colston headed the Biodefense Knowledge Center, led the Chemical and Biological Countermeasures Division, secured 13 patents, and received three R&D 100 awards. Co-founder Milanovich directed the Laboratory's Chemical and Biological National Security Program, and in 2002 was named a Lawrence Livermore Edward Teller Fellow. Both founders were also inducted into the Laboratory Entrepreneurs' Hall of Fame.

QuantaLife was honored as the "most promising company" at the Personalized Medicine World Conference in 2010. Later versions of ddPCR earned the Best New Life Sciences Product in 2013 and a Federal Laboratory Consortium Outstanding Commercialization Success Award. In 2011, Bio-Rad, Inc., acquired

Lawrence Livermore Director Bill Goldstein (left) congratulates former Livermore employee Bill Colston on his election to the Laboratory Entrepreneurs' Hall of Fame. Colston co-founded QuantaLife, Inc., which commercialized a breakthrough Livermore technology for detecting and identifying pathogens.

QuantaLife for $162 million. Bio-Rad continues to enhance the product. Bailey says, "We developed the technology for national security, but QuantaLife made it useful for medicine."

A Rigorous Selection Process

Livermore scientists and engineers who seek funding from the Laboratory Directed Research and Development (LDRD) Program must choose from among four project categories: Strategic Initiative (SI), Exploratory Research (ER), Laboratory-Wide (LW), and Feasibility Study (FS). SIs involve large multidisciplinary, cross-organizational teams and are funded for up to three years at $1.5 to $3 million per year. ERs represent investments in core competency areas and are funded typically for less than $1.5 million per year. LWs are small projects that serve as incubators for proposals from early-career personnel. (See "Program Supports Blazing New Trails," beginning on p. 13 of this issue.) FSs are funded at less than $175,000 for one year, but are considered for funding opportunities throughout the year.

During the first quarter of each calendar year, the Laboratory director issues a call to all scientific and technical personnel for LDRD proposals in the four project categories. All proposals are rigorously evaluated with criteria consistent with those used across the scientific community, in particular the National Science Foundation and the National Institutes of Health. Scientific and technical merit is a key element of the review process, as are innovation and creativity, potential impact on the technical field, qualifications of the researchers, available resources, and the proposed research approach.

Enhanced Hydraulic Fracturing

A major element of national security is energy security, and LDRD-supported efforts have helped to reduce U.S. dependence on imported oil. Hydraulic fracturing, also known as hydraulic stimulation, has revolutionized domestic hydrocarbon production and is providing the nation with an abundant source of oil and natural gas.

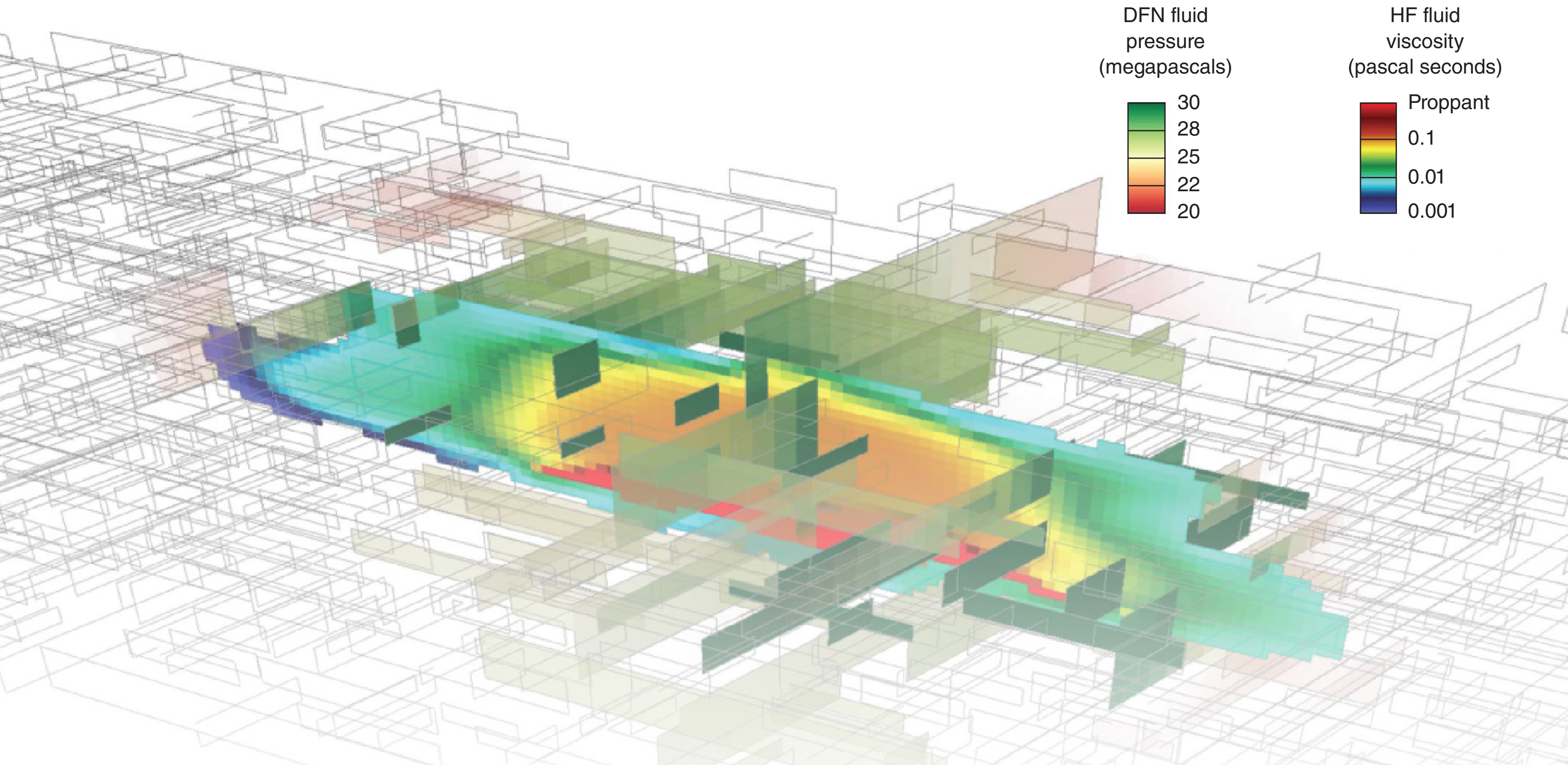
Fractures produced or reactivated during hydraulic stimulation provide an efficient pathway for the transport of hydrocarbons that are tightly bound within rock and wellhead. The process was initially developed in the 1980s and 1990s with the help of DOE funding. A typical hydraulic fracturing well begins as a vertical well that is subsequently steered to penetrate horizontally for many kilometers. A combination of water, viscous fluids, and sand is then pumped into the well at high pressure, opening fractures that liberate oil and gas.

However, hydraulic fracturing operations typically recover only a small portion of the available oil and gas, and energy producers wanting to maximize production struggle to understand the physical mechanisms that govern the hydraulic stimulation. In addition, longstanding concerns remain regarding the large amounts of water routinely used in the process, the potential contamination of aquifers, and the triggering of seismicity from water reinjection.

To increase hydraulic fracturing efficiency, decrease costs and environmental impacts, and enhance understanding of the hydraulic stimulation process, a Livermore team, funded by LDRD, developed GEOS, a 3D multiphysics supercomputer simulation code. GEOS is a powerful tool for predicting the behavior of Earth's subsurface and guiding oil and natural gas extraction from shale formations, thereby maximizing the yield of underground reservoirs.

"Conventional practices leave so much oil and gas in the ground that even a small increase in efficiency helps," says lead GEOS developer Randolph Settgast. He notes that well operators have limited information about how the rock fractures they create will form and propagate when subjected to high-pressure fluid injections. GEOS incorporates models of the physical processes that accompany hydraulic stimulation and control the formation and propagation of fractures. Using reservoir models representing the heterogeneous nature of the subsurface, GEOS predicts the response to stimulation, including the lateral and vertical extent of the fracture as well as its shape and aperture. GEOS simulates the growth of fractures over a spatial range extending kilometers—from near the well to the entire reservoir—and spans a temporal scale ranging from seconds to years. In this way, the code helps operators to more efficiently exploit the subsurface layer containing the most natural gas or oil. For example, the code seeks to guide decisions on the optimum spacing of production wells and recommend the best pumping schedules.

GEOS' development effort, which began under a 2011 LDRD SI led by geophysicist Rick Ryerson, took advantage of Livermore expertise in computational geoscience, high-performance computing, mechanical engineering, geomechanics, seismology, hydrology, and the experience of industrial partners. Currently, three GEOS-related LDRD initiatives are under way. One team, led by Joseph Morris, is modeling "dynamic stimulation," in which energetic materials are used to enhance hydrocarbon production in tight formations. Another LDRD group is analyzing stress and strain data from fiber-optic acoustic sensors inside a well to better characterize fracturing operations. A third team, led by Pengcheng Fu, is performing simulations to advise California's Division of Oil, Gas, and Geothermal Resources on the efficiency and environmental impacts



A GEOS simulation shows the growth of fractures caused by a horizontal hydraulic fracturing well pumping fluid into an oil-containing layer of subsurface shale. Color gradients correlate to the discrete fracture network (DFN) fluid pressure and hydraulic fracture (HF) fluid visocity. The full duration of the simulation is 102 minutes, about the time it takes to stimulate a 300-meter-long section of a production field.

of cyclic steam injection and hydraulic stimulation in California oil reservoirs.

Livermore researchers are also working with colleagues at Lawrence Berkeley National Laboratory as part of DOE's Exascale Computing Project to couple the GEOS code with a Lawrence Berkeley code that simulates pore-scale flow and geochemical reactions of fluids. Settgast explains, "Together, the coupled codes will allow us to simulate the performance of a vertical well ranging from the flow and chemistry of fluids in rock pores to large-scale fractures."

Two CRADAs, one with a small independent company and the other with a major oil producer, are aimed at validating the performance of GEOS under real-world conditions. Settgast says that working closely with the oil and gas companies has helped the group refine its goals. "The companies are looking for partners they can trust," he says. "They know the LDRD efforts are nonprofit, and we are upfront about the capabilities we do and do not have." GEOS is poised to become an important tool for energy security. The code could also be used to enhance operations at geothermal power plants.

Celebrating 25 Years of Success

With LDRD making possible national security advances on so many fronts, competition among scientists and engineers for this prized funding source remains fierce. (See the box on p. 11.) LDRD projects are selected on a highly competitive basis through rigorous management and peer-review processes, and only 1 in 10 proposals receives funding. However, researchers whose proposals are turned down receive valuable feedback about their submittals and are encouraged to apply the following year.

Applicants say that despite the intense competition for obtaining LDRD funding, the opportunity to pursue frontier science—and make an important research contribution—makes the effort more than worthwhile. LDRD-funded efforts have produced enormous payoffs from modest investments over the past 25 years. Another quarter century of outstanding results is just beginning.

—Arnie Heller

Key Words: additive manufacturing (AM), Center for Engineered Materials and Manufacturing, Cooperative Research and Development Agreement (CRADA), Department of Energy (DOE) Early Career Research Program, direct ink writing (DIW), droplet digital polymerase chain reaction (ddPCR), Exascale Computing Project, GEOS, hohlraum, hydraulic fracturing, Laboratory Directed Research and Development (LDRD) Program, Nanoscale Synthesis and Characterization Laboratory (NSCL), National Ignition Facility (NIF), polyelectrolyte enabled liftoff (PEEL), Presidential Early Career Awards for Scientists and Engineers, QuantaLife, Inc.

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