LDRD Quarterly Highlights

Mission Agility | Technical Vitality | Workforce Development

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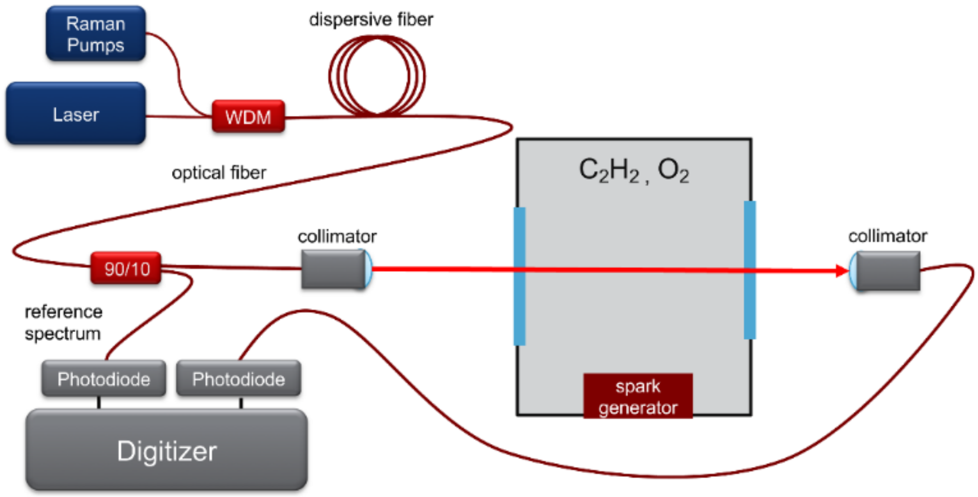
SDRD SITE-DIRECTED RESEARCH & DEVELOPMENT HIGHLIGHTS

NNSS team uses time-domain spectroscopy to measure transient infrared absorption spectra in gases

The NNSS has developed a diagnostic that uses time-domain spectroscopy to measure transient infrared absorption spectra in gases. Using a time-stretch Fourier transform approach, it can determine pressure, temperature, and gas concentrations with sub-microsecond time resolution for over two milliseconds. The technique measures spectra using fiber optics, photodetectors, and digitizers. No cameras or spectrometers are required.

Laser-based spectroscopic techniques that probe the rotational and vibrational spectra of molecules are often used to measure temperatures, pressures, concentrations, and material composition on short timescales to examine events such as shock waves in high pressure research, during the detonation of explosives, or in combustions studies. In many cases, a method that records high-resolution spectra on a sub-microsecond timescale under dynamic conditions is required.

Conventional high-speed recording methods map the spectrum into the spatial domain using a grating or prism to disperse the various wavelengths, and a streak or framing camera records the spectra. Such techniques have an inherent trade-off between high time resolution and long recording times. Furthermore, high-speed streak and framing cameras that can record in the short-wave infrared (SWIR), where many vibrational spectra exist, are uncommon.

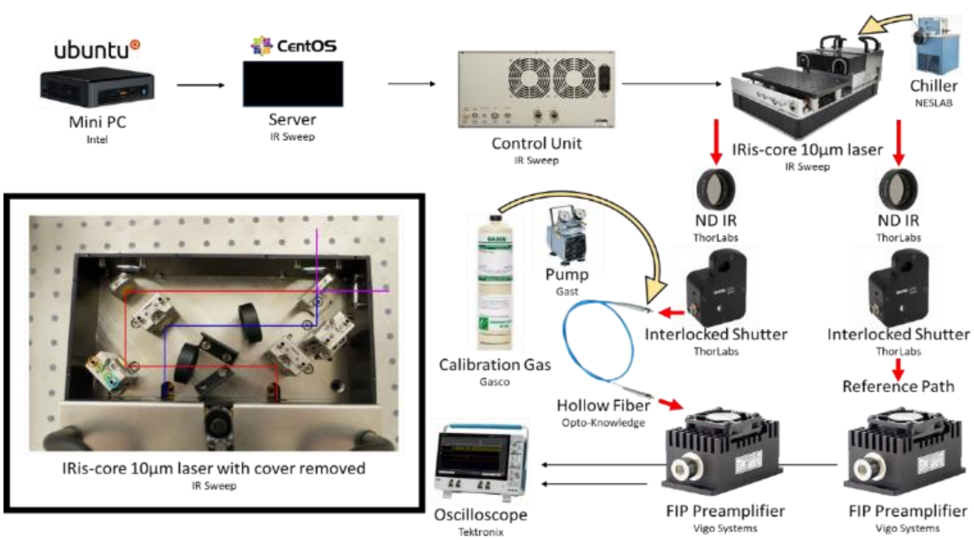


Experimental setup for time-domain spectroscopic measurements of temperature, pressure, and composition of gases during the combustion of C_2H_2 in O_2. A mode-locked 1550 nm laser is chirped and Raman amplified in highly dispersive fiber before passing through the combustion cell and being recorded by a photodiode. WDM is a wavelength division multiplexer.

Time-stretch spectroscopy, an alternative approach that overcomes these limitations, is also referred to as dispersive Fourier transform spectroscopy or photonic time stretch; the method disperses spectra into the time domain by creating different temporal path lengths for different wavelengths. The spectra can then be recorded with a single-point photodiode and oscilloscope. The system develop by NNSS operates at wavelengths ranging from 1520 to 1620 nm, where many rotational-vibrational spectra exist.

The full article describing this diagnostic and results were recently published in *Optics Express* (vol. 28, no. 20; https://doi.org/10.1364/OE.401737). *(DOE/NV/03624--0960)*

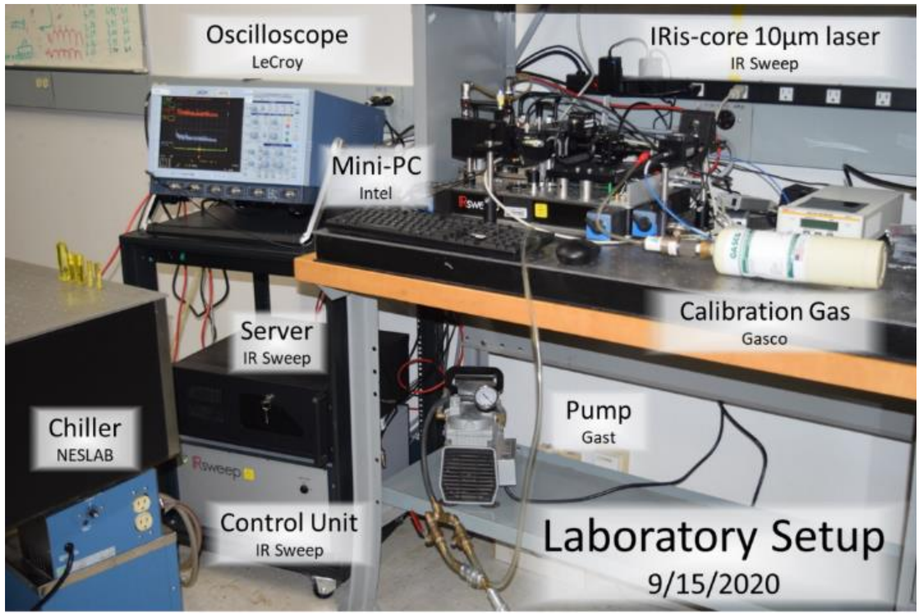
NNSS uses dual-comb spectroscopy to identify gases at speeds that mitigate turbulence effects



The dual-comb spectroscopy system schematic shows both the reference and hollow fiber paths.

A group at the NNSS Special Technologies Laboratory is developing a dual-comb spectroscopy system to be used in material detection scenarios. The system promises to outperform conventional Fourier transform spectrometers in precision, accuracy, and speed of collection with no moving parts. Due to its speed, this technique has the potential to mitigate turbulence effects.

Absorption spectroscopy is a standard technique for identifying gases of interest. Tunable diode laser absorption spectroscopy provides quantitative measurements, but its spectral range is often narrow and can be spoofed by gases that also absorb in the same region. Wider frequency absorption measurements can be more definitive, but using industry standard Fourier transform spectrometers is expensive and slow; these measurements are often degraded by the length of time required for making them. However, the dual-comb system is expected to have upgraded speeds that will effectively “freeze” atmospheric turbulence and mitigate its ability to degrade data. The researchers expect to acquire spectral measurements of materials of interest at resolutions of approximately 0.01 cm^{-1} over a range from 990 to 1010 cm^{-1} (roughly 9.9 to 10.1 microns).



The dual-comb spectroscopy system laboratory setup was used to collect data in FY 2020; further developments are forthcoming in FY 2021 prior to design of a field prototype.

The team has developed software, modeled a heterodyned signal, and applied cross correlation techniques to compensate for the drift in frequency; this worked extremely well in simulations. On a benchtop experimental setup in the laboratory the comb lasers were able to detect the heterodyne signal from the beating of the two laser combs. The team collected dual-comb data that compared an empty reference path to a calibration gas using a hollow-core fiber design to stand in for the gas cell in a standard gas detection setup. This relatively novel approach maximizes absorption path length and employs a minimum sample of gas. Continuing to test the capability of the fibers in the system, they have transmitted the combs through one fiber sans gas and also fitted a fiber to introduce and retain the gas inside itself while it simultaneously transports laser light.

Developing a dual-comb spectroscopy system in this wavelength region will serve two strategic purposes. It will develop a compact detector in a wavelength region that is of importance to chemical/biological and weapons detection agencies. It will also develop a knowledge base and expertise on dual-comb spectroscopy that can be expanded to other frequency regimes and other mission spaces. The final system would be paired with either an in-scene detector (such as already developed by the NNSS) or convenient in-situ reflectors such as bare metal surfaces (which can be easily located with infrared cameras) for a complete detection package. *(DOE/NV/03624--0958)*

NNSS R&D 100 awards winner and finalist have roots in SDRD

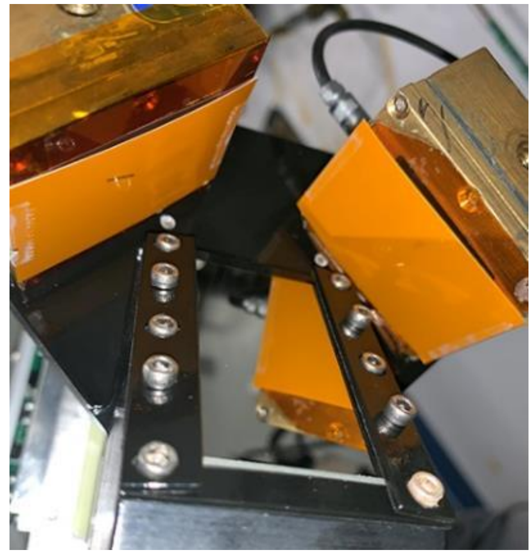
The NNSS’ X-ray Polarizing Beam Splitter (XRPBS) was named a winner of the 2020 R&D 100 Awards. The Intelligent Consequence Control by Aerial Reconnoiter Using Unmanned Systems (ICARUS) was a finalist.

The award-winning innovation recognized, the XRPBS, has the ability to separate an x-ray beam in two in order to measure each polarized beam simultaneously, which will be used for diagnostics within the NNSA enterprise. Developed in partnership with Sandia National Laboratories, Argonne National Laboratory and EcoPulse, it is the first x-ray polarizing beam splitter in existence.

"I see it as a diagnostic that will be involved with many different types of experiments and scientific research facilities," said NNSS Distinguished Scientist Howard Bender.

ICARUS equips unmanned aircraft systems with a payload of radiation, chemical, optical, LIDAR, and photographic detectors. The technology, developed by the NNSS in partnership with Unmanned Systems, Inc., H3D, Inc., and Virginia Tech.

ICARUS "provides an unmanned capability to do some of the dull, dirty, dangerous, and sometimes deep work where you don't want to send any type of human system—for example, a serious incident involving hazardous materials," said Bender. *(DOE/NV/03624--0959)*



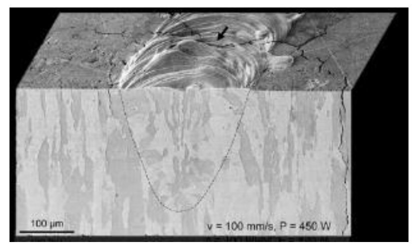
The XRPBS crystals and detectors in the setup used for polarization contrast measurements at the Advanced Photon Source synchrotron.

Lawrence Livermore National Laboratory

HIGHLIGHTS

Livermore researchers analyze real-time crack formation in 3D-printed tungsten

With the highest melting and boiling points of all known elements, tungsten is frequently used in applications involving extreme temperatures, including radiation shielding, and as plasma-facing material in fusion reactors. However, its widespread adoption has been hampered due to tungsten's inherent brittleness and the microcracking that occurs while using 3D printing to produce parts made from the metal.



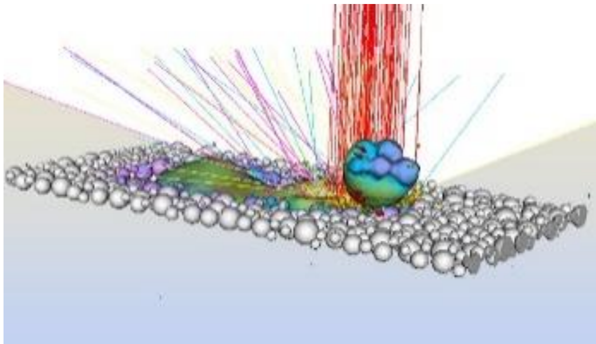
LDRD funding enabled LLNL scientists to observe—in real time—how microcracks initiate and spread in 3D-printed tungsten. Photos taken using a scanning electron microscope show how the microcrack network branches along the laser melt track on the surface, and can penetrate deep into the adjacent substrate material.

To characterize how and why these microcracks form, Lawrence Livermore National Laboratory (LLNL) scientists combined thermomechanical simulations with high-speed videos taken during a metal 3D printing process known as laser powder-bed fusion. Whereas previous research was limited to examining cracks post-build, for the first time, scientists were able to visualize the ductile-to-brittle transition in tungsten in real time.

This novel, real-time capability allowed them to observe how microcracks initiated and spread as the metal heated and cooled. The team was able to correlate the micro-cracking phenomenon with variables such as residual stress, strain rate, and temperature. By identifying the fundamental mechanisms behind cracking in 3D-printed tungsten, they established a baseline for future efforts to produce crack-free parts made from the metal.

According to Bey Vrancken, a Lawrence Fellow and the study's co-principal investigator, the novel capability can help investigators determine the most effective strategies to eliminate cracking and enhance the structural integrity of parts printed with tungsten. More information regarding Vrancken's research and related publications can be found on LLNL's website. *(LLNL-WEB-458451)*

Livermore investigators develop technique to reduce defects in 3D metal printing



Combining high-fidelity computer simulations with ultra-high-speed x-ray imaging, LLNL researchers discovered a way to reduce or eliminate defects in parts built through a 3D-printing process known as laser powder-bed fusion, which uses a laser beam to melt metal powder layer-by-layer to form 3D parts.

Along with collaborators at the Air Force Research Lab, LLNL scientists identified previously unknown dynamics in this 3D-printing process that “spatter” metal powder particles—which are ejected from the laser’s path and can land back on the parts, potentially leading to pore formation and defects. They developed a “power map” that dynamically adjusts the laser’s power output along its track, finding a “sweet spot” that can keep the melt pool stable. In addition, they discovered that pre-sintering the metal powder (fusing particles together prior to the build) can help reduce spatter and improve part reliability. Learn more about this LDRD-funded additive manufacturing research on LLNL’s website. *(LLNL-WEB-458451)*

Livermore investigators develop surrogate models that use advanced artificial intelligence to improve predictive simulation capabilities

Predictive simulation capabilities play a key role in many national security missions, and LDRD funding has supported several efforts aimed at improving the accuracy of complex predictive models. For example, scientists are exploring how surrogate models supported by neural networks can perform as well as, and possibly better than computationally expensive simulators—providing new insights into complicated physics problems.

LLNL researchers are exploring new ways to integrate experimental data, such as data generated by LLNL’s National Ignition Facility (right), with simulations conducted on LLNL’s Sierra supercomputer (left), using new deep learning methods that can boost the accuracy of predictive simulation capabilities.

LLNL researchers developed a surrogate model driven by deep learning that incorporates a multi-modal neural network capable of quickly and accurately emulating complex, data-rich scientific processes, such as the high-energy-density physics involved in inertial confinement fusion.

The team anticipates that deep learning can capture important relationships between data sources and provide a compact representation for all of them. It offers the potential to make simulations more flexible and accurate.

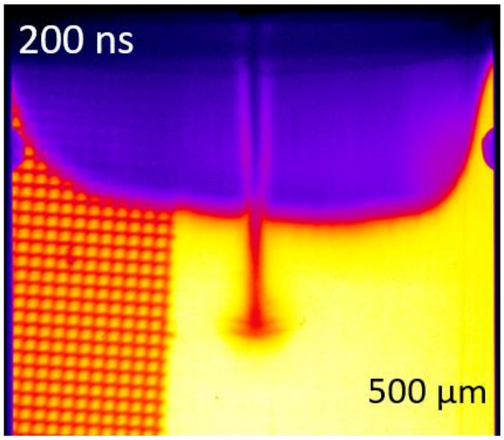
The project is part of LLNL’s broader cognitive simulation initiative, which focuses on transforming simulation science and enabling new approaches to predictive analysis for complex, data-driven problems. More information about this effort to improve predictive simulations through the use of artificial intelligence can be found on LLNL’s website. *(LLNL-WEB-458451)*

Livermore researchers improve codes used to simulate interactions between particles moving at high velocities

A team of LLNL scientists is exploring the interaction between ejecta—particles ejected from a material's surface following shock-driven processes that cause the micron-sized particles to travel at high velocities. For example, they are studying metal ejecta generated from copper and tin material samples during high-power laser experiments, comparing how the mass, velocity, and material phase (e.g., liquid or solid) influences particle interaction.

The research team is also improving hydrodynamics codes used to model phenomena that occur during these types of high-energy experiments. By feeding better experimental data into the hydrocodes, combined with data from molecular dynamics, scientists can conduct more realistic simulations at experimental scales.

Gaining a better understanding of ejecta interactions has a broad range of applications, such as spacecraft shielding, cold-spray welding, additive manufacturing, and understanding material strength at small scales.



A radiography image of an ejecta microjet traveling downward (with the laser drive coming from above), captured during experiments conducted by LLNL's research team as part of their efforts to characterize ejecta interactions.

(LLNL-WEB-458451)

Doctoral student Marco Echeverria (right) is collaborating with the LLNL research team to improve hydrodynamics codes used to model phenomena that occur during high-energy experiments. One of his mentors is LLNL physicist Alison Saunders (left).

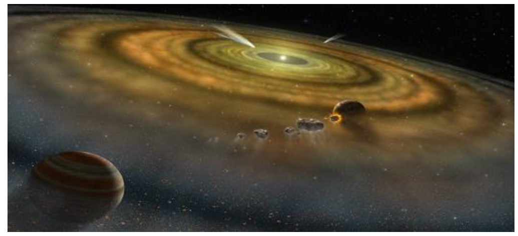
Echeverria is a GEM fellow, sponsored by LLNL. The National GEM Consortium is a network of national laboratories, universities and other organizations that enables students from underrepresented communities to pursue graduate education in science and engineering.

Echeverria is earning a doctoral degree in materials science and engineering. During a previous internship at LLNL, he learned about the Laboratory's computing infrastructure and molecular dynamics codes. He was also able to view experimental setups and interact in person with experimentalists. As a result, he was able to hit the ground running in his more recent work on the simulation efforts.

One of the benefits of the GEM program is that it helps build connections with mentors and employers, giving students an opportunity to explore environments where they might want to work after graduation.

According to Echeverria, he likes the close connection between experimental work and modeling that's possible in a national lab research environment. "It's exciting to be able to reverse-engineer simulation codes based on experimental results," he explained.

Livermore scientists analyze isotopes in meteorites to study solar system formation


Artist's conception of dust and gas surrounding a new planetary system. (Image courtesy of NASA)

LLNL scientists examined the potential timeframe for the formation of our solar system by studying isotopes found in meteorites. The research provides a link between astronomical observations of star formation and cosmochemical studies of solar system formation.

The oldest solids in our solar system are calcium-aluminum-rich inclusions (CAIs). Micrometer- to centimeter-sized CAIs are found in meteorites formed in high-temperature environments. In collaboration with scientists from the University of California, Santa Cruz, and the California Institute of Technology, LLNL investigators measured the concentration of molybdenum isotopes in CAIs taken from meteorites, including a meteorite known as Allende—the largest carbonaceous chondrite meteorite found on Earth. Findings indicate that the solar system formed much more rapidly than previously thought.

Learn more about this cosmochemical research and related publications on LLNL's website. *(LLNL-WEB-458451)*

Sandia National Laboratories

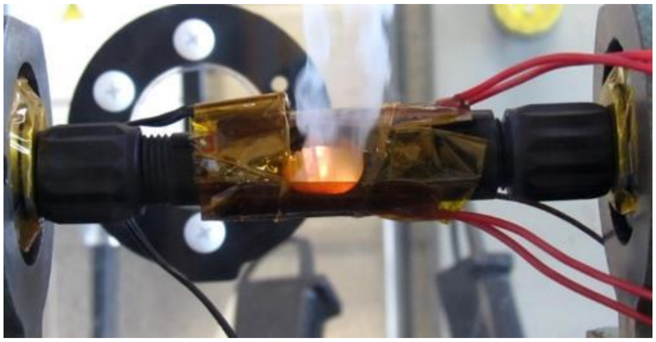
HIGHLIGHTS

Sandia developed materials help extinguish solar panel fires before they ignite

As solar panels become popular and their voltages increase, there is a need to have built-in capabilities to extinguish fires caused by arc-faults, which are high-power discharges of electricity that can create explosions or flash events due to damaged wires. Sandia National Laboratories researcher Kenny Armijo has spent 10 years working alongside other researchers at the labs and local company Guardian Sensors Inc. to understand and characterize these hazardous arc-faults. Their work led to development of electrical in-line connectors that automatically predict and prevent photovoltaic arc-faults before they can ignite electrical fires.

Sandia National Laboratories researcher Kenny Armijo uses an arc-fault generator that was developed by researchers to determine how dangerous arc-faults are. (Photo by Bret Latter)

"As solar panels become more efficient, they're able to produce more power," said Armijo. "More power means that they're going to have higher current and higher voltage levels. As you increase the current and voltage levels in next-generation solar panels, it becomes a bit more dangerous because as you increase the voltage, you get a higher propensity for arc-faults. This new self-extinguishing mechanism could solve that problem."



If there were a spark, a special polymer, developed by Sandia National Laboratories, within the in-line connectors would melt and a spring would extend inside the connector to facilitate a larger spark gap and stop the flames, as shown in this photo. (Photo courtesy of Kenny Armijo)

The in-line connector developed by Guardian Sensors — about an inch long and the diameter of a dime — contains a metal spring covered in a special type of self-extinguishing polymer material developed and tested at Sandia over the last five years. Like current connectors, the self-extinguishing mechanisms would link a series of solar panels like a string of Christmas lights that could operate together in a field or on a roof.

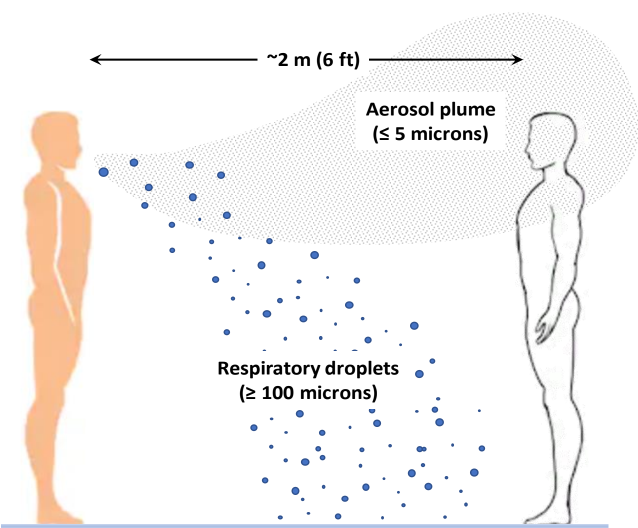
All connectors are susceptible to corrosion, damage or improper installation, which can lead to reliability issues, especially if there are tiny crevasses or breaks in the wires. Sparks and devastating fires can occur when high current and voltage run through damaged connectors, and unfortunately, there currently isn't a completely reliable way for the connectors themselves to prevent fire danger. The new device would fill that technology safety gap, Armijo said.

The new in-line connectors have been built to activate at temperatures above 185 degrees Fahrenheit. When that happens, the special self-extinguishing material melts, fills in the crevasses or breaks in the wires and extends the spring which increases the spark gap between wire conductors, so they can no longer produce energy that leads to heat and fires. A combination of the speed of the reaction and the material's fire-resistant properties will stop a fire before it starts — in less than 2 seconds — Armijo said.

The self-extinguishing materials used in the connectors were developed from Sandia-based research originating out of the LDRD program. *(SAND2020-1239)*

Modeling airborne transmission and exposure risks of SARS-CoV-2 at Sandia

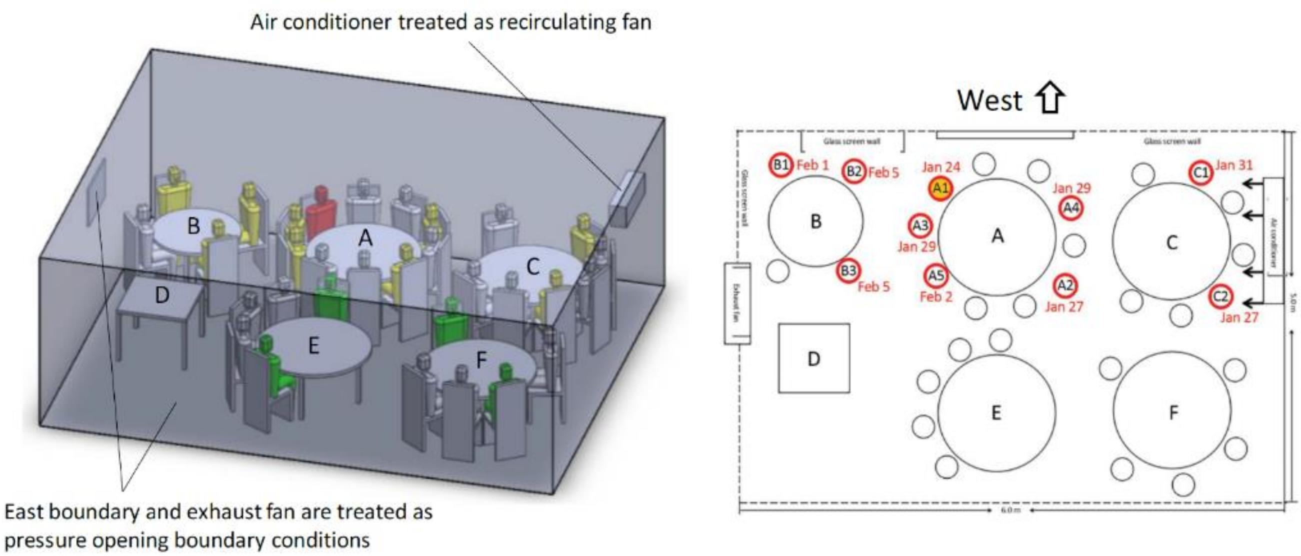
Due to the COVID-19 pandemic, many different guidelines have been issued to help prevent the spread of the virus. Case in point, people now stand six feet away from each other when interacting outside of their household to mitigate the spread of the virus. Where did the "six feet of social distancing" guideline come from?



Large droplets (>100 µm) are deposited quickly due to domination of gravitational force. Small droplets, or aerosols (<5 µm) are responsible for airborne transmission.

According to Sandia researcher, Cliff Ho, this six-foot guideline value was based on early studies indicating that larger droplets (>~100 microns) expelled during a cough or other expiratory event only travelled a maximum of 1–2 m (up to ~six feet) before falling to the ground. However, additional studies demonstrated that smaller more buoyant droplets ejected during coughing, sneezing, talking, or even breathing could be suspended for longer periods and carried much further. In Ho's research, computational fluid dynamics (CFD) modeling was utilized to simulate various events (e.g., coughing/sneezing vs. talking/breathing) to understand how various environmental factors could impact airborne pathogen transport and transmission. He assumed viral pathogens (droplet nuclei) were aerosolized such that the pathogen distribution and concentration could be represented by the concentration of the simulated exhaled vapor plume. “I introduced spatial and temporal concentrations into the modeling to develop quantified risks of exposure based on separation distance, exposure duration, environmental conditions such as airflow, and face coverings,” said Ho. “I could then determine the probability of infection based on spatial and temporal aerosol concentrations, viral load, infectivity rate, viral viability, lung-deposition probability, and inhalation rate.”

After defining cumulative distributions of infection and determining the most important parameters, the models and methods were applied to a case study in a restaurant located in Guangzhou, China, with an observed infection outbreak to verify the methodology, calibrate the model parameters, and perform studies of different ventilation configurations to determine measures to minimize the risk of airborne transmission. The tools and models yielded probabilities of infection that were qualitatively consistent with observations of infection rates at the different tables surrounding the index patient. Simulations confirmed that poor ventilation and recirculation increased pathogen concentrations and probability of infection. Increasing the fresh-air supply to the ventilation decreased the pathogen concentrations and probability of infection. This was observed through the increase of the fresh-air percentage by 10%, 50%, and 100% over 73 minutes. “The accumulated pathogen mass in the room,” noted Ho, “reduced by an average of ~30%, ~70%, and ~80%, respectively. This reduced the probability of infection by 11%, 37%, and 51%, respectively.”



Three-dimensional model of Guangzhou restaurant created in Solidworks (left) for use in CFD simulations based on configuration reported in Lu et al. [11] (right). Index patient in Solidworks model is highlighted in red, infected receptors are highlighted.

The models demonstrated wearing a face mask or face shield significantly reduced the forward plume propagation and normalized cumulative exposure by an order of magnitude. However, the vapor concentrations near the face were more persistent than without face coverings due to the reduced forward momentum.

Overall, results showed that social distancing significantly reduced the normalized cumulative exposure (by two orders of magnitude) and allowed time for dilution and dispersion of the expelled viral plume. Other models showed that being upwind or crosswind of the source of the cough also significantly reduced risk while being directly downwind of the cough increased exposure risks since lateral dispersion was confined.

In short, the issued guidance indicating that people should stand at least six feet apart and wear masks, in addition to staying upwind, is solid and can help to reduce probability of viral transmission. In addition, public gathering places, such as stores, gyms, and restaurants, can help decrease likelihood of infectious spread by increasing fresh air ventilation through centralized systems. *(SAND2020-10253)*

Three of Sandia's 2020 R&D awards rooted in LDRD

Physicists keep an eye on Nobel prizes; mathematicians, the Fields Medal. Inventors of useful programs and devices get their own moments of recognition when the R&D 100 Awards are announced each fall.

The contest — held and published annually since 1963 — is sometimes referred to as "the Oscars of invention." The winning lists are created by teams of examiners identifying the 100 most technologically significant products each year from an international pool of submissions sent in from government labs, universities and private corporations. The contest is sponsored by R&D World Magazine, the successor to R&D Magazine. This year, Sandia researchers earned six awards. Below are the three projects rooted in LDRD.

REDUCING RISK — Sandia computer scientist Vince Urias and his team earned a 2020 R&D 100 Award for developing HECATE, a software supply chain and assurance platform. (Photo by Randy Montoya)

HECATE: High-density Evaluator of Commercial-off-the-shelf Applications for Trust and Efficacy

Principal Investigator: Vince Urias

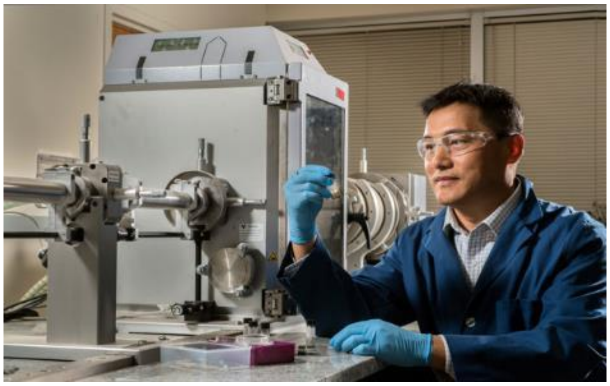
The number of software supply-chain attacks has grown to an unprecedented degree over the past decade. HECATE, a software supply chain and assurance platform, reduces risks for commercial and open-source software users. The platform addresses these threats through a virtual environment that simulates real, physical devices.

The platform distinguishes between benign, anomalous and suspicious behaviors. Intruders set off an alarm if they include an unrequested update that changes a program's behavior or requests access to privileged features in the user's system. HECATE provides a testing ground that attackers can't detect and therefore can't lie to, offering a yardstick to determine how much trust to accord a new addition.

Binary Solvent Diffusion for Fabrication of Large Nanoparticle Supercrystals

Principal Investigator: Hongyou Fan

Researchers used nanotechnology and chemistry to self-assemble gold nanoparticles into millimeter-sized supercrystals. These supercrystals exhibit crystal facet-dependent optical properties that provide an enhanced molecular-sensing capability.



SUPERCRYSTALS — Sandia materials scientist Hongyou Fan and his team earned a 2020 R&D 100 Award for using nanotechnology and chemistry to turn gold nanoparticles into supercrystals for optoelectronics, photovoltaics and surface catalysis. (Photo by Randy Montoya)

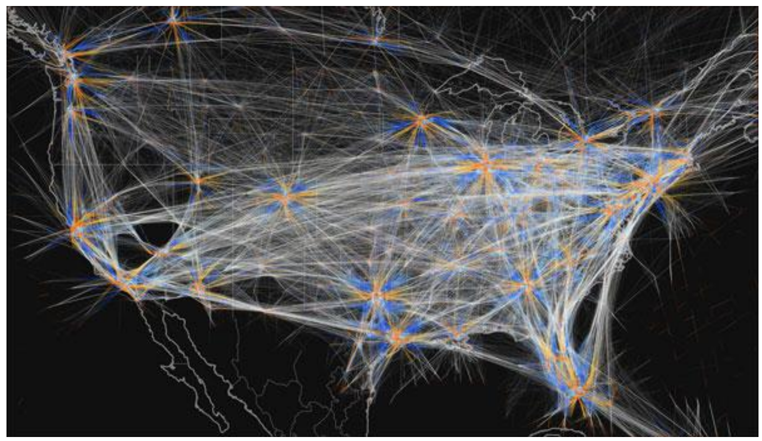
An inexpensive, large-scale production method uses a simple solvent diffusion process for seeding and crystal growth. The supercrystals obtained through this process also exhibit potential applications in optoelectronics, photovoltaics and surface catalysis.

Tracktable

Principal Investigators: Danny Rintoul, Andy Wilson, Chris Valicka

Tracktable applies advanced machine-learning techniques to large trajectory data sets, searching for shapes and patterns in space and time by providing a mathematical framework. The method organizes, searches and quickly analyzes millions of patterns, grouping similar shapes and extracting unusual trajectories without first requiring a definition of the term "normal," which might eliminate from consideration shapes worth studying.

By treating time as a variable similar to space, Tracktable enables searches for collective behavior and patterns over long periods of time. Fast search techniques predict paths and destinations of moving objects by comparing observed paths to historical databases of trajectories. *(SAND2020-1164)*



FINDING PATTERNS IN BIG DATA — This color map shows take-offs (red ends) and landings (blue ends) for all the flights in the U.S. from a single day. A Sandia team has earned a 2020 R&D 100 Award for creating Tracktable, a technology that uses machine learning.

Los Alamos NATIONAL LABORATORY EST. 1943

HIGHLIGHTS

Six Los Alamos 2020 R&D awards rooted in LDRD

Los Alamos National Laboratory technologies brought in eight R&D 100 Awards presented by R&D World magazine, and six have roots in LDRD.

"These awards reflect some of our great work that both benefits humanity and advance the frontiers of science," said LANL Director Thom Mason.

Below are the six projects rooted in LDRD.

Click the icons for associated videos.

AMANZI Advanced Terrestrial Simulator

Principal Investigator: David Moulton

Amanzi-ATS is an open-source software that includes the most complete suite of surface/subsurface physical processes to model complex environmental systems across multiple scales. Amanzi–ATS has been used to analyze pristine local watersheds, wildfire impact on watersheds, subsurface contaminant transport at legacy waste sites, the effect of a warming climate on the Arctic tundra, and groundwater in fractured porous media. Los Alamos led the joint entry with Oak Ridge National Laboratory, Lawrence Berkeley National Laboratory, and Pacific National Laboratory. This work has benefited from timely and critical support from LDRD. Related LDRD projects include: Predicting Climate Impacts and Feedbacks in the Terrestrial Arctic (20120068DR); Critical Watersheds: Climate Change, Tipping Points, and Water Security Impacts (20150397DR); and Adaptation Science for Complex Natural-Engineered Systems (20180033DR).

Video link: https://www.youtube.com/watch?v=mVibEU7npI0&feature=youtu.be

Multi-Burn Solid Rocket

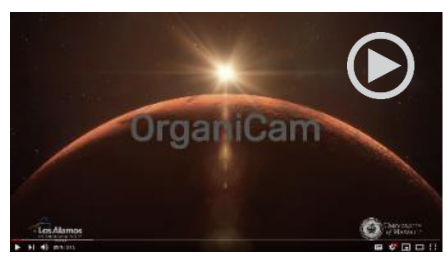
Principal Investigators: Nick Dallmann, Bryce Tappan, Mahlon Wilson

Solid rockets are high thrust, safe, scalable, and can be stored for long periods. However, they traditionally only provide a single burn per motor. The Multi-burn Solid Rocket is a revolutionary system providing multiple independent thrusts from a single solid rocket. This new capability could provide agile maneuverability for even the smallest and lowest cost satellites. The Earth's orbital zones are an important natural resource. The Multi-burn Solid Rocket could help protect this resource by enabling satellites to avoid orbital debris and to de-orbit at the end of life. This work is a direct outcome of a LDRD project, "ERIS: Electrolysis Rocket Ignition System" (20180382ER).

Video link: https://www.youtube.com/watch?v=RVQr2vEsIXU&feature=emb_log+o

OrganiCam

Principal Investigators: Roger Wiens and Patrick Gasda



OrganiCam is the first camera for noncontact, nondestructive biodetection in remote environments and space. It opens exciting frontiers in space exploration and the search for signs of life beyond the Earth. The compact laser-induced fluorescence imaging camera with Raman spectrometer could identify organic molecules and biosignatures in Martian caves, icy-moons, and asteroid surfaces. OrganiCam's robust design for extreme environments, portability, simple operation, and low power requirement build on the Lab's 50+ years designing robotic instruments for space applications. Los Alamos led the joint entry with University of Hawai'i. This work is a direct outcome of a LDRD project, "OrganiCam: A High-Sensitivity Radiation-Hardened Imaging Organic Detector For Space and

Programmatic Applications" (20180244ER). It also benefited from a FY14 LDRD project, "Remote Raman-LIBS Spectroscopy (RLS) Signature Integration" (20140033DR).

Video link: https://www.youtube.com/watch?v=DYUHAzaOKvM&feature=youtu.be

QUIC-Fire

Principal Investigators: Rodman Linn

The Quic-Fire software is the first fast-running, laptop-capable, 3D fire-atmosphere feedback model for complex wildfire and prescribed fire scenarios. It simulates critical influences of 3D vegetation structure, variable winds, interaction between multiple fires, and complex topography at meter-scale spatial resolutions. QUIC-Fire transforms fire and fuel manager's ability to assess risk, optimize fuel treatments, and plan prescribed burns to prevent catastrophic wildfires. Rodman Linn of Los Alamos, Scott Goodrick of the USDA Forest Service, and J. Kevin Hiers of Tall Timbers Research Station led the team of Los Alamos researchers. The modeling software QUIC was developed and funded through a FY15 LDRD project, "Critical Watersheds: Climate Change, Tipping Points, and Water Security Impacts" (20150397DR).

Video link: https://www.youtube.com/watch?v=3uVhUXB4b84&feature=youtu.be

Smart Microbial Cell Technology

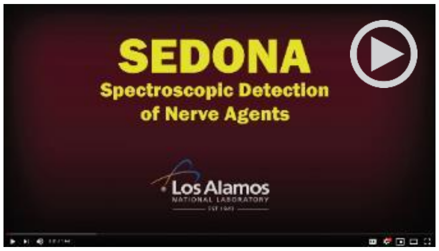
Principal Investigator: Ramesh Jha

Biocatalysts are essential for food production, pharmaceuticals, specialty chemicals, renewable energy, and environmental cleanup. Current methods to find biocatalysts are slow. Smart Microbial Cell Technology scans genetic variations to optimize a single enzyme or microbial cell to generate a product efficiently. It selects rare mutations needed for biocatalyst optimization orders of magnitude faster than current screening methods. A custom sensor reporter gene circuit causes cells to fluoresce when they are making the target product. When coupled to flow cytometry, a million biocatalyst variants can be screened in hours. LDRD funded development of this technology through a reserve grant, "Genomics and Biomanufacturing" (20160656ER).

Smart Microbial Cell Technology also received a Silver Special Recognition Award for Market Disruptor-Services, which highlights any service from any category as one that forever changed the R&D industry or a particular vertical within the industry.

Video link: https://www.youtube.com/watch?v=_QueFOT2Yzk&feature=youtu.be

Spectroscopic Detection of Nerve Agents



Principal Investigator: Robert Williams

Spectroscopic Detection of Nerve Agents (SEDONA) is the only portable screener to accurately detect the chemical nerve agents in unopened bottles, providing results in seconds. Current airport detection system cannot scan for the threat of toxic organo-phosphorus nerve agents and insecticides. The SEDONA portable system screens *through* an unopened bottle using the principles of nuclear magnetic resonance spectroscopy. The system could be deployed and operated with minimal training. SEDONA dramatically reduces the likelihood of a successful nerve agent attack at airports, government buildings, embassies, sporting events, concerts, and political rallies. The work draws on data originally generated in a LDRD project, "Fieldable Chemical Threat Mapping by Multi-modal Low Magnetic Field Nuclear Magnetic Resonance Signatures" (20170048DR).

Video link: https://www.youtube.com/watch?v=CiJO1vGg9UY&feature=youtu.be

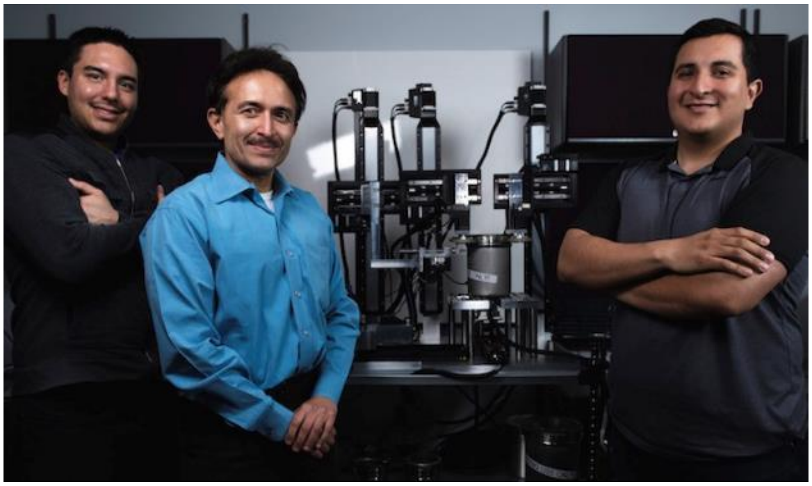
The R&D 100 Awards

The prestigious "Oscars of Invention" honor the latest and best innovations and identify the top technology products of the past year. The R&D 100 Awards span industry, academia and government-sponsored research organizations.

Since 1978 Los Alamos has won more than 170 R&D 100 Awards. The Laboratory's discoveries, developments, advancements and inventions make the world a better and safer place, bolster national security and enhance national competitiveness. See all of the 2020 R&D 100 Awards. Read more about the LANL's past R&D 100 Awards. *(LA-UR-19-31248)*

Los Alamos researchers re-imagine testing of nuclear material containers

Dubbed the Nation's Plutonium Center of Excellence for R&D by the National Nuclear Security Administration since 2008, the Los Alamos Plutonium Facility (PF-4) has long been home to essential research and development (R&D). Recently, a project funded through LDRD has come up with a new way to test nuclear material containers used at PF-4. The team calls their system the Modular Integrated Non-destructive Test System (MINTS). Once the MINTS technology is put to use in PF-4, the team envisions wider applications across other sites within the NNSA complex that use similar storage containers.



LDRD researchers at Los Alamos display the Modular Integrated Non-destructive Test System that will soon be installed in LANL's Plutonium Facility (PF-4) vault for container testing.

From mentorship to MINTS

Los Alamos researcher Raj Vaidya has long had a passion for mentoring, but the classified nature of his work made it difficult to invite in students. So, he set out to find a mission-oriented project that could function in an unclassified setting. At the time, he couldn't have known that his idea would bloom into an important project for national security.

With a small team of students, Vaidya began a project to investigate standardized nuclear storage material containers. It wasn't long before the team discovered unexpected corrosion in their container testing, which called for new levels of surveillance. So, the team applied for LDRD funding to continue to pursue their work, with a new goal of transitioning from destructive testing of containers to non-destructive.

Superpower vision = greater efficiency

The nuclear material containers known as SAVY containers (named for the initials of their inventors) are currently tested by unloading and cutting out sections in order to surveil their structural health. This process is very time consuming, leads to expensive losses, and adds to the waste flow. Non-destructive testing would mean, simply, seeing through metal and understanding the character of a container, without ever opening it.

The result, after two years of research, was the Modular Integrated Non-destructive Test System (MINTS). Vaidya describes:

"Once we narrowed down the technology, we found that a combination of three techniques — ultrasonic testing, eddy current array, and laser interferometry, coupled with a sophisticated gantry system and control logic — would give us all the information we needed about what was going on in these containers, without having to open any single one of them."

A SAVY container, which holds nuclear materials, is non-destructively tested with Ultrasonic and Laser Interferometer on the left, while Eddy Current Detectors traverse the bottom surface of the container.

In the upcoming months, pending COVID-related delays, the team will move the MINTS table into the PF-4 vault, which is home to all nuclear material storage containers that need frequent testing.

"In production, there are quite a few support functions that have to be attended to at the same time, such as waste management and nuclear materials storage," Vaidya said. "Both of those have to be in place to run operations in PF-4. This new process helps keep that storage and waste safe, so this is all quite integral to the mission."

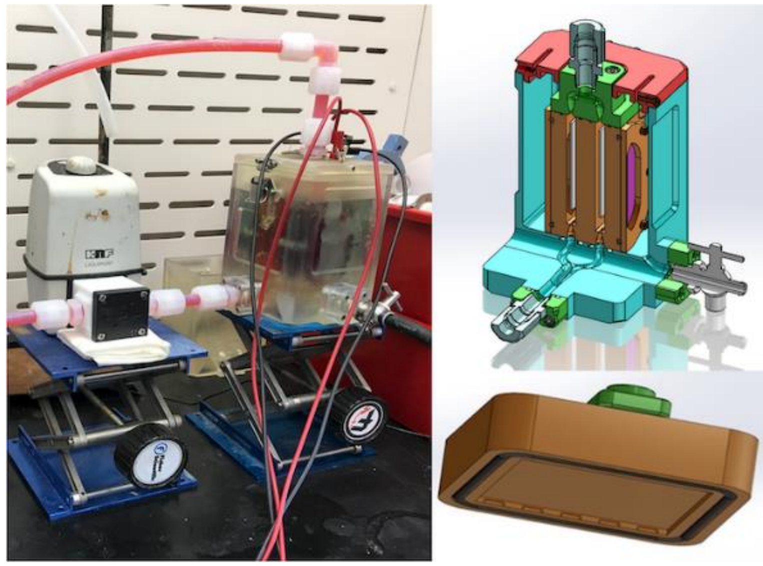
Once the MINTS technology is put to use in PF-4, the team envisions a wider application across other sites within the NNSA complex. Notably, the team was recognized this year by the International Symposium on the Packaging and Transportation of Radioactive Materials. *(LA-UR-20-30290)*

Researchers at Los Alamos develop new technologies to improve decontamination of gloveboxes

As PF-4 ramps up over the course of several years for the plutonium pit mission, both efficiency and safety are critical. A team of LDRD researchers at Los Alamos recently completed a project which, among other achievements, may have the solution for safely decontaminating the many aging gloveboxes that need to be replaced.

In the context of radiological work, gloveboxes are the large containers where nuclear materials can be safely housed and manipulated by employees. They are exactly like they sound: a giant box with attached sets of gloves that keep the contamination from getting out, serving as a barrier between the worker's hands and the materials. The High Efficiency Automated Leaching of Gloveboxes (HEAL-GB) team, led by Los Alamos researcher Ben Karmiol, developed new technologies to improve decontamination of gloveboxes and other metal components in PF-4.

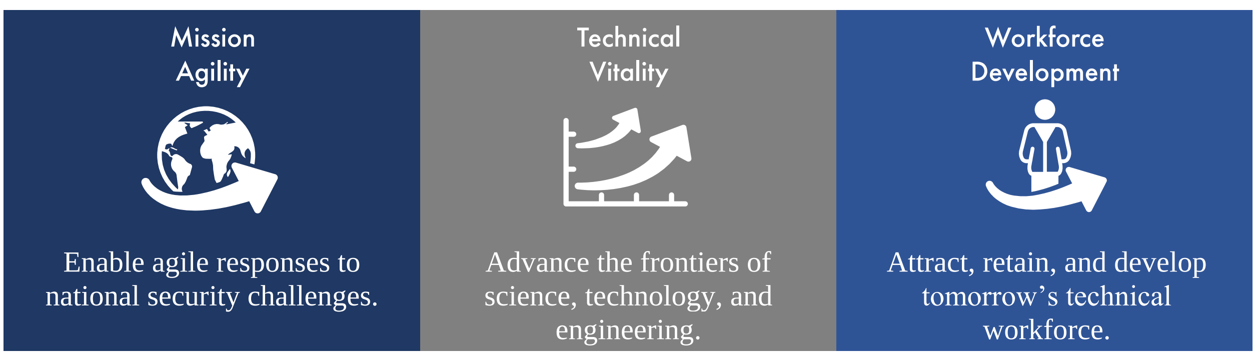
You can't just throw a box that has housed radioactive material in the trash, and the standard decontamination process can be time-consuming, not always effective, and possibly hazardous to workers due to its strenuous manual nature. The HEAL-GB team developed two new systems — one using suction, and the other using a bath or submersion — to more efficiently and safely decontaminate gloveboxes and other contaminated metal components.



Parts of a glovebox hood cleaning unit developed by the Los Alamos LDRD project that worked to find a new way to decontaminate PF-4 gloveboxes.

A growing team effort

Karmiol says that now that the LDRD portion of the project has wrapped, the team has received other funding to continue developing the technology for use, with the goal of applying it by the end of FY21. The progress over the past two years has been evident in the technology advancements made to the HEAL-GB system, but also in scope of the team itself. *(LA-UR-20-30290)*



This newsletter, published quarterly, features LDRD and SDRD work done by Lawrence Livermore, Los Alamos, Nevada National Security Site and Sandia. For additional issues, visit www.https://NNSA-LDRD.lanl.gov. This newsletter is approved for unlimited release. *(LA-UR-20-30372).*

For more information

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