LAWRENCE LIVERMORE NATIONAL LABORATORY





Scientific Discoveries Change Lives and Fuel Economic Growth

The year 2020 presented unique and unforeseen challenges throughout the world with the arrival of COVID-19. Global economies were shut down, huge swaths of the workforce faced unemployment, education systems were re-designed, mass transportation and air travel declined as much as 80 percent, and some medications, personal protective equipment, and medical devices were in serious short supply. The world scrambled for solutions as the virus continued to spread.

Although the challenges manifested in different forms, those related to public health loomed the largest. In response, the United States and other countries turned to innovation and technology to gain an advantage over the virus. Perhaps the most significant technological contribution to the global fight involves the power of the nation's supercomputers. The DOE made available its deep knowledge and supercomputing hardware to private industry for the development of COVID-19 therapeutics and vaccines. One example involves LLNL researchers who for the first time combined artificial intelligence/machine learning, bioinformatics, and supercomputing to help discover candidates for new antibodies and pharmaceutical drugs to combat the virus.

Approximately fifty LLNL technologies have been leveraged to help fight this pandemic, and the Lab's Innovation & Partnerships office (IPO) has served as an access point for interested industrial partners. IPO developed express licenses for companies wishing to use LLNL IP for COVID-19-related applications. These short, nonexclusive, time-limited licenses enable rapid technology deployment by the private sector. The IPO accelerated the execution of numerous Cooperative Research and Development Agreements so technologies could be further refined with industrial partners.

For decades, LLNL's research has produced innovation and technology that has improved the human condition. This is not unique to 2020. When the pandemic is gone, LLNL will continue its mission, and the IPO will encourage commercialization, foster entrepreneurship, and promote the value of partnerships.

Director, Innovation & Partnerships Office

-Richard A. Rankin

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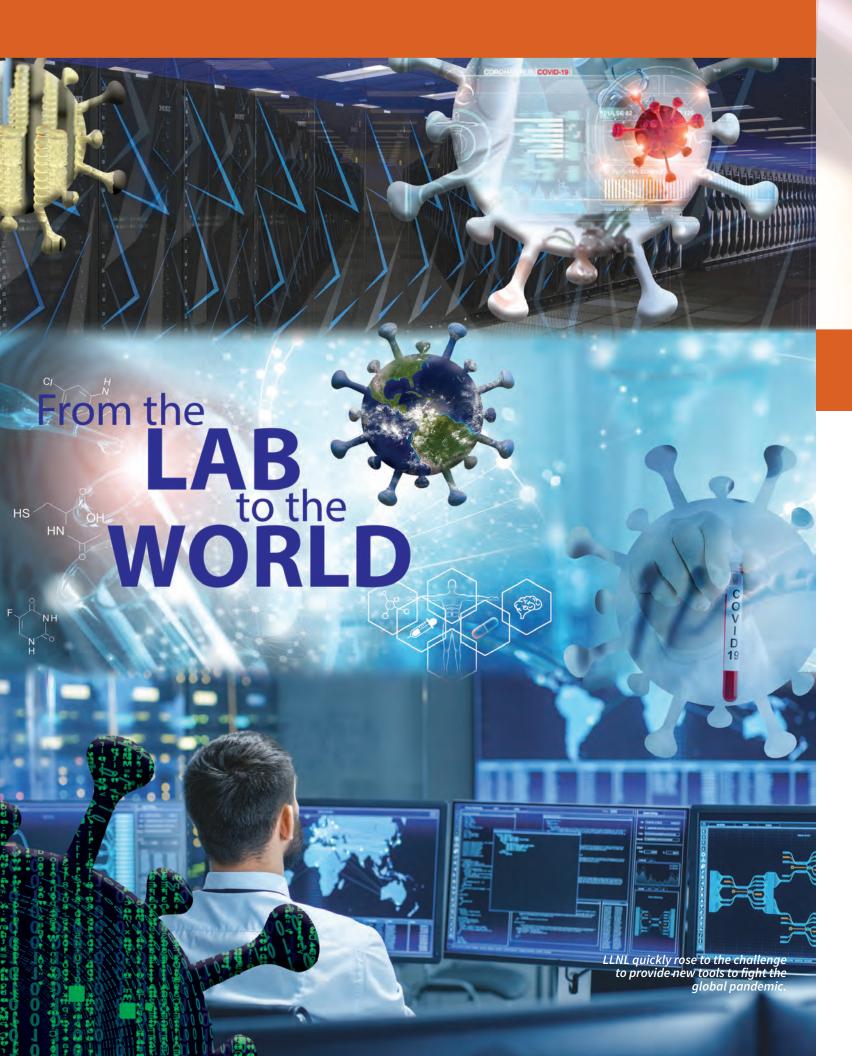




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EXECUTIVE SUMMARY

The IPO identified approximately 50 hardware and software technologies useful in the fight against COVID-19. In coordination with LLNL Office of General Counsel, the team developed express licenses for companies to use LLNL IP for COVID-19-related applications.

When the World Health Organization declared coronavirus disease 2019 (COVID-19) a global pandemic on March 11, the nation braced for the upheaval that the novel SARS-CoV-2 would cause in virtually every sector of our society. This year's IPO annual report highlights some of the COVID-19 work, including a prototype ventilator design, novel 3D printed nasal swabs for sample collection, and rapid PCR thermocycling for a SARS-CoV-2 test kit. Many other Laboratory efforts are highlighted here including: using quantum science to optimize the quantum—classical interface, artificial intelligence to predict material properties, new additive manufacturing (AM) techniques that overcome cost and time constraints, and an optical encoder device to digitize high-power electronic signals. Partnerships with industries and research institutions enhance core capabilities and provide sponsors with world-class science and technology (S&T) solutions, such as: a cold spray AM technique that preserves a material's functional properties, lightweight and deformable mirrors for directed energy systems, compact telescopes for nanosatellites, and a simulation framework for RAS proteins.

The National Labs Entrepreneurship Academy, Energy-I-Corps, and National Lab Accelerator programs bring together scientists and engineers (S&Es) and mentors from industry, and FedTech and I-GATE support startups. InnovationXLab summits and HPCIC events boost capabilities in computational S&T, and the Livermore Valley Open Campus, and the Advanced Manufacturing Laboratory spur public—private partnerships.

Laboratory talent was recognized in 2020 by many awards, including: a national Federal Laboratory Consortium award; four R&D 100 awards, and one silver Special Recognition award; a 'Best in Class' award from DOE's Technology Transfer Working Group, and five Office of Technology Transitions Technology Commercialization Fund awards. As the Laboratory continues to address the needs in national security and other important global challenges, its investments will strengthen the nation's ability to anticipate the threats on the horizon to keep our country safe.





LLNL Joins the Fight against Coronavirus

"The National Nuclear Security Administration is eagerly lending its worldclass supercomputing resources to combat COVID-19 in collaboration with OSTP and other agencies."

> Lisa E. Gordon-Hagerty, DOE undersecretary for Nuclear Security and NNSA administrator

to address patient volume. 2.000 Cephid's SARS-CoV-2 diagnostic tests

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Coronavirus disease 2019 (COVID-19) has touched millions of lives since

it was first identified in Wuhan, China in December 2019. COVID-19 quickly spread to the United States as well as every other country and was deemed a global pandemic on March 11. Caused by the novel coronavirus SARS-CoV-2, the disease manifests in a range of symptoms and severity.

To assist the nation in its fight against COVID-19, the IPO reviewed LLNL's extensive IP portfolio to identify which LLNL technologies and/or software might aid in the fight against the disease and identified approximately 50 applicable technologies. The IPO worked with the Office of General Counsel at LLNL to develop express licenses for companies wishing to use LLNL IP for COVID-19related applications. These short, nonexclusive, time-limited licenses were designed for expedited execution to enable rapid technology deployment by the private sector.

Innovative LLNL Technologies Join the Fight

In addition to opportunities for licensing LLNL technology, IPO assisted in facilitating research and testing partnerships. During the first few months of the pandemic, hospitals across the U.S. faced shortages of mechanical ventilators. A "skunkworks" team at LLNL worked tirelessly to prototype a ventilator design for quick and easy assembly from readily available parts. IPO posted a Technology/ Business Opportunity for this technology, and the company BioMedInnovations (BMI) responded with interest.

To facilitate the time sensitive project, IPO accelerated the execution of a Cooperative Research and Development Agreement (CRADA) with BMI. Under the CRADA, BMI and LLNL are developing a commercial ventilator, based on LLNL's prototype design, under the brand SuppleVent. The ventilator is designed to meet the functional requirements of COVID-19 patients suffering from Acute Respiratory Distress Syndrome and other conditions that cause serious breathing difficulties. The FDA authorized the prototype for emergency use so that hospitals could use the device to provide relief in places where ventilators are in short supply.

Internal Laboratory efforts are also contributing in the fight against the pandemic. The unique capabilities of LLNL's Advanced Manufacturing Lab (AML) proved invaluable in the evaluation of novel 3D printed nasal swabs for biological sample collection. Researchers working in the AML identified the best designs and ensured the swabs performed as required. One such design received FDA exemption for immediate use.

Current licensees of LLNL technology also played an important role. In March, Cepheid, a company founded on LLNL technology, received an emergency use authorization from the FDA for SARS-CoV-2 diagnostic tests. Cepheid licensed technology from LLNL on microfabricated silicon heaters for PCR that enabled fast thermocycling. In May, the FDA granted another LLNL licensee, BioRad, emergency use authorization for their SARS-CoV-2 Droplet Digital PCR (ddPCR)

Supercomputers Advance Research for Treatment

The White House has spearheaded a COVID-19 High Performance Computing (HPC) Consortium to provide COVID-19 researchers with access to the world's most powerful HPC resources, including ten NNSA supercomputers, to advance the pace of scientific discovery in the fight to stop the virus. The unique public-private consortium includes Lawrence Livermore, Argonne, Los Alamos, Oak Ridge, and Sandia national labs; Massachusetts Institute of Technology and Rensselaer Polytechnic Institute; National Science Foundation and NASA; and IBM, Amazon, Google, Microsoft, and Hewlett Packard.

Researchers submit COVID-19-related proposals via an online portal, and a panel of scientists and computing researchers assess the public health benefit of the work. Consortium members are volunteering free compute time and resources on their machines to researchers whose proposals are chosen by the panel.

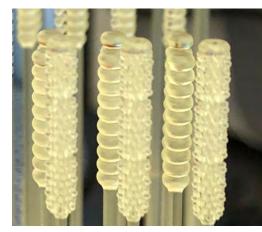
DOE Resources Highlight IPO Technologies

LLNL COVID-19 technologies and collaborative research were also highlighted in the COVID-19 section of the DOE's OTT resource for innovators through its Lab Partnering Service (LPS). Livermore's IPO highlighted more than 50 technologies and success stories related to COVID-19 on the LPS site. Supported by DOE's OTT, the LPS initiative allows U.S. innovators to readily access vital resources and connect and partner with experts at DOE's 17 national laboratories in the fight against the virus.





SuppleVent, a ventilator developed by LLNL and mass produced by North Carolina-based medical device startup company BioMed-Innovations is designed to help COVID-19 patients breathe.



Swabs were 3D-printed at LLNL from a biocompatible. surgical-grade resin and tested in the Laboratory's Advanced Manufacturing Laboratory.



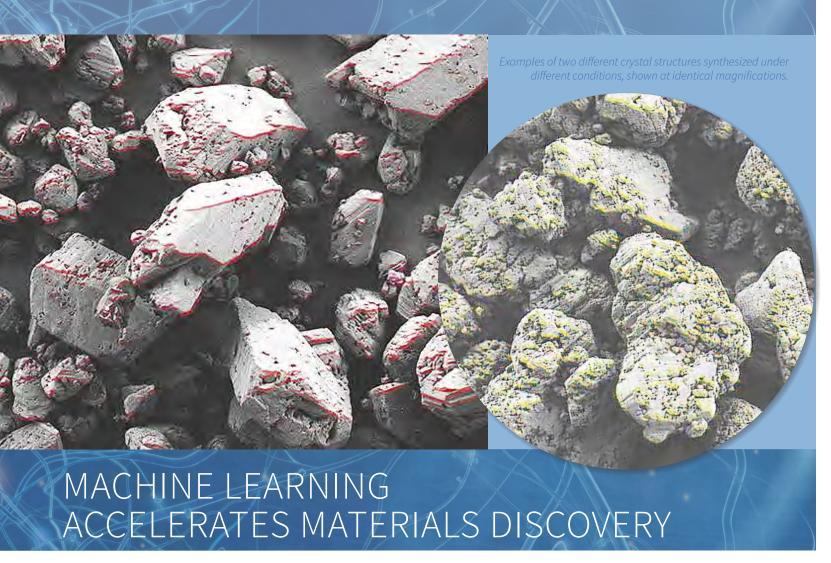




LLNL research pushes the limits of computational and experimental capabilities and builds deeper knowledge within LLNL's core competencies.

The Laboratory's multidisciplinary teams work together to apply advances in science and technology to address problems of national and global importance. Transformational research includes quantum science, artificial intelligence (AI), radio frequency photonics, additive manufacturing (AM), and drug and vaccine delivery. Activities highlighted in this section include:

- Applying new materials development to advance quantum science to synthesize materials, fabricate modular devices, optimize the quantum classical interface, design quantum computing systems, and develop new sensing and imaging capabilities;
- Leveraging advances in AI by extracting information from nanomaterials
 publications, employing simple models to predict material properties, and
 creating a machine learning (ML) framework that provides a trust score to
 quantify confidence in predictions;
- Meeting the growing needs in communication systems with several novel innovations including an optical encoder device that enables digitization of high-power electronic signals;
- Overcoming the time and cost limitations of traditional AM with a system that creates objects in 3D all at once, and another solution that generates a video portraying the complete rotation of projections of the 3D object; and
- Helping the healthcare industry by developing a platform for drug and vaccine delivery using nanolipoprotein particles.



Predicting Material Properties Using a Novel Machine Learning Pipeline

Challenge:

A grand challenge in materials science is to reduce the development and optimization cycle from materials conception to deployment. To achieve this, researchers need to understand the relationships between process, structure, properties, and performance (PSPP). Previous attempts to understand PSPP were hindered by a lack of data and the complexity of the problem. Recent technology advances have enabled the collection of large quantities of high-quality data. However, the sheer volume of data makes it difficult for scientists to separate salient information from noise.

Solution:

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A group of LLNL scientists, led by Yong Han, are developing approaches that address these challenges by leveraging advances in AI, ML, and data science.

Extracting materials process and structure information via publications: The team has developed ML tools that extract and structure information from the text and figures of nanomaterials articles using state-of-the-art natural language processing image analysis, computer vision (CV) and visualization techniques. In addition to processing articles' text, microscopy images of nanomaterials are automatically identified and analyzed to determine morphologies and size distributions.



To enable users to easily explore the database, Han's team also developed a browser-based visualization tool.

Predicting material properties: LLNL scientists have developed a novel pipeline that employs an ensemble of simpler models to reliably predict material properties. The team used their framework to predict properties of crystalline compounds and identify new, potentially stable compounds with bandgaps attuned for solar cell applications.

Understanding material performance: The LLNL team developed a novel approach to predict material performance. By applying CV and ML based on scanning electron microscopy images of feedstock materials, the team trained models to predict material performance, reducing error by 24% over current approaches. Furthermore, they did this without fabricating and physically testing a part. In addition, the team showed that ML models can discover informative materials attributes, which domain experts had underutilized previously.

Using explainable data to increase confidence in predictions: With imbalanced data, standard methods for assessing ML models break down and lead to distorted conclusions. LLNL scientists created a general-purpose, explainable, and reliable ML framework, which provides a trust score to better quantify the confidence in the predictions. The new system shows that the performance loss due to models' simplicity can be overcome by exploiting correlations among different material properties.

Collaboration:

The LLNL team partnered with Carnegie Mellon University to enable powerful, data efficient representation learning by developing new approaches for learning highly expressive models with small amounts of labeled data. This work bridges two predictive modeling approaches—Bayesian non-parametrics (BN) and deep learning (DL). The new approach enjoys the data-efficiency of BN and high representation power of DL. These models are being applied to a broad range of tasks on feedstock materials where scientists must make reliable inferences based on limited data.



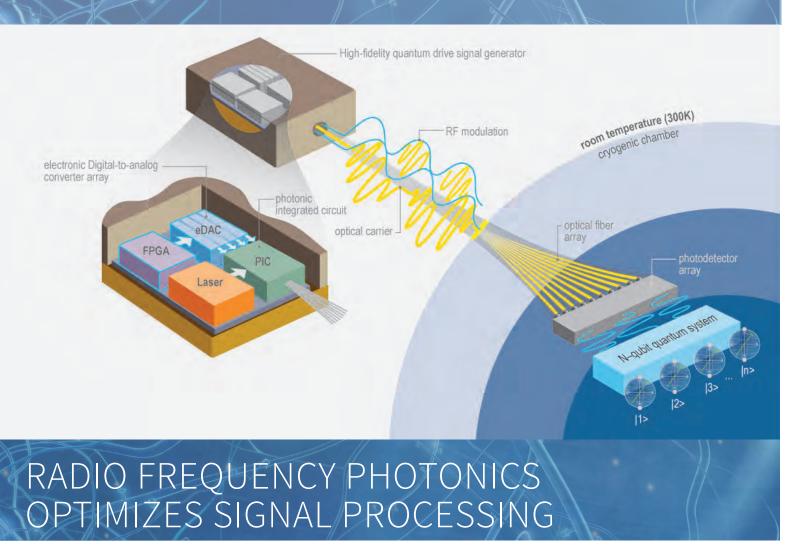
The Feedstock Optimization project brings together an interdisciplinary team from materials science, computer science, and data science, to advance technologies in material development and discovery.



Impact:

The LLNL team is making impacts in both materials science and computer science. So far, their research has advanced ML in materials science by extracting information from publications about materials processes and structure, saved time and money by reducing the need for fabrication and testing, and reduced the error rate of material property prediction. The team has also applied their ML tools to extract information from SARS-CoV-2 and COVID-19 literature, which is now being analyzed for its utility in accelerating COVID-19 research.





Low noise, high dynamic range high frequency signal processing

Challenge:

1101

Generating and detecting microwave signals with low noise and high fidelity is crucial in communication systems, radars, signal processing, radio astronomy, satellites, GPS navigation, spectroscopy, and in time and frequency metrology. Noise and interference are the most important factors limiting the performance of existing signal processing systems. Systems that implement electronics-based analogue-to-digital converters (ADCs) suffer from multiple noise sources, such as thermal noise and sampling jitter, the latter being particularly important for applications with high signal bandwidth since effective noise scales linearly with signal. For this reason, ADC performance typically drops with high bandwidth, driving up cost dramatically. For example, a typical mid-tier ADC chip can measure 2 GHz electronic signals with 1450 levels of resolution and costs \$150, while a 20 GHz commercial oscilloscope provides only ~81 resolvable levels at over a thousand times the cost.

To mitigate these issues, analog optical links offer a promising technology for applications such as radio frequency (RF)over-fiber, antenna remoting, and photonic-assisted ADCs featuring reduced noise characteristics and resilience to electromagnetic interference. However, one of the primary limitations of intensity-modulated analog optical link technology is high noise stemming from successive electronic-to-optical and optical-to-electronic conversions.

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Many electro-optic modulation techniques exist that strive for high modulation efficiency by increasing modulation depth of the modulated RF signal, resulting in higher signal-to-noise ratio. However, fundamental limitations exist for all such technologies, resulting in tradeoffs in RF bandwidth, optical power handling, and/or insertion loss.

Solution:

LLNL researchers in the National Ignition Facility Directorate's DoD Technologies RF Photonics Group have explored phase modulation solutions to this signal processing challenge. Optical frequency combs offer phase noise characteristics that are orders of magnitude lower than are available from commercial microwave references. The researchers recognized that by converting the intensity information into phase, the magnitude of the converted information is no longer limited to 100% modulation depth, but instead can span multiple 2π radians without clipping. In a suite of five new patent applications, the researchers proposed several novel innovations including an optical encoder device they refer to as a helix encoder because the mapping of intensity to phase can be viewed as encoding the pump intensity information into a helix, with the third dimension represented by the total number of 2π radian windings. This technology innovation enables digitization of high-power electronic signals via unlimited optical phase wrapping that uses noise cancellation and calibration algorithms to achieve an extremely large dynamic range

Collaboration:

Several aerospace and defense contractors are seeking high dynamic range, low noise, ADC and digital-to-analog converter technology solutions using photonics. Potential partners have been in talks with the RF Photonics group throughout the year, and some have evolved into new CRADA collaborations to commercialize the Lab's revolutionary new RF photonics technologies and secure the future licensing opportunities they offer.

High dynamic range direct-to-millimeter wave photonics offers low noise and high linearity for quantum computing applications.

Impact:

LLNL's RF photonics technologies enable lower noise and higher dynamic range, high-frequency signal processing that is not possible with conventional all electronic or even analog optical techniques. Applications span a variety of areas including millimeter wave signal processing, quantum computing, and 5G communications networks.







Creating a 3D printed object in a single step

Challenge:

Conventional AM prints parts layer-by-layer, each layer taking about one minute. This time-consuming approach is not suitable for high-volume manufacturing involving a hundred or more parts. In addition, the traditional approach often results in undesirable roughness and unsupported structures or disconnected islands of material that will connect to another layer by an overhang or a span that cannot be formed layer by layer.

Solution:

LLNL scientist Maxim Shusteff is leading a team that is exploring a new approach in AM that uses a holographic image that is broken down into three projections, allowing researchers to create objects in 3D all at once. Each projection represents a different orthogonal view of the desired object. A diode laser generates a primary beam that passes through an array of optical components and is patterned into the three projections spaced apart from each other inside the beam. Together they form a single 3D image. The projected image overlaps two prism mirrors and a glass chamber, which contains a photopolymer resin and photoinitiator. Two of the three composite image segments are directed by the mirrors into the chamber at right angles while the third projection shines head-on into the chamber. As these beams perpendicularly intersect in the chamber, the free-floating 3D structure forms in the resin as its photopolymer absorbs the light energy.

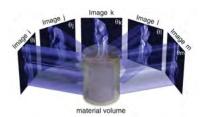
A second solution the researchers are studying is computed axial lithography (CAL). The CAL method is similar to computed tomography but uses visible light instead of x rays. The CAL system generates a video portraying the complete rotation of projections of the 3D object. Instead of using three images, the system uses a sequence of 1,440 images, or 4 per degree of rotation. These video images travel through a lens and into a resin chamber whose rotation rate is synchronized with the video frame rate. Each image is a different 2D pattern of light and enters the resin from a different angle. By summing the images, the system creates a distributed 3D energy dose inside the resin. With multiple rotations, the dose becomes sufficient to cure desired regions while leaving undesired regions in liquid form. The structures cure upon completing up to three full rotations.

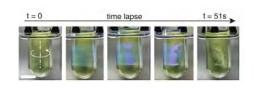
Collaboration:

LLNL is collaborating with three partners, a Pennsylvania dental supply company, a California startup specializing in advanced materials for AM, and a Texas bioprinting company. These projects are developing not only the 3D-printing machines, but also the materials necessary to 3D-print the project-specific component.

"We may not always be able to fabricate a part by spinning it around in CAL or not always have access to all sides to use holographic lithography. However, the chances are we can make any structure using one technique or the other or some combination of both."

Maxim Shusteff,
 LLNL Microtechnology Engineer



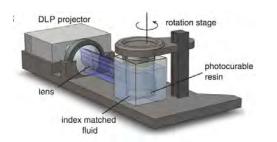




A miniature representation of Auguste Rodin's "Thinking Man" volumetrically printed using computed axial lithography

Impact:

Since volumetric manufacturing is faster, cheaper, and offers more geometric versatility than other polymer-based methods, researchers believe that this approach will open a significant new direction for AM.







Driving targeted development to advance national security

Challenge:

"In order for the United States to maintain its global economic edge, Federal investment must be made in research and development efforts focused on industries of the future, such as artificial intelligence, quantum information science, biotechnology, and next generation wireless networks and infrastructure, advanced manufacturing, and synthetic biology," reads a section of the Industries of the Future bill introduced by Senator Roger Wicker in January 2020. As an industry of the future, quantum information science aims to uphold US national security and economic competitiveness. In this rapidly developing interdisciplinary field, academia, industry, and government organizations must partner in innovative research and development to provide transformative solutions to modern challenges in science, national security, and industrial competitiveness.

Solution:

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LLNL's multidisciplinary research teams are exploring novel solutions in a variety of quantum science and technology areas, including:

- Synthesizing and tuning materials with special quantum properties;
- Designing and fabricating modular devices and systems to enable future scalability of quantum platforms;

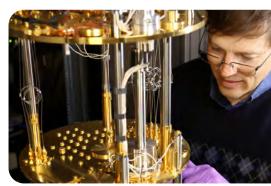
- Leveraging our expertise in photon science to develop and optimize the quantum—classical interface;
- Developing algorithms and advanced control techniques for quantum systems;
- Designing and evaluating full-stack, prototype quantum computing systems;
- Exploiting quantum phenomena to develop new sensing and imaging capabilities.

Collaboration:

LLNL is collaborating in many quantum science activities. Two notable partnership areas are:

Quantum Design and Integration Testbed (QDIT): With support from DOE and NNSA, LLNL is fostering a unique research environment with a "co-design" approach—a collaborative development environment where users' needs inform the system design process. LLNL's QDIT focuses on collaborative co-design involving quantum system developers and quantum application scientists. A multidisciplinary team is developing novel algorithms for various applications. Current partners include UC Berkeley and UC Merced.

Quantum Sensing: LLNL is working with the private sector to develop and field-test advances in quantum sensing that offer the speed and sensitivity needed for national security and defense applications. For nearly a decade, LLNL has collaborated with U.S.-based AOSense, Inc., to develop sensors and algorithms for detecting the gravity signature of nuclear material—a useful sensing technology for screening vehicles at border crossings and other sensitive areas. LLNL and AOSense are also investigating the use of atom-interferometer gyroscopes for internal navigation—devices that enable "dead reckoning" navigation, providing high-precision navigation in areas where GPS navigation is not viable. Additionally, LLNL is working with Vector Atomic to develop mobile quantum sensors for inertial navigation that incorporate LLNL-developed micromirror array technology. Vector Atomic is leveraging LLNL's Advanced Manufacturing Laboratory to adapt the laser-based technology for use in a demanding mobile environment.



Inside a test bed's dilution refrigerator. Gold-plated cans contain qubits, which are connected by wires to the rest of the assembly. Recirculating helium progressively cools the structure from top to bottom, with each circular plate introducing a colder phase. (Photo by Carrie Martin.)

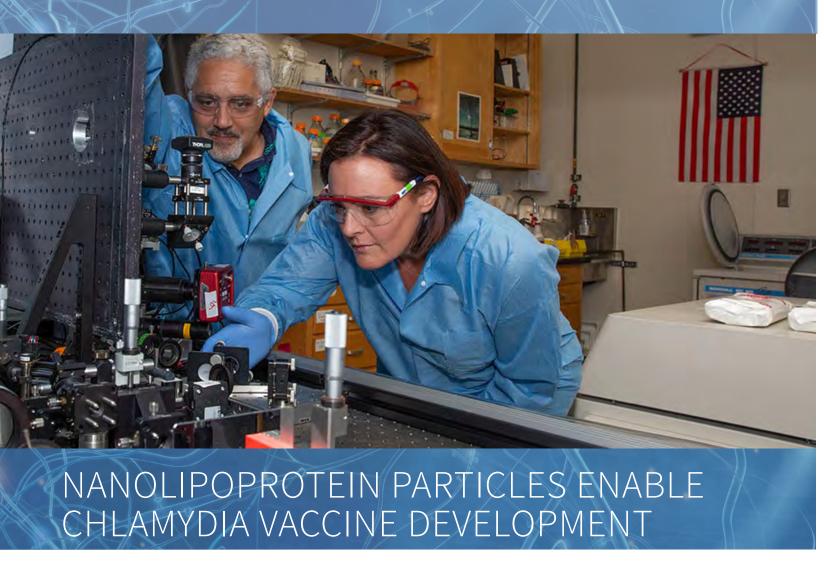
Impact:

Quantum information science promises future innovations for national security, computing, communications, and Al. These innovations could transform long-established industries such as manufacturing, biotechnology, transportation, and financial services. LLNL's partnerships in developing new quantum sensing capabilities, such as cold-atom gravity gradiometry and inertial motion sensors, will support LLNL's efforts to address mission-relevant challenges ranging from improved threat detection to GPS-free advanced navigation. Our materials development efforts yield materials that meet the rigorous requirements for effective quantum systems, while our quantum computing partnerships bring us closer to demonstrating a fully programmable quantum system with powerful simulation capabilities. These partnerships grow our abilities to address some of the most complex national security problems.









A novel platform for the targeted delivery of a chlamydia vaccine

Challenge:

Chlamydia trachomatis (Ct) is the most common sexually transmitted bacterial pathogen in the world. The U.S. Centers for Disease Control and Prevention estimates that at least 1.7 million U.S. cases of chlamydia were diagnosed in 2017, 45 percent of which were in women from the age of 15 to 24 years. Most infections are asymptomatic, but left untreated can lead to pelvic inflammatory disease, infertility, and ovarian cancer. There is no vaccine against chlamydia despite several decades of intensive research. Previous studies have shown that immunization with a highly expressed membrane protein of this pathogen can provide significant protection against infection if its native structure is preserved. However, formulating and delivering this type of vaccine remains a major hurdle.

Solution:

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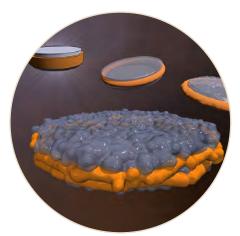
For the past decade, LLNL researchers have been developing and refining a platform for drug and vaccine delivery that has led to the creation of a strategic portfolio of intellectual property. The patented platform is based on tiny, disk-shaped structures called nanolipoprotein (NLP) particles. These closely resemble a type of cholesterol that moves fats through the bloodstream. To study the effects of these NLP vaccines, researchers carried out tests on experimental animals. The results indicated that when antigens and adjuvants are attached to NLPs through a relatively simple process, the resulting vaccine elicits a stronger and more targeted immune response than when the components are administered separately. The size of NLPs (8–25 nanometers in diameter) is ideal for leveraging natural pathways for entry into cells, particularly immune cells relevant to vaccine delivery.

In 2019, the National Institutes of Health established, through its National Institute of Allergy and Infectious Diseases, five-year funding for the Cooperative Research Center for NanoScaffold-based Ct Vaccines. Center researchers will leverage NLPs to explore solutions for both the development and the delivery of an effective Ct vaccine. First, they will identify the most promising antigen formula to protect against the pathogen and explore how to administer it via an NLP delivery platform that preserves the molecule's structure as it is delivered. Then, they will test the vaccine to move the work toward clinical trials.

Collaboration:

The Center, which is led by Matthew Coleman at LLNL and Luis de la Maza at UC Irvine, will leverage expertise from three institutions:

- UC Irvine researchers, including a leading expert in Ct biology, will develop models that mimic the response of Ct human infections.
- Using these models, LLNL scientists who developed the nanotechnology platform will refine NLP formulations for use in Ct vaccine development and delivery.
- UC Davis health researchers will test and establish the safety and efficacy of the vaccine formulations.



NLP particles can be used to create vaccines by attaching vaccine elements such as antigens, molecules that are bound by antibodies, and adjuvants, molecules used in vaccine development to enhance the immune response.

Impact:

The Center will leverage a multidisciplinary team of experts in immunology and nanotechnology for developing and testing a new type of vaccine to prevent sexually transmitted infections caused by the Ct pathogen, providing a viable pathway to address this widespread public health threat. The collaboration is expected to further advance the nanotechnology delivery platform and will form the basis for future efforts to deliver drugs and vaccines to fight other infectious diseases.



Researchers who will participate in the Cooperative Research Center for NanoScaffoldbased Ct Vaccines include: (left to right) Sean Gilmore, Sandra Peters, Amy Rasley, Dawn Whalen, Brent Segelke, Wei He, Patrik D'haeseleer, Matt Coleman and Nick Fischer. (Not pictured: Alex Noy, Joe McKeown, Dina Weilhammer, and Megan Shelby.)







Partnerships Boost Economic Development

Public-private
partnerships help drive
additive manufacturing,
computing, and health
industries to develop
new hardware and
software with capabilities that benefit
NNSA, DOE, and other
government agencies.

Strategic partnerships combine LLNL's expertise in areas such as additive manufacturing (AM), high performance computing (HPC), simulation, and pathogen detection, with expertise from industry and research institutions to overcome technology gaps. For example:

- LLNL and TTEC are developing a new cold spray technique to coat a wide variety of substrates, such as metals, ceramics, glasses, and organic foam materials while maintaining the materials' functional properties;
- The National Ignition Facility and Optimax Systems, Inc. are using Labdeveloped AM processes to produce high-energy laser lightweight and deformable mirrors for directed energy systems;
- LLNL's Space Science & Security Program and Tyvak Nano-Satellite Systems, Inc. are using LLNL's monolithic telescope (MonoTele) technology to build compact, robust telescopes for nanosatellites;
- Laboratory researchers are partnering with collaborators to develop a viral sensing diagnostic platform that can be tuned to identify a specific pathogen based on isothermal amplification of the genetic sequence;
- DOE and NCI are bringing together scientists from LLNL, LANL, the National Cancer Institute's Frederick National Laboratory for Cancer Research, ORNL, San Jose State University, and IBM Corporation to develop a first-of-its-kind multiscale simulation framework to predictively model the dynamics of RAS proteins and their interactions with lipids;
- LLNL's continuing collaboration with other DOE national labs in the HPC4
 Energy Innovation is applying HPC to challenges associated with manufacturing, materials in energy technologies, and mobility technologies and systems.







LLNL researchers have previously demonstrated 3D printing as a viable route to produce glass optical components with both novel structures and compositions. By combining with Projection Microstereolithograhy 3D printing techniques, low density "green bodies" are first printed in desired shapes from specially formulated silica-containing pastes or resins. Then, using conventional heat treatment techniques, the green bodies are converted to full density, structural glass, forming geometries ranging from monoliths to open lattices. For this collaboration the material and optical properties of LLNL's printable silica-titania formulations rival conventionally prepared optical grade ultralow expansion glass.

Exploring Additive Manufacturing of Lightweight Reflective Optics

LLNL's National Ignition Facility and New York-based Optimax Systems, Inc. have formed a new optical technology development collaboration. Optimax is a highprecision, custom optics manufacturing company serving semiconductor, aerospace, defense, medical, and imaging markets. The company has been engaged in government-sponsored research for several years. Most recently, Optimax won a Missile Defense Agency (MDA) Phase II STTR entitled: Additive manufacturing and thin film coating development for lightweight-directed energy reflective optics. The directed energy (DE) community has identified high-energy laser lightweight and deformable mirrors and low stress mirror coatings as key component-level technology gaps for existing and future DE systems.

Optimax became interested in partnering with LLNL after learning about the Laboratory's advances in 3D printed direct-ink-write glass optics and projection micro-stereolithography, research primarily funded by the Laboratory Directed Research and Development Program. Optimax saw the advantage in using Labdeveloped AM processes to achieve architected structures with higher stiffness-toweight ratios when compared to those attainable by conventional lightweighting via selective material removal. By combining LLNL's AM of lightweighted mirror substrates along with Optimax's low-stress, low-loss, high laser damage threshold coatings, the company could realize large format, lightweight, high-performance mirrors for directing laser energy over long ranges for targeted results.

The partnership's goal is to extend LLNL's technology into a commercial capability for producing large, lightweight mirrors to the same high-performance standards demanded by the DE community. MDA's sponsorship of the project has enabled Optimax to continue movement towards its commercialization goal of being the premier service provider of custom optics and coatings for the DE market.

Collaboration Develops Innovative Telescopes for Nanosatellites

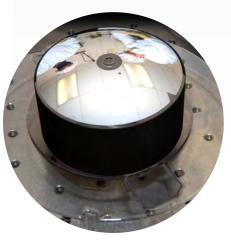
A new CRADA collaboration between LLNL's Space Science and Security Program (SSSP) and Irvine, California-based Tyvak Nano-Satellite Systems, Inc. is developing compact, robust telescopes for nanosatellites. Tyvak Nano-Satellite Systems is an industry leader that delivers optimized, end-to-end satellite solutions. The four-year, \$6 million CRADA combines LLNL's Monolithic Telescope (MonoTele) technology with Tyvak's high-reliability spacecraft.

Developed over an eight-year period, LLNL's MonoTele space telescopes range in size from one inch (called the mini-monolith) to 14 inches. The MonoTele technology provides imaging for nanosatellites that are about the size of a large shoebox and weigh less than 22 pounds, and microsatellites that are about the size of a dorm refrigerator and weigh up to several hundred pounds.

The MonoTele concept was inspired by the mirror design used for the Large Synoptic Survey Telescope which is due to come online in Chile in 2023 and is expected to image some 20 billion galaxies. The MonoTele consists of a space telescope fabricated from a single, monolithic-fused silica slab, allowing the optic lens to operate within tight tolerances. This approach does not require on-orbit alignment, greatly simplifying spacecraft design and favorably affecting spacecraft size, weight, and power needs.

Under this CRADA, LLNL and Tyvak expect to develop additional MonoTele-type telescopes capable of operating in other wavelength bands, such as ultraviolet and short-wave infrared, and as a spectrometer instrument. The telescopes will be demonstrated in space and will feature compact, low-power focus mechanisms for missions requiring agile optics technology. The MonoTele nanosatellite imaging payloads will serve Earth observation, space situational awareness, and satellite navigation initiatives. Tyvak will provide the spacecraft and integrate the MonoTele into their payloads configured to ensure survivability in a demanding launch and on-orbit environments.





The four-year, \$6 million CRADA will combine LLNL's Monolithic Telescope technology with Tyvak's expertise producing high-reliability spacecraft.

SPOTLIGHT

A space telescope, dubbed the V4 and an identical twin to this one, flew on LLNL's GEOstare1 mission, where it was employed to demonstrate the utility of nanosatellites for space situational awareness.

> From left: LLNL optical engineer Brian Bauman, mechanical designer Darrell Carter and Alex Pertica, the acting program leader for the Lab's Space Science and Security Program, look over several small space telescopes, three of which have already flown in space.



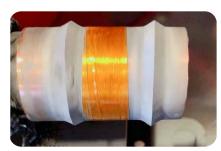




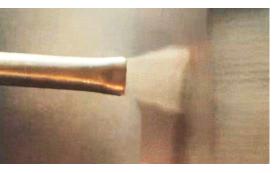
TTEC



This versatile cold spray control unit allows precise control of gas temperature and pressure, as well as additional in-line diagnostics during the spray process.



Supersonic particles of bismuth telluride are sprayed from the nozzle to deposit on a glass substrate.



Cold Spray of Brittle Materials Opens the Door for Low-Cost Functional Coatings

Versatile cold spray (VCS), developed through a partnership between LLNL and industry partner TTEC, is a new cold spray technique that deposits a broad range of brittle and glassy materials onto any substrate. The innovative VCS nozzle design and powder particle size distribution enables the deposition of the brittle materials, driven by an embedding and interlocking process that achieves near-theoretical density while maintaining both mechanical and functional properties. Unlike many AM techniques, particularly existing spray technologies, VCS can coat a wide variety of substrates, such as metals, ceramics, glasses, and medium density organic foam materials.

"Cold" refers to the temperature of the gas, which is typically less than 500°C, below the material's melting point. Conventional cold spray has been used successfully on steel, copper, chromium, and other ductile materials. However, with the exception of conventional cold spray's capability in adding corrosion resistant coatings, the technology can only repair or patch materials rather than add functionality. When applied using conventional cold spray, the particles in brittle, functional materials tend to shatter on impact rather than build a high-density deposit.

Unlike with most competitive AM techniques, materials applied with VCS maintain their functional properties. This capability, combined with VCS's portable design opens the door to creating thermoelectric generators and other functional components such as magnets and insulators on industrial components with complicated form factors.

In addition, sequential deposition of different materials will allow the complete AM of complex devices composed of combinations of metallic, semiconductor, magnetic, and thermal and electrical isolation materials. VCS can also uniformly coat complex shapes such as the inside or outside of pipes. This feature, combined with VCS's portability, enables the technology to apply coatings on equipment already installed in industrial facilities, transforming fixed pieces of existing equipment into functional devices, depending on the coating selected.

Strips of p- and n-type thermoelectrics (grey ridges) deposited on the outside of a copper pipe, forming a basic thermoelectric generator to harvest waste heat radiated from the pipe's contents.

Technology Commercialization Funds Projects to Mature Laboratory Innovations

In June, the DOE's Office of Technology Transitions (OTT) awarded nearly \$1.4 million in support of five LLNL projects. The funds are part of OTT's Technology Commercialization Fund (TCF) which helps mature laboratory projects for commercial potential. With matching investments from the Lab or a commercial partner, these efforts advance the commercialization of promising cutting-edge technologies and strengthen partnerships between DOE's national laboratories and private sector companies to deploy these technologies to the marketplace. Since 2016, twenty-one LLNL research teams have participated in the program.

The TCF was created by the Energy Policy Act of 2005 to promote promising energy technologies by supporting not just entrepreneurs, but all private sector efforts to engage with the DOE national laboratory complex. DOE received more than 220 applications for 2020 TCF funding, with project teams engaging more than 130 different partners across multiple diverse disciplines.

Below is a list of LLNL's 2020 TCF projects and their partners:

Advanced Magnetic Radiation Shielding for Nuclear Energy Application

- American Ceramic Technology, Escondido, California
- Ames Laboratory, Ames, Iowa

Materials Design Simulator: A Practical Tool for Advanced Alloys Development

• MolyWorks, Cloverdale, California

System Integration of Rationally Designed Dilute Alloy Catalysts for Energy-Efficient Electrochemical CO₂-to-Fuel Conversion

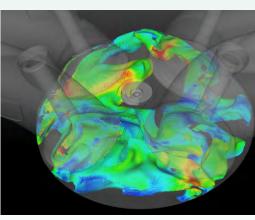
- Opus-12, Berkeley, California
- TOTAL American Services, Inc., Hopkinton, Mass

Zero-order Reaction Kinetics: Enabling the Use of Detailed Chemical Kinetics in Combustion Simulations

- Convergent Science, Madison, WI.
- Gamma Technologies, LLC, Westmont, II

Micro-liter Fuel Ignition Tester for Accelerated Discovery of Advanced Combustion Fuel

Partner TBD



LLNL's R&D 100 award winning Zero-RK software package drastically reduces the time it takes to simulate chemically reacting systems by as much as three orders of magnitude compared to state-of-the-art commercially available solvers.

\$240,000

\$250,000

\$250.000

\$545,000

\$100.000





TECHNOLOGY IMPACTS



The method uses a sample from a nasal or oral swab. The heater for the single-tube method is built by Symbient Product Development.

Single-Tube Isothermal Amplification Diagnostics

LLNL scientists invented a viral sensing diagnostic platform based on isothermal amplification of the genetic sequence. The highly sensitive diagnostic tool can be tuned to identify a specific pathogen. As a proof of concept, the team demonstrated the patented technology's ability to detect *E. coli*, methicillin resistant *Staphylococcus aureus* (MRSA), and the virus that causes foot-and-mouth disease in cattle.

Through internal funding, the team is adapting the platform to enable identification of the genomic sequence of the SARS-CoV-2 RNA virus. Because the pathogen inactivation step would also destroy the enzyme used to amplify the RNA virus, the sample is transferred to a second tube containing a reagent to amplify the genetic material of the pathogen. The team has also built a prototype heater for this process.

A California company is in active discussion to license the technology for the detection of the H1N1 influenza virus strain responsible for flu pandemics such as in 1918 and 2009. The company is also in active discussion for commercializing the technology for the diagnosis of COVID-19 under a non-exclusive license that LLNL has made available under a special provision to support rapid dissemination and commercialization of technologies that are relevant for combating the COVID-19 pandemic.



[24]











Scientists are adapting the single-tube technology to test for RNA viruses such as CoV-2. In this process, an oral sample swab is inserted into a tube that is heated to inactivate the pathogen. The sample is then transferred to a second tube containing a reagent to amplify the genetic material of the pathogen. The tube is heated again, and a preloaded colorimetric dye displays a visible color change for positive results.

Modeling Protein Interactions to Improve Outcomes for RAS-related Cancers

Cancer is the second leading cause of death in the United States, killing nearly 600,000 people each year. Nearly a third of all cancers are driven by constitutively active (oncogenic) mutations in RAS proteins that account for a high percentage of pancreatic (~95%), colorectal (~45%), and lung (~35%) cancers. RAS proteins localize to the plasma membrane where they can propagate growth signaling, leading to cancer. The specific localization of RAS to different regions of the plasma membrane may be important for the activation of signaling. Despite tremendous progress in RAS biology over the past three decades, no therapies are currently available.

Analyzing RAS proteins on the molecular level

A team of LLNL scientists and their collaborators developed a first-of-its-kind multiscale simulation framework to predictively model the dynamics of RAS proteins and their interactions with lipids, the organic compounds that help make up plasma membranes. The framework, known as the Multiscale Machine-Learned Modeling Infrastructure (MuMMI), was first presented at the International Conference for High Performance Computing, Networking, Storage and Analysis (SC19), where it won the conference's Best Paper award. MuMMI uses machine learning to identify areas of interest to "zoom in" to and analyze on a molecular level, a novel approach developed to study the dynamics of protein—lipid interactions. MuMMi is capable of simulating the interactions between RAS proteins and different types of lipids to investigate RAS dynamics on a macroscale and on a molecular level.

The macro-to-micromodel simulations allow researchers to see how RAS proteins interact on a cell membrane at biologically relevant time and length scales, generating data that can be tested experimentally at Frederick National Laboratory for Cancer Research (FNLCR) to ensure the models are representative of actual biological results. The models will help FNLCR and the National Cancer Institute (NCI) carry out experiments, test predictions, and generate more data that will feed back into the model, creating a validation loop to improve the accuracy of models.

MuMMI was developed as part of the Molecular Level Pilot project in the Joint Design of Advanced Computing for Cancer program, a collaboration between the DOE and NCI. The multidisciplinary team comprises more than 40 computational scientists, biophysicists, biologists, chemists, and statisticians from LLNL, LANL, NCI/FNLCR, ORNL, San Jose State University, and IBM Corporation.

A multidisciplinary team from LLNL, LANL, NCI, and other institutions is using machine learning as a virtual magnifying glass to study regions of RAS protein/lipid simulations in high detail.



University of Tennessee professor Jack Dongarra (left) and SC19 Papers Chairs Michelle Mills Strout and Scott Pakin (far right) presented LLNL computer scientists (l-r) Francesco Di Natale, Harsh Bhatia and Peer-Timo Bremer with the Best Paper award. Co-authors included more than a dozen LLNL scientists as well as researchers from the National Cancer Institute/Frederick National Laboratory for Cancer Research, LANL, ORNL, and IBM.







The HPC4Mfg program pays laboratories up to \$300K for industry access to HPC resources and expertise while industry pays at least 20% of project costs.

From September 2019 through June 2020, DOE has awarded \$4.7M for 16 new HPC4Mfg projects. LLNL has expanded its involvement with the HPC4Mfg program in FY20 through partnerships with:

- Owens Corning and St. Gobain Reducing glass furnace spectral
- OxEon Energy Optimizing synthetic
- Flawless Photonic Reducing loss in fiber optic transmissions
- Guardian Glass Applying machine learning tools to glass furnace
- Arcelor Mittal Designing new high strength steel alloys

HPC4 Energy Innovation

The HPC4EI program consists of three programs, HPC4Manufacturing, HPC-4Mobility, and HPC4Materials, which leverage the world-class computational resources at the national laboratories that connect with industry to advance the national energy agenda. Companies submit concept papers and if accepted, a laboratory scientist is assigned to help the company develop a full proposal. Winning proposals are selected by how well the technology advances the state of the art, the technical feasibility of the team, the project's impact on industry, and its need for HPC systems.

HPC4Mfg Program

The goal of the HPC4Mfg program is to enhance the adoption and advancement of HPC by addressing manufacturing challenges such as optimizing production processes, enhancing product quality, and speeding up design and testing cycles while decreasing energy consumption.

LLNL leads the program and is joined by LBNL, and ORNL. Six additional national laboratories participate in the program as executers of selected projects. HPC4Mfg offers a low-risk path for U.S. manufacturing companies interested in adopting HPC technology to advance clean energy technologies and increase energy efficiency while reducing the risk of HPC adoption. DOE labs involved in the HPC4Mfg program include LLNL, LBNL, and ORNL.

HPC4Mobility Program

In FY19, DOE announced an opportunity to fund up to \$1M in projects to create new knowledge tools, insight, and technology solutions that increase mobility energy productivity for individuals and businesses through the new HPC4Mobility program. The HPC4Mobility program brings together industry partners and DOE laboratory scientists to work on short-term, collaborative projects focused on applying HPC to challenges associated with mobility technologies and systems.

ORNL leads the program and is joined by LLNL, NREL, PNNL, LBNL, and ANL. The HPC4Mobility program offers a low-risk path for U.S. companies and local municipalities interested in adopting the application of HPC, modeling, simulation, and data analysis to address key challenges in developing, modifying, and/or qualifying new or modified software, hardware, and implementation solutions that perform well in complex mobility systems. The first two projects in this portfolio were awarded in fall 2019.

HPC4Mtls Program

In FY20, DOE announced an opportunity to fund up to \$2M in projects related to improving materials exposed to severe or complex environments through the new HPC4Mtls program. The HPC4Mtls program brings together industry partners and DOE laboratory scientists to work on short-term, collaborative projects and focuses on applying HPC to challenges associated with materials in energy technologies.

LLNL leads the program and is joined by ORNL, National Energy Technology Laboratory, LANL, and PNNL. HPC4Mtls offers a low-risk path for U.S. manufacturing companies interested in adopting the application of HPC, modeling, simulation, and data analysis to address key challenges in developing, modifying, and/or qualifying new or modified materials.

LLNL partners with PPG Industries to increase the understanding of corrosion inhibitors in automobile coatings.

LLNL/NASA Agreement Leads to Joint Satellite Mission

A multi-year collaboration between LLNL's Space Science and Security Program (SSSP) and Maryland-based NASA Goddard Space Flight Center (GSFC) culminated in a December 5, 2019 launch into orbit of a joint climate science mission comprising a Livermore small satellite bus and a NASA GSFC laser heterodyne radiometer (LHR) for sensing greenhouse gas concentrations in the atmosphere.

SSSP, with sponsorship from the National Reconnaissance Office, created the CubeSat Next Generation Bus (CNGB) architecture. The joint mission with NASA was primarily funded by the Laboratory Directed Research and Development Program.

With the Space Act Agreement in place, NASA installed the LHR into Livermore's CNGB to complete the integrated 6U satellite called "MiniCarb." By collecting sunlight passing through slices of Earth's upper troposphere and lower stratosphere, LHR was designed to detect the amount of sunlight absorbed by methane and carbon dioxide. Researchers would then use absorption spectra to measure the concentrations of these greenhouse gases. The bus design features flexibility; transparency; and mechanical, electrical, and software standardization. Although initially defined for a 3U CubeSat comprising three 10 cm x 10 cm modules, CNGB is scalable to larger configurations.



From September 2019 through June 2020, DOE awarded \$1.5M for five new HPC4Mtls projects to improve U.S. energy technologies through HPC.













The Laboratory invests in its capabilities and people through a variety of programs. Some join scientists and engineers (S&Es) with mentors from industry to develop a business concept around a market need

- programs. The latest spring 2020 cohort utilized three LLNL technologies, and

Investments often also result in awards. Some of the awards received in

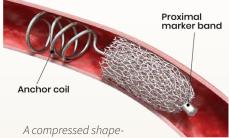
LLNL events and collaborative environments spur innovation and creative

- facturing, and the October summit on quantum information science and technology;
- The Livermore Valley Open Campus (LVOC), and the Advanced Manufacturing Laboratory (AML); and
- The High Performance Computing Innovation Center (HPCIC).



LLNL has won:

37 national FLC awards to date



A compressed shapememory-polymer foam is delivered by catheter to an aneurysm sac within the brain. Once it is activated by temperature change, the foam expands to match the sac's contours.

FLC Technology Transfer Awards

National Award for IMPEDE Embolization Plug

After winning a 2019 Far West Regional Federal Laboratory Consortium (FLC) award for Outstanding Commercialization Success and a 2019 R&D 100 award, the IMPEDE Embolization Plug was nominated and won a 2020 National FLC award for Excellence in Technology Transfer.

The development of the IMPEDE Embolization Plug started at LLNL. When the inventor moved to a new institution, his grant funding went with him, and it led to a first-of-its kind inter-institutional agreement (IIA) and new way to successfully transfer the technology. The IIA provided the new institution access to a significant portfolio of background intellectual property (IP) for the polymer material, and it provided LLNL access to future IP.

Without the complete lab-to-market efforts of the nominated team, a life-saving medical product may not have reached the marketplace. Blood flow through diseased or damaged vessels puts patients at increased risk of stroke, severe pain, uncontrolled bleeding, and even death. The IMPEDE Embolization Plug, incorporating an LLNL-developed polyurethane shaped memory polymer, operates as a physical barrier to obstruct or reduce the rate of blood flow in peripheral blood vessels. The device's surface area increases as much as 1,000 times greater than other embolizing technologies, which initiates clotting more effectively in the target blood vessel.

IMPEDE provides easy delivery and minimal risk of device migration. Preclinical studies indicate that the high surface area provided by IMPEDE leads to improved long-term healing compared to other embolizing devices, decreasing risks associated with retreatment. More than 200 patients have been treated successfully with the device with no reported adverse effects. The IMPEDE Em-

bolization Plug received 501(k) clearance from the FDA in 2018. The IMPEDE-FX, which enables physicians to embolize in greater lengths, received FDA 501(k) clearance in 2019.

Charted in 1974, the FLC is a nationwide network that helps accelerate the transfer of technologies from federal laboratories into the marketplace. It comprises more than 300 federal laboratories, agencies, and research centers.

LLNL Nominates Four Technologies/Partnerships for Far West Regional FLC Awards

LLNL nominated four technologies/partnerships under three different categories for a Far West Regional FLC award in 2020.

Outstanding Technology Development

Versatile Cold Spray (VCS)

VCS, developed through a partnership between LLNL and industry partner Thermoelectric Technologies (TTEC), is a new cold spray technique that deposits a broad range of brittle and glassy materials onto any substrate. VCS opens the door to creating thermoelectric generators and other functional components such as magnets and insulators on industrial components with complicated form factors.

In-air Drop Encapsulation Apparatus (IDEA)

IDEA creates microcapsules of consistent size and composition at a rate 100 times faster than current microfluidic-based, monodisperse capsule production techniques and up to 1,000 times faster when incorporated with a multi-nozzle design. By overcoming past production shortcomings, IDEA opens the market to many more microcapsule applications for greater global impact, whether delivering life-saving drugs or enabling carbon dioxide capture and reuse to combat greenhouse gas emissions. A partnership with a Silicon Valley-based biotech startup company, Artveoli, will deliver on IDEA's promise by incorporating IDEA microcapsules for carbon capture to improve indoor air quality.

LLNL has won:

36 regional FLC awards to date









Outstanding Commercialization Argon license of RaFTS

LLNL and Argon Electronics Limited (UK) executed a license for LLNL's innovative technology, Radiation Field Training Simulator (RaFTS). The partners also formed a CRADA to facilitate the development of an ultra-realistic radiation simulator tool for first responders. RaFTS provides a first responder training solution that can be used to protect against acts of radiological or nuclear terrorism and respond to their subsequent aftermath.

Researchers from LLNL and Argon Electronics Ltd. conduct a test with the Radiation Training Field Simulator (RaFTS). From left: Dave Trombino, Erik Swanberg, and Josh Oakgrove, from LLNL; Phil Dunn of Argon, Greg White of LLNL, and Steven Pike of Argon.

Outstanding Partnership LLNL and BioMedInnovations

LLNL and medical device startup company BioMedInnovations (BMI) have reached an agreement to develop a commercialized ventilator that can be easily built from readily available parts. Branded as SuppleVent™, the ventilator is designed to meet the functional requirements of COVID-19 patients suffering from Acute Respiratory Distress Syndrome and other serious breathing difficulties.



BioMedInnovations lead engineer Gokhan Yildiz works with LLNL to develop the first SuppleVent™ ventilator for COVID-19 patients.

1321

IMPEDE Embolization Plug (Analytical/Test)

R&D 100 Awards

IMPEDE is a medical device that reduces blood flow to blood vessels outside of the brain to decrease health risks. Researchers from LLNL, Santa Clara-based Shape Memory Medical Inc. and Texas A&M University developed the IMPEDE Embolization Plug. The device offers 100–1,000 times greater surface area than current technologies to more effectively initiate clotting in the target vessel and divert blood flow away from at-risk regions. To date, more than 100 patients have been successfully treated worldwide with IMPEDE with no reported adverse effects.

In FY19, LLNL researchers garnered four R&D 100 awards for inventions recog-

nized as some of the top 100 science and technology innovations worldwide

and one silver Special Recognition award for being a market disruptor.

Spack: A Package Manager for HPC Systems (Software/Services) and Silver Special Recognition for Market Disruptor

Spack is an easy-to-use, versatile, and scalable software package management tool for HPC scientific applications. It simplifies and accelerates building and customizing software by automating the build workflow, thus reducing deployment time for large software stacks from weeks to hours. Spack is widely available as open source software and has a large and active community of more than 400 contributors.

169 R&D 100 awards received by LLNL since 1978

4 R&D 100 technology innovations awards and 1 silver Special Recognition award received by LLNL innovators in FY19



Columbia University

École Polytechnique Fédérale de Lausanne

Fermi National Accelerator Laboratory

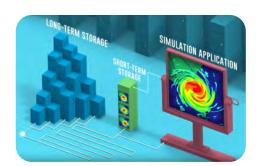
Iowa State University

Kitware, Inc.

National Energy Research Scientific Computing Center

Perimeter Institute; University of Hamburg University of Illinois at Urbana–Champaign University of Iowa





The Scalable Checkpoint/Restart Framework is a software package that allows HPC simulations to take advantage of hierarchical storage systems.



MC-15 is portable, weighs 47 pounds, and is faster than any other available neutron multiplicity detector. In addition, it requires little training to operate.

SCR Framework: Accelerating Resilience and I/O for **Supercomputing Applications (Software/Services)**

The LLNL team, with support from ANL, developed the Scalable Checkpoint/ Restart (SCR) Framework 2.0 software. Using SCR, the input/output performance of scientific simulations can be improved by hundreds of times, with the results produced in significantly less time than they could be using traditional methods. This is important because HPC applications simulate real-world phenomena that impact our daily lives.

Next Generation Multiplicity Detector (MC-15) (Analytical/Test)

MC-15 is an instrument that can quickly identify and assess nuclear-based threats. Scientists from LLNL and SNL assisted a team led by LANL researchers, who developed the next generation multiplicity detector (MC-15) instrument to help emergency response teams quickly identify and assess nuclear-based threats. MC-15 uses the technique of neutron multiplication to quantify special nuclear materials such as plutonium and uranium.

IPO on the "Spot"

The IPO received a Laboratory Spot award for exceptionally rapid development and execution of agreements in response to a U.S. Southern Command (USSOCOM) solicitation during the COVID-19 shelter in place order. USSOCOM sought to utilize Government Use Rights for the multi-stage bypass suppressor technology developed and patented by LLNL. To support this effort, IPO developed a solicitation-specific non-disclosure agreement (NDA), a Government Use Agreement (GUA), and a solicitation-specific ALE3D4I application form that provides the necessary access to LLNL computational resources. IPO staff members coordinated with Legal and Computing to develop these agreements and ensured they were aligned with LLNL requirements and the USSOCOM call. IPO worked with the 14 selected bidders to ensure the NDA and GUA were executed. Through a meticulously coordinated effort, IPO was able to review and execute this process for all 14 bidders in just four weeks.

Director's Award

LLNL's IPO received a Director's Office Silver award in recognition of the teamwork and extra effort associated with quickly and efficiently obtaining the necessary CRADA approvals for the development of an emergency stopgap ventilator that could be used for patients fighting COVID-19. Originally dubbed NERVe (Novel Emergency Response Ventilator} and later called SuppleVent, the device meets the requirements of a mechanical ventilator, but is portable and much less expensive than traditional medical ventilators. The FDA evaluated the prototype and authorized it for emergency use.

DOE's TTWG "Best in Class" **Awards**

DOE's Technology Transfer Working Group (TTWG) recognized IPO business development executive Genaro Mempin and LLNL scientists Patrick Dempsey and Chris Spadaccini with a Best in Class national technology transfer award for their considerable efforts in furthering economic development. The award, given for novel initiatives that spur economic development, was focused on LLNL's 14,000 square-foot, AML which is designed for shoulder-to-shoulder R&D in a laboratory setting. More than ten partnerships have been established since the AML was completed in 2018, and the waiting list continues to grow. Current participants are developing designs for automotive, aerospace, and optics applications or seek to improve existing additive manufacturing quality.

In this first-of-its-kind collaboration center, industry researchers partnering with LLNL experts are free to share ideas and develop manufacturing innovations across workstations and wet labs while maintaining proprietary research within partitioned areas. A viewing corridor enables visitors to observe R&D activities. The facility features manufacturing systems at industry scale plus research tools too expensive or specialized for most companies to have on hand. Partners have access to LLNL's HPC modeling and simulation capabilities to quickly optimize manufacturing processes and remain competitive.

The TTWG awards are selected by a team of representatives comprising technology transfer professionals from the national laboratories, single purpose research facilities and production facilities, and the DOE NNSA field offices. The awards were given for five categories: intellectual property management, licensing, partnering, economic development, and innovative lab facilities. The TTWG strives to improve the technology transfer activities of the laboratories/ facilities and the DOE by promoting DOE laboratory technology transfer policy in a mutually beneficial, supportive, and non-adversarial working environment that encourages open communication, teamwork, and professional development.

This year's award marks the second straight year that LLNL has won a TTWG Best in Class honor.

"Winning our second Best in Class award serves as recognition for the outstanding work done by Lab employees in their efforts to fulfill the Lab's technology transfer mission,"

-Richard A. Rankin, Director Innovation & Partnerships Office November 26, 2019

"Our talented and dedicated researchers apply themselves to solving some of today's most challenging problems. These awards serve as recognition that their innovative work has a deep impact on industry, our nation, and the world."

> -Bill Goldstein, LLNL Director Newsline, 2020













Open Resources Foster Collaboration

Laboratory Collaboration Zone

The LVOC was established in 2011 to serve as a meeting space for collaborative, unclassified research and development work between LLNL and Sandia-California researchers and colleagues in industry and academia. The LVOC Collaboration Zone launched with the HPCIC and continues to grow with multiple construction projects under way, expanding collaboration and partner-ship opportunities with the private sector.

The motivation for the Collaboration Zone stems from current and future national security challenges that require increased partnerships with the private sector in order to understand threats and deploy solutions in areas such as energy and environmental security, economic security, cyber security, HPC, and non-proliferation. Targeted academic alliances and industrial partnerships will help foster educational opportunities and future research collaborations.

Advanced Manufacturing Laboratory

On January 23, officials from NNSA and LLNL gathered with elected leaders and industry professionals to dedicate and tour the AML, a collaborative hub that spurs public—private partnerships. These partnerships "spin in" technological advancements that positively impact the Lab's national security mission while also supporting the commercialization efforts of private partners. The 14,000-square-foot facility is located in the LVOC.

The building serves as a tribute to LLNL's commitment to push the boundaries in advancing technology while engaging the community and the broader private sector. The AML's impact on the Lab's industry partners was apparent throughout the January event, as representatives from several companies spoke



LLNL's Manyalibo "Ibo" Matthews introduced a group of visitors and Lab employees to several research machines aimed at exploring new processes of metal additive machines.

to the advantages of having access to the Lab's expertise, equipment, novel materials, and unique manufacturing processes, many of which are not yet commercially available.

One of the many early Lab partnerships spawned from the AML is with General Electric, which has installed a large metal additive machine in the facility as part of an agreement with LLNL to accelerate metal 3D-printing processes for part production in aerospace and other applications. Vector Atomic, a Pleasanton, California-based start-up that is partnering with the Lab on quantum sensor approaches to ultra-precise global positioning, has been an "early beneficiary" of the AML, winning a large outside contract.

High Performance Computing Innovation Center

LLNL's HPCIC provides industry and academia with a platform to align projects with the Lab's mission and HPC capabilities. In turn these activities enhance the HPC skills of the Lab workforce. HPCIC fosters many collaborative events that help companies and universities increase their capabilities by utilizing HPC to accelerate innovation and competitiveness.

The RAND Corporation, the University of California, and the UK Science and Technologies Facilities Council are strategic partners that add value to the Lab's mission by broadening capabilities. In FY20, the first Advanced Strategic Computing/Renesselaer Polytechnic Institute HPC doctoral fellow graduated. Camille Bilodeau defended her award-winning thesis involving the use of molecular dynamics and machine learning for drug discovery following three years of on-site practicums and DOE Advanced Simulation and Computing Program. The HPCIC also provides institutional support for the DOE HPC4EI program by fostering ideas, proposals, and staff engagements at LLNL.

The HPCIC typically hosts 1,000 events and 10,000 visitors annually. Some of the events are: 3D printing workshops for teachers, "Passport Days" for Lab families, 24-hr "hackathons" for staff skills development, and "Meeting of the Minds" events for LLNL and SNL staff, students, and professionals.

A new LVOC facility for the HPCIC staff will be ready for occupancy in FY21. The modern building will have 100 staff offices that LLNL programs can use, and a separate conference hall for large meetings. The current HPCIC facility will remain available as a multi-use meeting facility.







HPCIC's first Renesselaer Polytechnic Institute fellow, Camille Bilodeau, completed her award-winning doctoral studies in combining simulations and deep learning methods to understand and predict molecular properties.





ENGAGING ENTREPRENEURS



In November 2019, 37 S&Es learned key entrepreneurial skills at the UC Davis Bishop Ranch campus.

Entrepreneurial Programs

When faced with a grand challenge, LLNL's best and brightest have come up with revolutionary ideas to solve problems in national security, health, energy, and other areas of our life. Entrepreneurs are creative, hardworking innovators who think outside the box to achieve big goals in business. LLNL's IPO sponsors and manages programs to enhance the entrepreneurial skills of the LLNL workforce to spur innovation and seed commercialization of LLNL intellectual assets.

National Labs Entrepreneurship Academy

Since 2015, LLNL's IPO has partnered with the UC Davis Graduate School of Management to host six academies teaching LLNL and Sandia-California scientists and engineers (S&Es) the fundamentals of entrepreneurial business. Each three-day course teaches S&Es communication skills for working with funding sponsors. The program focuses on the value of a technology to solve a problem that people care about, rather than focusing on the technology alone. For example, private investors want their capital to grow in the marketplace; government sponsors want their capital to solve an important national problem. In both cases, the skilled team offering a value proposition with highest return on investment will get funded.

In November 2019, 37 S&Es participated in the Academy, bringing the total trained to 250 since 2015. The eighth Academy will be taught in November 2020.

National Lab Accelerator

Laboratory solutions to problems important to the U.S., such as energy challenges, are implemented through the business sector; therefore, it is important for LLNL S&Es to have some knowledge in working with businesspeople. The LLNL-hosted National Lab Accelerator is a DOE Office of Technology Transitions

(OTT)-funded program designed to train national laboratory S&Es in optimizing the flow of laboratory-developed technologies into the private sector to create value for the US economy. With a stronger understanding in business, S&Es are able to better communicate a value proposition with businesspeople. The knowledge also increases the likelihood of moving technologies developed at the national laboratories into the hands of those who can create value. The Accelerator program provides S&Es the opportunity to work with experienced external business mentors who help them develop a value proposition and business concept around a market need and a technology. Their work culminates in a pitch competition in which their knowledge and business model communication are judged by Bay Area and Silicon Valley investors.

IPO hosted the National Lab Accelerator program in 2017, 2019, and is in the midst of the program in 2020. There are currently six LLNL S&Es working with business mentors to develop business models and pitches applying LLNL technologies to a market need.

The LLNL participants will compete against each other in an LLNL-hosted Accelerator Pitch Event, and the winner will move on to compete against trained S&E pitchers from other DOE national laboratories in a daylong National Lab Accelerator Pitch Event. As in the past, this event is expected to attract a wide audience, including national lab participants and tech transfer officials, as well as angel investors, venture capitalists, entrepreneurs, and business community representatives from the greater Bay Area and Silicon Valley, including groups such as Keiretsu Forum, Band of Angels, Life Science Angels, CleanTech Open, Harvard Angels, Venture Capital Roundtable, among others.

DOE OTT will award a cash prize for the best presentation and technology business model with the greatest potential for moving from the lab to the marketplace.

Entrepreneurial programs started at LLNL in 2015, since then:

- 250 S&Es trained through the Academy
- 23 LLNL Accelerator participants matched with business mentors
- 7 Energy I-Corps teams performed in-depth customer discovery
- 6 LLNL technologies included in FedTech cohorts working to create new companies



Moonguake

Fostering Inclusive Behaviors through Real Play

MoonQuake is an innovative experiential learning tool for increasing awareness of inclusion and promoting cooperative behaviors, performance, and productivity. Developed by a multidisciplinary team at LLNL, MoonQuake allows participants to build inclusive behaviors through a unique learning experience based on serious gaming methodology.









Energy I-Corps

Established in 2015, DOE's Energy-I-Corps pairs teams of researchers with industry mentors to train entrepreneurs in moving technologies toward commercialization. LLNL was one of the initial laboratories to pilot the Energy-I-Corps program. S&E participants go through an intensive two-month training in which the researchers define technology value propositions, conduct customer discovery interviews, and develop viable market pathways for their technologies. Researchers return to LLNL with a framework for industry engagement to guide future research and inform a culture of market awareness.

Seven LLNL teams have participated in Energy I-Corps since 2015. The latest team, led by LLNL scientists Patrick Campbell and Steven Hawks, participated in Cohort 10 in the fall of 2019, interviewing customers and developing a business model for their water desalination technology, e-IonSorb.



FedTech

FedTech is a D.C.-based startup studio and accelerator that builds startups around deep technology from federal laboratories, universities, and corporations. It is a valuable resource to the entrepreneurial programs provided by the IPO. Since 2018, LLNL's IPO worked with FedTech to match Laboratory technologies and S&Es with FedTech-recruited entrepreneurs. FedTech entrepreneurs work with LLNL scientists to perform a key step of customer discovery and market validation, and in some cases startup formation, to bring Lab technologies to the market. Since 2018, seven S&Es have participated in this program with the latest spring 2020 cohort utilizing three LLNL technologies in their program:

- Komal Kampasi Implantable Optoelectrode for Optogenetics
- Razi Hague Deep Brain Stimulation Electrode
- Ryan Goldhahn and Priyadip Ray Autonomous Al Sensor Network

Two of the three technologies are the basis for two new start-ups that will incorporate and apply for SBIR funding with the help of a newly developed, Phase 2 program being offered by FedTech.



The Department of Defense's Defense Advanced Research Projects Agency (DARPA) funded LLNL to develop an implantable neural interface with the ability to record and stimulate neurons within the brain for treating neuropsychiatric disorders. The technology will help doctors to better understand and treat post-traumatic stress disorder, traumatic brain injury, chronic pain, and other conditions.

I-GATE

i-GATE Innovation Hub and Daybreak Labs

LLNL, through IPO, maintains a close connection to the regional economic development ecosystem. Located within the innovation and investment hub that is the San Francisco Bay Area, LLNL is lucky to have a community ready to support and benefit from LLNL technology commercialization.

The i-GATE Innovation Hub, originally founded through a collaboration between the City of Livermore, Sandia-California, and LLNL aims to support startups and economic development in the Tri-Valley region of California. i-GATE's work is particularly centered around the national labs as anchors of innovation. i-GATE manages a life sciences and hard tech incubator called Daybreak Labs (formerly Switch Labs). Daybreak Labs provides biological research facilities and prototyping equipment to help life sciences and hardware startups get started and grow quickly. i-GATE's incubation programs have supported a number of high-tech startups that are commercializing technologies originally developed at LLNL. Three startups with ties to LLNL (Savion Aerospace, Metal Monomers, and New Frontier Aerospace) are currently incubated in the facility.

A successful i-GATE alumni company is SafeTraces, an LLNL licensee of DNATrax technology. SafeTraces has obtained \$20M in funding including \$3M in FDA, NIH, and NSF grants. Investors include UL, Bunge, Spero Ventures (Omidyar Network fund), and S2G Ventures. The company has grown its business, created 23 jobs in the San Francisco Bay Area, and filed for six patents, creating significant intellectual property. SafeTraces recently expanded its offices to an 8,000 ft² laboratory/office in Pleasanton, California and relocated its research and development facility to Livermore, further contributing to the regional economy.

In the past year, i-GATE has continued their successful NextTech Speaker Series connecting Bay Area founders, investors, executives, and technology developers with the life sciences community in the TriValley and greater East Bay. i-GATE also held the second annual Tri-Valley Life Sciences Summit, with an audience of more than 350 local life sciences professionals and entrepreneurs. A poster session preceded the Summit, with technologists from LLNL, UC Davis, UC Merced, and Sandia's California site presenting to experienced local entrepreneurs. i-GATE also manages the Tri-Valley Connect and Tri-Valley Bio branding websites, which identify and highlight the Tri-Valley as a hub of innovation with the goal of recruiting and retaining key talent that will benefit the entire regional innovation ecosystem.











HIGHLIGHTING CAPABILITIES

"Bringing together industry leaders, DOE leaders and *cutting edge researchers* from national labs to discuss the value of innovation and emerging technological areas is a great benefit to the technology transfer commercialization pipeline."

> —Hannah Farquar, PhD LLNL Business Development Executive & InnovationXLab Representative

InnovationXLab Summits

InnovationXLab summits, hosted by the DOE OTT, convene key industry representatives to showcase the unique technical resources and capabilities of the 17 DOE national laboratories, and how they can be leveraged by private companies, investors, universities, and other organizations. Laboratory IPO commercialization experts and Laboratory scientists and management work together to participate and reap the benefits of commercial connections and partnership leads developed at these strategic events.

At a January Biomanufacturing Summit, Sarah Baker, LLNL's deputy group leader for the Functional Materials Synthesis and Integration Group, moderated a panel on "Leaping Toward Profitability."

Planning continued for other InnovationXLab Summits as they were moved to virtual events due to COVID-19 restrictions. For both the InnovationXLab Quantum Information Science and Technology (QIST) Summit, and the CarbonX Summit, IPO will host virtual exhibits of LLNL capabilities and licensable technology.

The QuantumXLab virtual exhibit will focus on an emerging intellectual property portfolio of quantum-coherent devices and materials. Also highlighted will be a long-term industry partnership in quantum sensing with AOSense, Inc. and LLNL's Quantum Design and Integration Testbed (QuDIT).

The CarbonX exhibit will profile intellectual property portfolios on carbon capture, storage, sequestration, and re-utilization, as well as LLNL's ongoing focus on analysis of solutions for carbon dioxide reductions in a new carbon economy.

Promoting Technology Commercialization

In an effort to lower barriers to innovation, DOE selected 12 projects as part of its Practices to Accelerate the Commercialization of Technologies (PACT) program. Each PACT project was chosen to enhance the potential for commercialization of national laboratory technologies and increase collaboration between industry and lab researchers. LLNL is participating in five projects and leading one—Open Source Software: Seeds of Commercialization. Below are descriptions for the five projects that will involve LLNL.

Open Source Software

The project seeks to identify and validate value propositions for open source software developed and released by LLNL, and by extension all of the DOE national laboratories. The project is validating strategies for probing and accelerating LLNL open source software use and impact to the private sector.

Lab Innovation Networking Center (LINC)

The Lab Innovation Networking Center (LINC) project provides a single portal to the four DOE national laboratories in the San Francisco Bay Area (LLNL, Sandia-California, SLAC National Accelerator Laboratory, and LBNL), linking corporations, startups, and investors to DOE's world-class research and unique facilities. LINC's mission is to accelerate innovation in the region by being a multifaceted resource for Bay Area institutions.

Technology Transfer Researcher Liaison Program

The Technology Transfer Researcher Liaison program's goal is to improve communication between research organizations within a larger research institution and the institution's technology transfer office, which improves IP productivity. The ORNL-led project provides LLNL with an opportunity to rethink and improve its current "Liaison" program.

Accelerating Commercialization by Connecting Inventions to Maturation (ACCLAIM)

ACCLAIM seeks to connect national laboratory-developed technologies to federal government accelerators that are intended to identify, mature, and otherwise support technologies for deployment in national security applications. The initiative will enable DOE labs to understand goals and interests of the different federal technology accelerators and technology maturation programs, identify potential roles and pathways for contribution from DOE national laboratories, and define a path forward for strategic alignment.

Diversity and Inclusion in InVentorship and EntrepReneurship Strategies and Engagement – Women (DIVERSE-W)

The inclusion project seeks to better understand and frame diversity and inclusion (D&I) issues, including participation rates for women in inventorship and entrepreneurship; best practices for D&I from both inside and outside of DOE that are yielding results; and strategies for new and innovative inclusion programs that can be piloted.

The program, originally developed by the DOE's Office of Technology Transitions provided \$2.5 million for the 12 projects. These PACT projects engage all 17 national laboratories, one NNSA facility, and six external partners for a total of 24 participating entities.



The project goal of DIVERSE-W is to increase female participation within the national laboratories' tech transfer programs to spur innovation and enhance the potential for commercialization of lab technologies.

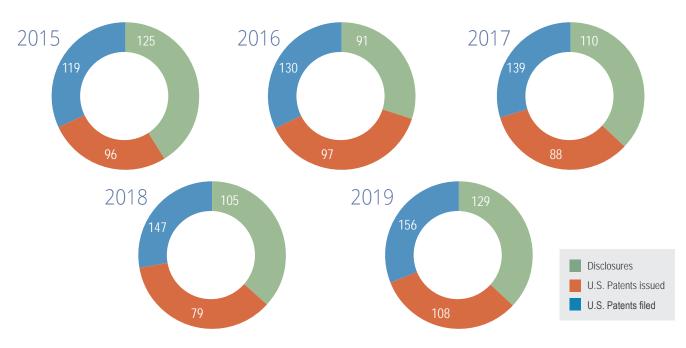


METRICS

While narratives that describe scientific discoveries at LLNL provide evidence of innovation in action, they do not tell the whole story. Here, we share metrics that serve as quantitative indicators of our success in transferring technology from LLNL to commercial partners.

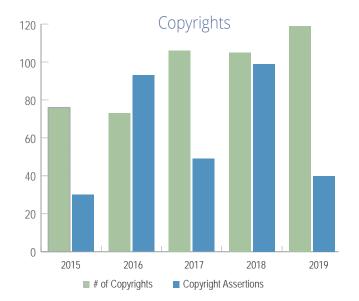
Intellectual Property

LLNL-based inventions were protected by more than 1,000 issued patents and patent applications, including provisional patents, from 2015 to 2019.



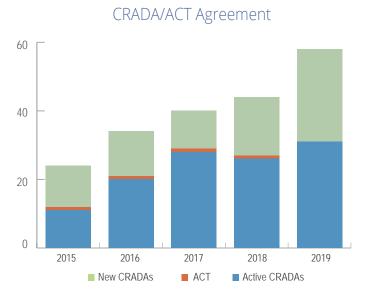
LLNL obtained more than 300 copyright assertions, helping protect our scientists' intellectual property from 2015 to 2019.

|44|

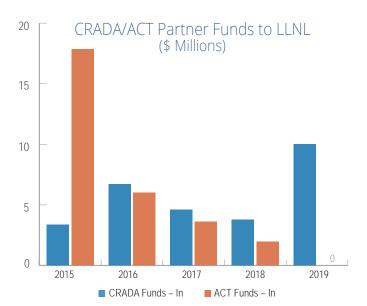


Industry Agreements

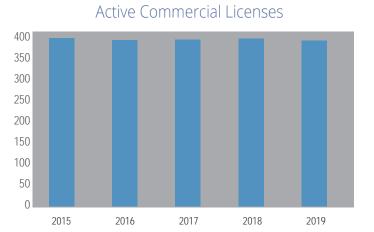
LLNL had nearly 200 active CRADAs from 2015 to 2019, which helped our scientists transform promising technology into marketable products.



Funds received by LLNL from our CRADA and ACT partners play a key role in our technology transfer activities.



LLNL had nearly 2,000 active commercial licenses from 2015 to 2019.







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