LDRD Quarterly Highlights

Mission Agility | Technical Vitality | Workforce Development

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Lawrence Livermore National Laboratory

HIGHLIGHTS

Livermore team explores the source of asymmetries in ICF implosions

Scientists are now one step closer to understanding the gap between simulations and inertial confinement fusion (ICF) experiments conducted at LLNL's National Ignition Facility (NIF) due to LDRD-funded research aimed at analyzing experimental data to improve implosion performance.

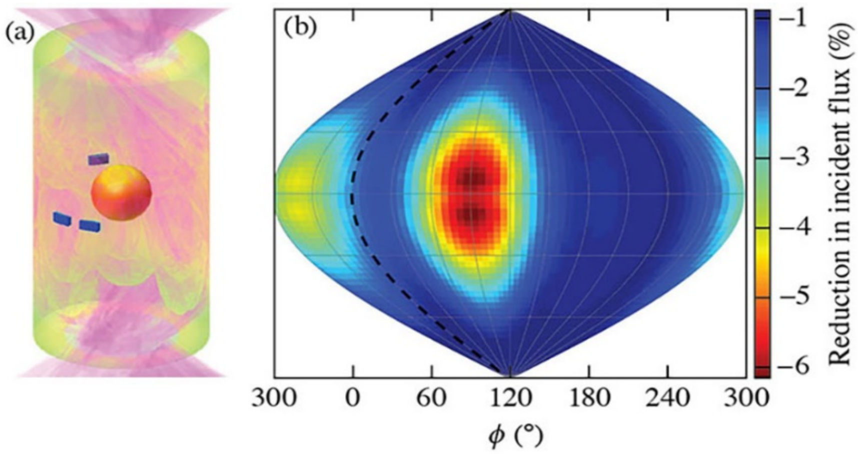
ICF experiments aim to ignite a propagating fusion burn wave in deuterium-tritium fuel. To achieve ignition, the fuel must reach a self-heating state in which the energy produced exceeds energy loss from expansion, thermal conduction, and radiative cooling.

The best-performing ICF implosions have begun to show the effects of fusion self-heating, but these experiments still underperform on 2D simulations.

By analyzing data from several years of high-yield ICF experiments, researchers found a correlation between the velocity of the hot-spot implosion and the asymmetry of fuel areal-density (the combined thickness and density of the imploding frozen fusion fuel shell).

"We know that asymmetry is a principal degradation factor of implosion performance," said LLNL physicist Dan Casey. "We found that 3D asymmetry does exist and is correlated between two key measurements. These results lay the foundation for subsequent work to track down the sources of the asymmetries."

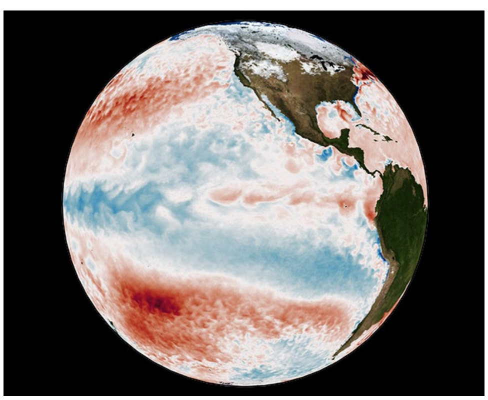
According to physicist Hans Rinderknecht, who conducted this work while serving as a Lawrence Fellow at LLNL, “We found that most of the implosions performed in the last three years at NIF had an unintentional asymmetry that ‘pushed’ the implosion to one side instead of imploding it uniformly, resulting in some wasted energy.”



LLNL researchers analyzed overlapping datasets to identify factors that may limit ICF implosion performance. The figure above illustrates their approach, depicting (a) a model of the capsule in a laser-irradiated hohlraum, with the typical size and position of diagnostic windows shown in blue; and (b) the calculated reduction of radiation flux on the capsule in a 3-window hohlraum, assuming complete radiation loss through the windows.

Using two overlapping datasets—hot-spot velocity versus density asymmetry—investigators started plotting them together, and “the shared pattern popped right out,” said Rinderknecht. “The two supporting datasets, from two different and independently vetted diagnostics, confirmed one another across so many shots with such different conditions that it became clear something real and significant was going on.” More information regarding the team’s findings related to ICF implosions can be found on LLNL’s website. *(LLNL-WEB-458451)*

Livermore researchers analyze natural variations to resolve a climate puzzle



Sea-surface temperature anomalies illustrating a La Niña event, which results in widespread warming of the atmosphere and ocean lasting several months. (Image courtesy of NOAA Coral Reef Watch.)

New research shows that naturally occurring climate variations help to explain a long-standing difference between climate models and satellite observations of global warming.

Satellite measurements of global-scale changes in atmospheric temperature began in 1978. Relative to most model simulations, satellite data has consistently shown less warming of Earth’s lower atmosphere, leading some researchers to conclude that climate models are too sensitive to greenhouse gas emissions, and thus are not useful for making future climate change projections. However, after analyzing hundreds of simulations from the newest global climate models, LLNL investigators recently discovered that the model-versus-satellite difference is largely driven by natural variations in the Earth’s climate.

“Natural climate variability has likely reduced the observed warming during the satellite-era,” said LLNL climate scientist Stephen Po-Chedley, who first joined LLNL as a Lawrence Fellow. Although it is well-known that natural variability can produce decade-long periods of subdued warming, this study demonstrated that it also can play an important role over 40-year timescales that are relevant to satellite records.

More information regarding the team’s climate science research can be found on LLNL’s website. *(LLNL-WEB-458451)*

Livermore team conducts earthquake simulations with the highest-ever resolution using the Lab's supercomputing resources

Geoscience experts at LLNL conducted supercomputer simulations of a magnitude 7.0 earthquake on a fault located near the Laboratory—representing the highest resolution ground motion simulations achieved to date for an event of this scale.

Investigators used the SW4 code developed at LLNL and Livermore's Sierra supercomputer to conduct the simulations. The simulations resolved rapidly varying shaking with broader band frequencies up to 10 Hz, doubling the resolution of previous runs. Seismic waves as short as 50 meters were resolved across a regional-scale domain. Previous simulations lacked the performance and memory to model such high-frequency motions over such a large domain.

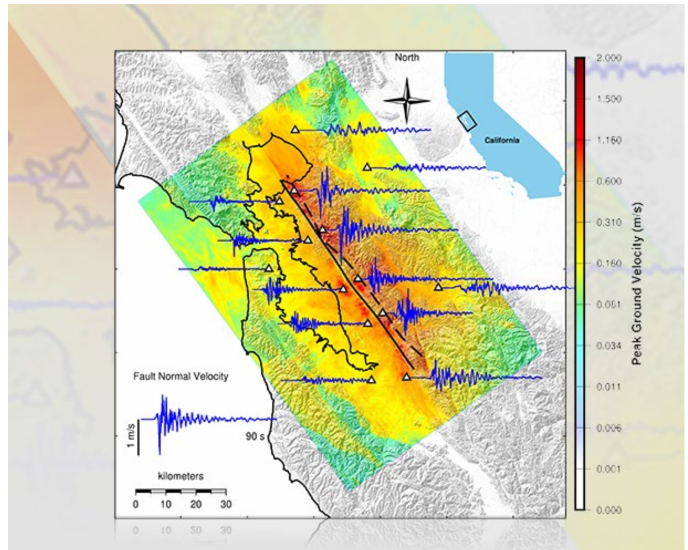


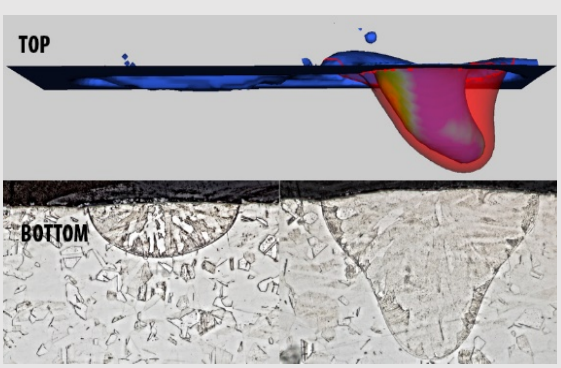
Illustration depicting the high-resolution simulations of seismic activity using LLNL's supercomputers. The figure depicts the simulated strength of shaking from a magnitude 7.0 earthquake showing peak ground velocity (colorbar) and seismograms (blue) at selected locations (triangles).

According to LLNL seismologist Arthur Rodgers, who led the LDRD-funded study, as computing power increases, such earthquake simulations will become easier and more accessible to scientists and engineers. These types of simulations can be used to evaluate shaking intensities at specific sites and model the response of engineered structures, enhancing our ability to evaluate potential seismic hazards and the risk of damage to our infrastructure.

More information regarding the team's seismic simulations using supercomputers can be found on LLNL's website. *(LLNL-WEB-458451)*

Livermore researchers measure electron emission to improve understanding of 3D laser-based metal printing

During an LDRD-funded project aimed at improving the reliability of 3D laser-based metal printing techniques, LLNL investigators measured the emission of electrons from the surface of stainless steel during laser processing, using a custom testbed system and a current preamplifier that measured the flow of the electrons. They captured thermionic emission signals to identify phenomena that can produce defects, advancing our understanding of laser-material interaction dynamics in this metal 3D printing technique. More information regarding this investigation of the use of thermionic emission sensing to detect laser-driven phenomena can be found on LLNL's website. (LLNL-WEB-458451)



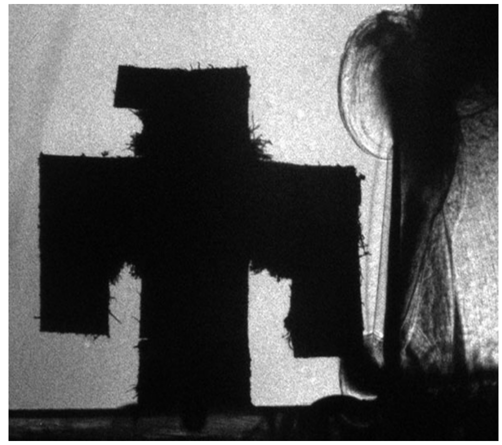
The top image shows a multi-physics simulation of laser-induced melting of stainless steel, showing the electron emission signal primarily produced at the front of the surface depression.
The bottom image depicts cross-sections of laser tracks produced in stainless steel. Monitoring of the thermionic emission can detect transition between conduction (left) and keyhole (right) mode-welding regimes.

Sandia National Laboratories

HIGHLIGHTS

Thin explosive films developed at Sandia provide snapshot of how detonations start

Using thin films—no more than a few pieces of notebook paper thick—of a common explosive chemical, Sandia researchers are studying how small-scale explosions start and grow.



An image from a test detonation of a thin explosive film, about as thick as a few pieces of notebook paper, with a thunderbird-shaped barrier the size of the thunderbird on Sandia business cards. The "shimmering" lines to the right of the thunderbird are the shock waves from the explosion, detected by schlieren imaging, a technique that can detect differences in air density. View the video. (Photo courtesy of Eric Forrest)

Sandia is the only lab in the U.S. that can make detonatable thin films like these for experiments that advance the fundamental knowledge of detonations. The gathered data improved a Sandia-developed computer-modeling program used by universities, private companies, and the Department of Defense to simulate how large-scale detonations initiate and propagate.

"It's neat, we're really pushing the limits on the scale at which you can detonate and what you can do with explosives in terms of changing various properties," said Eric Forrest, lead researcher on the project. "Traditional explosives theory says that you shouldn't be able to detonate at these length scales, but we've been able to demonstrate that, in fact, you can."

The research team shared their work studying characteristics of the thin films and the explosions they produce in two papers recently published in ACS Applied Materials and Interfaces and Propellants, Explosives, Pyrotechnics.

The team used PETN, also known as pentaerythritol tetranitrate, which is a bit more powerful than TNT, pound for pound. It is commonly used by the mining industry and by the military. Typically, PETN is pressed into cylinders or pellets for use. The research team instead used a method called physical vapor deposition—also used to make second-generation solar panels and to coat some jewelry—to "grow" thin films of PETN.

In collaboration with New Mexico Institute of Mining and Technology, the team developed a specialized setup, using schlieren imaging, to see the shock wave despite the smoke and debris from test explosions. The imaging technique can detect differences in air density similar to the way our eyes detect the shimmering of a hot highway.

Julio Peguero, now a Sandia employee, first started working on the project in 2018 as a mechanical engineering master's student from New Mexico Tech and then as a Sandia intern. He used data from the experiments to refine Sandia's explosives computer-modeling program. The program, called CTH, can be used for applications, such as determining how to best shape explosive charges while drilling for oil.

Peguero plotted the velocity of the shock waves above the films with and without gaps and adapted the computer program to better match the experimental results on very thin films. The team engineered thin films with cracks in the middle of various sizes—ranging from one-third the width of a human hair to 1 1/3 the width of a hair—to better understand the reliability of thin films and how detonations can fail. The team found that gaps around the size of a hair could stop a detonation from continuing.

The research was funded by Sandia's Laboratory Directed Research and Development program. *(SAND2021-1226 E)*

Sandia scientists use 3D-printed rocks, machine learning to detect unexpected earthquakes

Sandia geoscientists used 3D-printed rocks and an advanced, large-scale computer model of past earthquakes, to understand and prevent earthquakes triggered by energy exploration.

Injecting water underground after unconventional oil and gas extraction, or fracking, geothermal energy stimulation and carbon dioxide sequestration all can trigger earthquakes. Of course, energy companies do their due diligence to check for faults—breaks in Earth's upper crust that are prone to earthquakes—but sometimes earthquakes, even swarms of earthquakes, strike unexpectedly.

Sandia geoscientists studied how pressure and stress from injecting water can transfer through pores in rocks down to fault lines, including previously hidden ones. They also crushed rocks with specially engineered weak points to hear the sound of different types of fault failures, which will aid in early detection of an induced earthquake.

To study different types of fault failures and their warning signs, Sandia geoscientist Hongkyu Yoon needed a bunch of rocks that would fracture the same way each time he applied pressure—similar to the pressure caused by injecting water underground. Natural rocks collected from the same location can have vastly different mineral orientation and layering, causing different weak points and fracture types.

Several years ago, Yoon started using additive manufacturing, or 3D printing, to make rocks from a gypsum-based mineral under controlled conditions, believing that these rocks would be more uniform. To print the rocks, the team sprayed gypsum in thin layers, forming 1-by-3-by-0.5 inch rectangular blocks and cylinders. As he studied the 3D-printed rocks, Yoon realized that the printing process also generated minute structural differences that affected how the rocks fractured. This piqued his interest, leading him to study how the mineral texture in 3D-printed rocks influences how they fracture.

"It turns out we can use that variability of mechanical and seismic responses of a 3-D printed fracture to our advantage to help us understand the fundamental processes of fracturing and its impact on fluid flow in rocks," Yoon said. This fluid flow and pore pressure can trigger earthquakes.

For these experiments, Yoon and collaborators at Purdue University made a mineral ink using calcium sulfate powder and water, printed a layer of hydrated calcium sulfate about half as thick as a sheet of paper, and then applied a water-based binder to glue the next layer to the first. They printed the same rectangular and cylindrical gypsum-based rocks with some layers running horizontally, and others vertically. They also changed the direction in which they sprayed the binder to create more variation in mineral layering, and then squeezed the samples until they broke. When they examined the fracture surfaces using lasers and an X-ray microscope, they noticed the fracture path depended on the direction of the mineral layers.

Sandia geoscientist Hongkyu Yoon holds a fractured 3D-printed rock. He squeezed 3D-printed rocks until they cracked and listened to the sound of the rocks breaking to identify early signs of earthquakes.

They also monitored acoustic waves coming from the printed samples as they fractured, which indicated signs of rapid microcracks. Afterward, they combined the sound data with machine-learning techniques that can identify patterns in seemingly unrelated data to detect signals of minute seismic events.

After analyzing a surprise earthquake at a geothermal simulation site in Pohang, South Korea, Sandia geoscientist Kyung Won Chang said he needed to consider more than the stress of water pressing on the rocks. In addition to that deformation stress, his complex computational model also needed to account for how that stress transferred to the rock as the water flowed through pores in the rock itself.

The team plans on applying and scaling up machine-learning algorithms to detect previously hidden faults and identify signatures of geologic stress that could predict the magnitude of a triggered earthquake. In the future, they hope to use those stress signatures to create a map of potential hazards for induced earthquakes across the United States. Within five years they hope to apply many different machine-learning algorithms to identify signals of seismic events faster and more accurately than conventional monitoring systems. View the video (all video footage was taken prior to the COVID-19 pandemic.)

Kyung Won's research effort, as well as Yoon's initial work, were funded by Sandia's Laboratory Directed Research and Development program. (*SAND2021-3279 O)*

New Sandia study on submarine permafrost suggests locked greenhouse gases are emerging

Something is lurking beneath the Arctic Ocean. While it's not a monster, it has largely remained a mystery. According to 25 international researchers who collaborated on a first-of-its-kind study, frozen land beneath rising sea levels currently traps 60 billion tons of methane and 560 billion tons of organic carbon. Little is known about the frozen sediment and soil—called submarine permafrost—even as it slowly thaws and releases methane and carbon that could have significant impacts on our climate.

To put into perspective the amount of greenhouse gases in submarine permafrost, humans have released about 500 billion tons of carbon into the atmosphere since the Industrial Revolution, said Sandia geosciences engineer Jennifer Frederick, one of the authors of the study published in IOP Publishing journal Environmental Research Letters.

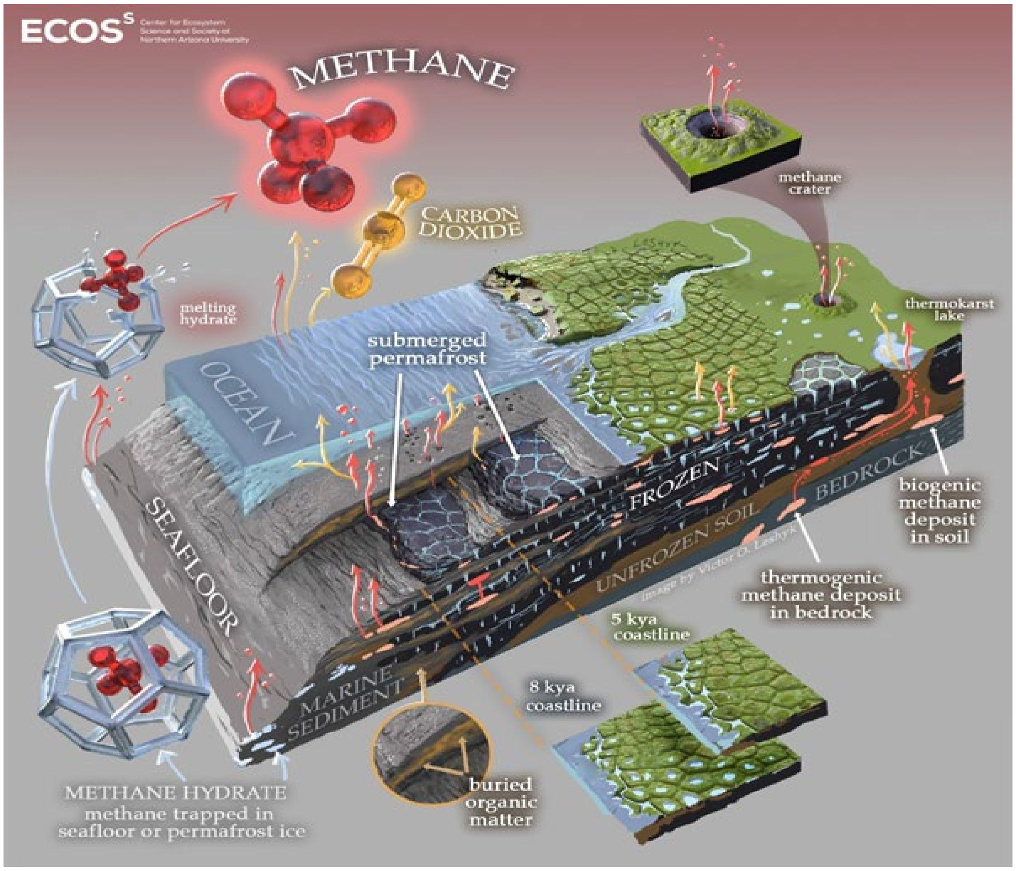
While researchers predict that submarine permafrost is not a ticking time bomb and could take hundreds of years to emit its greenhouse gases, Frederick said submarine permafrost carbon stock represents a potential giant ecosystem feedback to climate change not yet included in climate projections and agreements.

"It's expected to be released over a long period of time, but it's still a significant amount," she said. "This expert assessment is bringing to light that we can't just ignore it because it's underwater and we can't see it. It's lurking there, and it's a potentially large source of carbon, particularly methane."

The study, conducted through an expert assessment, sought answers to several central questions: What is the current extent of submarine permafrost? How much carbon is locked in submarine permafrost? How much has been and will be released? And, what is the rate of release into the atmosphere? The participating experts answered questions using their own scientific skills, which included modeling, data analysis, or literature synthesis.

Frederick, one of the original advocates of the study, has been modeling submarine permafrost for almost 10 years and answered the questions through the lens of her research, which is primarily in numerical modeling. She said she uses published material for model inputs or works directly with researchers who visit the Arctic and provide datasets.

"I hope this study begins to unite the research community in submarine permafrost," said Frederick. "Historically, it's not only been a challenging location to do field work and make observations, but language barriers and other obstacles have challenged international scientific progress in this area."



This artistic diagram of the subsea and coastal permafrost ecosystems emphasizes greenhouse gas production and release. (Artwork by Victor Oleg Leshyk, Northern Arizona University.)

The team estimates that submarine permafrost has been thawing since the end of the last glacial period 14,000 years ago, and currently releases about 140 million tons of carbon dioxide and 5.3 million tons of methane into the atmosphere each year. This represents a small fraction of the total human-caused greenhouse gas emissions per year, about the same yearly footprint as Spain.

Modern greenhouse gas releases are predominantly a result of the natural response to deglaciation, according to the study. Experts suggest that human-caused global warming may accelerate greenhouse gas release, but due to lack of research and uncertainties in this area, determining causes and rates of the release will remain unknown until better empirical and modeling estimates are available.

Almost every expert involved in the study mentioned the permafrost knowledge gap, which makes it harder for scientists to anticipate changes and reduces the reliability of estimates of carbon pools and fluxes, as well as the thermal and hydrological conditions of permafrost. Frederick said that while there is a wealth of ongoing research on terrestrial permafrost, submarine permafrost hasn't been taken on like this before, and hasn't been the subject of nearly as much international collaboration.

The amount of carbon sequestered or associated with submarine permafrost is relevant when compared to the amount of carbon in terrestrial permafrost and what's in the atmosphere today. "This is an example of a very large source of carbon that hasn't been considered in climate predictions or agreements," she said.

Her work on the study was funded by the Laboratory Directed Research and Development program, which enables Sandia scientists and engineers to explore innovative solutions to national security issues. The program serves in part as a proving ground for new concepts in research and development and fosters scientific discovery to propel the Labs' missions. *(SAND2021-0523 E)*

Early career researcher at Los Alamos leads successful effort to sharpen our picture of activity on Earth

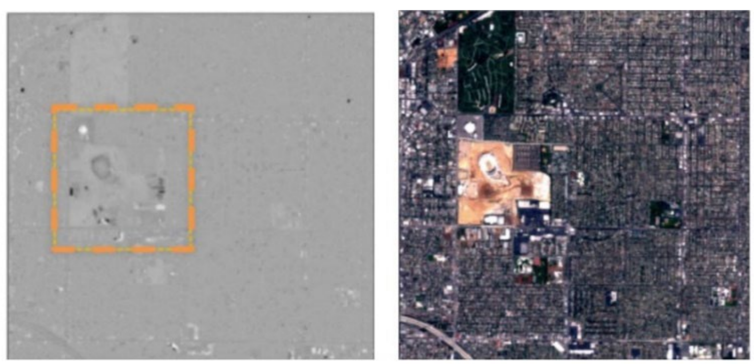
The ability to accurately detect changes to Earth's surface using satellite imagery can aid in everything from climate change research and farming to human migration patterns and nuclear nonproliferation. But until recently, it was impossible to flexibly integrate images from multiple types of sensors—for example, sensors that show surface changes (such as new building construction) versus sensors that show material changes (such as water giving way to sand). Now we can, thanks to LDRD early career researcher Amanda Ziemann, her team, and their new algorithmic capability—and in doing so, we obtain a more frequent and complete picture of what's happening on the ground.

Watch this video to learn how observing the construction of the new Los Angeles Rams Stadium provided information that may be useful to national security.

Ziemann's team developed a flexible mathematical approach to identify changes in satellite image pairs collected from different satellite modalities, or sensor types that use different sensing technologies, allowing for faster, more complete analysis. It's easy to assume that all satellite images are the same and, thus, comparing them is simple. But the reality is quite different. Hundreds of different imaging sensors are orbiting the Earth right now, and nearly all take pictures of the ground in different ways.

To test their method, the team looked at images of the construction of the new Rams stadium in Los Angeles starting in 2016. They began by comparing images from various multispectral sensors, as well as synthetic aperture radar (SAR) images, over the same date range to see which modalities picked up which changes. For example, in one case, the roof of a building beside the stadium was replaced, changing from beige to white over several months. The multispectral imaging sensors detected this change because it was related to color and material. However, SAR did not detect the change, as they expected. In addition, they determined that SAR was highly sensitive to surface deformation due to moving dirt piles, whereas multispectral imagery was not.

When they integrated the images using their new algorithmic capability, they were able to see both types of changes—surface and material—at a much faster rate than if they had focused on a single satellite. This had never been done before at scale, and it signals a fundamental shift in how satellite imagery is analyzed.



The left image depicts a change-detection map of the construction of the Rams Stadium in Los Angeles over the course of three years derived from Sentinel-1 SAR (synthetic aperture radar) and Sentinel-2 multispectral imagery. The image on the right is a Sentinel-2 true-color composite of the same area. The black marks on the change-detection map show unusual changes; gray indicates common changes; and white illustrates persistent anomalies. Sentinel-1 and Sentinel-2 are Earth-observing satellites operated by the European Space Agency (ESA). Image credit: LANL (left), ESA (right)

Geospatial change detection using heterogeneous satellite data streams has been a longstanding challenge in the science and national security communities. Ziemann's LDRD project that concluded in FY20 was a success, demonstrating fundamental results for multi-sensor anomalous change detection. The doors opened from these results are significant, allowing for the potential to use any and all available satellite imagery when, for example, rapidly responding to an unexpected event.

Work performed by Amanda Ziemann was supported by the LANL-LDRD program via project 20180529ECR *(LA-UR-21-22322)*.

Read more: https://www.space.com/satellite-imagery-advance-expert-voices

Researchers at Los Alamos develop a new Artifical Intelligence tool that makes vast data streams intelligible and explainable

[Making sense of vast streams of big data]() is getting easier, thanks to an artificial-intelligence tool developed at Los Alamos National Laboratory. SmartTensors sifts through millions of bytes of diverse data to find the hidden features that matter, with significant implications, ranging from health care to national security, climate modeling to text mining, and many other fields.

The SmartTensors software was developed under a current Los Alamos LDRD project (20190020DR) led by Boian Alexandrov and titled, "Tensor Networks: Robust Unsupervised Machine Learning for Big-Data Analytics" *(LA-UR-21-21940).*

The SmartTensors tool developed by Los Alamos LDRD researchers can sort through massive data streams to find key features, making the data understandable. Image credit: Newswise

New fabrication method at Los Alamos paves way to large-scale production of perovskite solar cells

A new, simpler solution for fabricating stable perovskite solar cells overcomes the key bottleneck to large-scale production and commercialization of this promising renewable-energy technology, which has remained tantalizingly out of reach for more than a decade.

"Our work paves the way for low-cost, high-throughput, commercial-scale production of large-scale solar modules in the near future," said LDRD researcher Wanyi Nie, who is the corresponding author of the paper, which was recently [published in the journal Joule](). "We were able to demonstrate the approach through two mini-modules that reached champion levels of converting sunlight to power with greatly extended operational lifetimes. Since this process is facile and low cost, we believe it can be easily adapted to scalable fabrication in industrial settings."

Perovskite photovoltaics, seen as a viable competitor to the familiar silicon-based photovoltaics on the market for decades, have been a highly anticipated emerging technology over the last decade. Commercialization has been stymied by the lack of a solution to the field's grand challenge: scaling up production of high-efficiency perovskite solar cell modules from the bench-top to the factory floor.

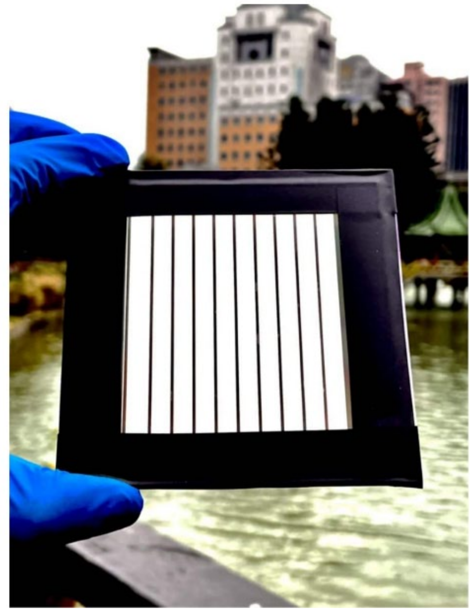
The team, in collaboration with researchers from National Taiwan University (NTU), invented a one-step spin coating method by introducing sulfolane as an additive in the perovskite precursor, or the liquid material that creates the perovskite crystal through a chemical reaction. As in other fabrication methods, that crystal is then deposited on a substrate.

The new process allowed the team to produce high-yield, large-area photovoltaic devices that are highly efficient in creating power from sunlight. These perovskite solar cells also have a long operational lifetime.

Through a simple dipping method, the team was able to deposit a uniform, high-quality perovskite crystalline thin film covering a large active area in two mini-modules, one of about 16 square centimeters and the other nearly 37 square centimeters. Fabricating uniform thin film across the entire photovoltaic module's area is essential to device performance.

The mini modules achieved a power conversion efficiency of 17.58% and 16.06%, respectively—among the top reported to date. The power conversion efficiency is a measure of how effectively sunlight is converted into electricity.

For other perovskite fabrication methods, one of the major roadblocks to industrial-scale fabrication is their narrow processing window, the time during which the film can be laid down on the substrate.



LANL's mini perovskite photovoltaic module has an active area of 36.6 cm2.

To get a uniform crystalline film that's well bonded to the layer below it, the deposition process has to be strictly controlled within a matter of seconds.

Using sulfolane in the perovskite precursor extends the processing window from 9 seconds to 90 seconds, forming highly crystalline, compact layers over a large area while being less dependent on the processing conditions.

The sulfolane method can be easily adapted to existing industrial fabrication techniques, which helps to pave the path toward commercialization.

Work performed by Wanyi Nie and Shreetu Shrestha was supported by the LANL-LDRD program via project 20180026DR *(LA-UR-21-22266)*.

A perovskite is any material with a particular crystal structure similar to the mineral perovskite. Perovskites can be engineered and fabricated in extremely thin films, which makes them useful for solar photovoltaic cells.

DOE investments in solar energy and perovskites in the news

The Hill (Budryk) reported in March that Secretary of Energy Jennifer Granholm announced that DOE is aiming to cut solar energy costs "by 60 percent by 2030." In addition, Sec. Granholm "announced a further $128 million in funding aimed at cutting the cost of deploying solar energy and hastening development." According to the article, the announcement "includes concentrating solar-thermal power (CSP) projects, which capture heat from sunlight and use the energy to power engines or turbines." Another $25 million, will go to "demonstrating a next-generation CSP power plant constructed by Sandia National Laboratories."

> *"DOE will put another $40 million toward research and development of perovskites, splitting the $40 million among 22 perovskite development projects."*

Axios (Geman) reported in late March that DOE is "targeting solar costs of 3 cents per kilowatt-hour by 2025" and "2 cents by 2030." According to the article, it "replaces a prior goal of hitting that 3-cent target by 2030 and comes as costs have already been coming down for years." In addition, DOE "announced roughly $128 million in new funding for various solar efforts, including $40 million for various outside R&D and performance validation initiatives for technologies that use a family of materials called **perovskites**." These efficiencies bring DOE in the same range as commercially available multi-crystalline silicon solar cells.

SDRD
SITE-DIRECTED RESEARCH & DEVELOPMENT
HIGHLIGHTS

NNSS plumbs the bright side of dark-field x-ray microscopy

Material defects affect a material's properties and performance under extreme conditions, and defect behavior at the onset of plasticity can now be visualized by deploying dark-field x-ray microscopy (DFXM) imaging techniques at x-ray facilities. An SDRD project team is developing a statistical analysis approach for DFXM imagery to characterize and quantify defect behavior and optimize the parameters of compound refractive lenses (CRLs) for alignment with the x-ray beam.

Dislocations Quantified

Recent developments in DFXM help us measure the detailed structure of crystalline materials with high sensitivity, presenting opportunities for dynamic compression. As DFXM images crystalline materials along their diffraction peaks, it maps the strain and lattice tilt, providing detailed maps of grain boundaries, dislocations, twins, and stacking faults deep inside crystals. In order for a new ultrafast DFXM (uDFXM) technique to be developed and fully adapted to shock physics, as part of a project led by Lawrence Livermore National Laboratory, NNSS is developing associated analytical methods and mathematical calibration and alignment tools, enabling the first experiments with uDFXM to directly measure how defects initiate large-scale deformations in materials.

Dislocations, a type of edge defect, are found in aluminum crystals. One focus of this project has been the development of analytic tools to identify and track dislocations from the initial aluminum experiments at the European Synchrotron Radiation Facility (ESRF). Dislocations appear in uDFXM images as bright/dark region pairs. Their behavior can be quantified by identifying them within frames, as well as tracking them through frames. Stationary wavelet transforms were implemented to extract the bright region of each dislocation and to inform a fast marching method to extract the corresponding dark region.

A series of image processing steps was subsequently applied to obtain the full object of interest, each of which was unambiguously identified and tracked with application of a Kalman filter coupled with a Munkres assignment, allowing for collection of relevant statistics. The accompanying figure shows the resulting statistical characterization of the glide and climb axis movement of tracked defects for an ESRF experiment on an aluminum crystal.

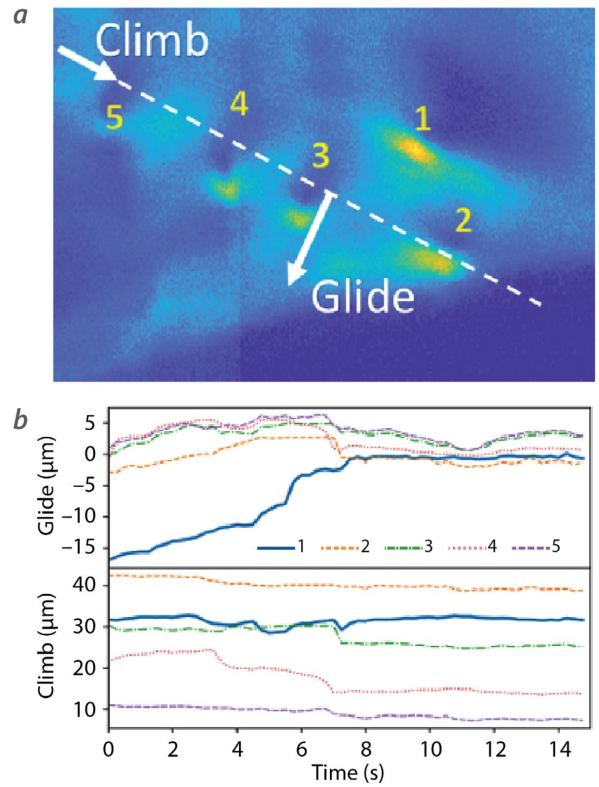


Figure depicting statistical characterization of experiment. (a) A uDFXM image subset from an ESRF experiment with five labeled dislocation defects at one point in time, with the glide and climb and climb planes annotated. (b) Plots of the glide and climb locations through time for each of the five dislocations, as tracked with our analytic methods.

Automated CRL Alignment

A second focus of this project is designing an automation for CRL alignment. Manual alignment requires approximately 100 to 5,000 sampling measurements, corresponding to ~1 to 4 hours per lens, usually once per day during beamtime shifts. The NNSS team automated this process using a downhill simplex optimization approach. The approach was then extended to accommodate beam instability observed at x-ray free-electron lasers (XFELs) and other optical sources such as high-energy lasers.

These newly developed, high-energy XFELs now provide the opportunity for uDFXM to image defects at the native timescales over which they form when externally driven. With uDFXM and specialized analytical methods, we can measure how the lattice deforms in the first nanosecond of a shock wave and obtain data to study the defect dynamics that cause the onset of plasticity.

These data will inform a century of untested theoretical models that predict how these nanometer-sized defects initiate large-scale transformations, with mechanisms that may differ because of crystal size, conditions, and grain boundaries. *(DOE/NV/03624--1037)*

NNSS designs new lab apparatus for studying particle-laden supersonic gas flows

An SDRD team is building a capability to support modeling of radio frequency (RF) emissions and high-explosives particulate evolution in a controlled environment using a shock tube and well-characterized particulates. The shock tube overpressure apparatus (STOA) is a revised design housed in a dedicated new anechoic chamber at the NNSS Special Technologies Laboratory. Along with associated diagnostics and software, this system will help experimenters understand the contributions that carbonaceous detonation soot makes to RF and optical signatures. It will also support millimeter-wave radio frequency attenuation studies through dynamic particle plumes.

The revised STOA design is particularly focused on reducing contamination from previously released particulates in the chamber and will provide more efficient filtration and venting of pressurized gas. Additional design work will refine in-nozzle sample delivery by positioning small sample quantities above the nozzle/vent to optimize inter-particle charging and to more rapidly introduce particles into the standing shock wave that appears above the vent. Simulations of dynamic pressure and velocity were performed to determine the suitability of proposed nozzle designs, several of which will be 3D-printed and tested in the STOA.

Using new analysis tools developed under this SDRD in FY 2020, comparison between readily diagnosable shock tube experimental results and Lawrence Livermore National Laboratory (LLNL) hydrodynamic and electrostatic simulations were made. This comparison demonstrated that shock tube experiments replicate essential aspects of shock phenomena in a high-explosives fireball and can be used to inform and validate models.

To improve analysis of RF and optical shock tube data, MATLAB code was written and used to analyze data collected in 2019. This analysis supported LLNL models of hydrodynamic and electrostatic behavior of particulates in shock waves. Software was also developed to determine ultraviolet-visible-near-infrared light transmission through a cloud of diamond particles (of varying size) using Lorentz dispersion and modified Mie attenuation models. Detonation soots varying from mostly graphitic to ~50% diamond:graphitic mixtures are being acquired and will be tested in the STOA in FY 2021.

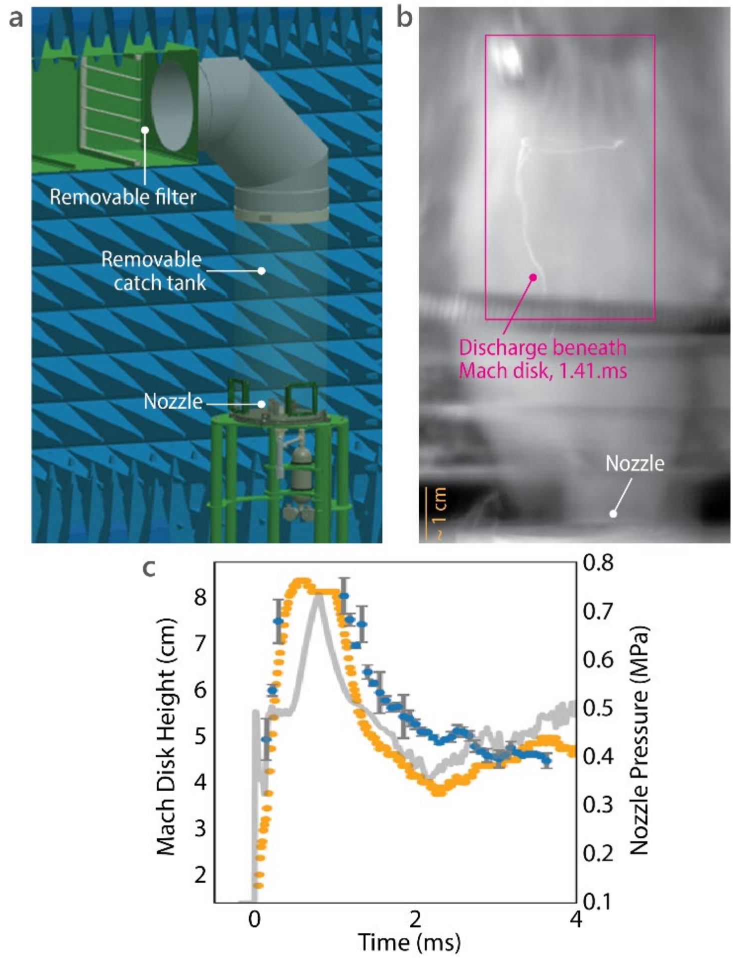


Figure depicting experimental work, done in collaboration with Lawrence Livermore National Laboratory. (a) STOA design in anechoic chamber (ducting to exterior not shown). (b) image of ring-shaped and vertical discharge constrained by standing shock wave (Mach disk). (c) Mach disk height above nozzle in experiment (blue) vs. LLNL simulation (yellow-orange), and nozzle pressure (gray).

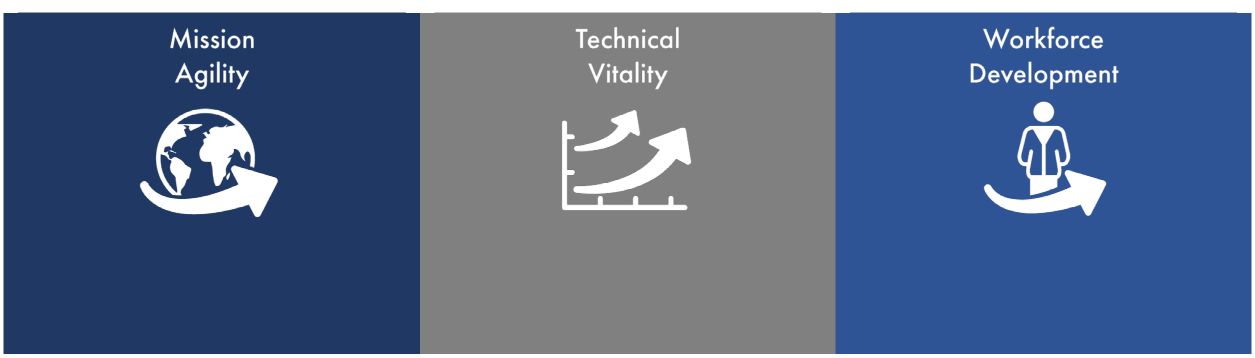
The University of Oregon will provide Faraday cups to measure particle charge. They are studying particle-to-particle charging on diamond, graphite, and raw Comp B detonation soot using fluidized beds and vibrating ramps.

From the Laboratory to the Field

Models are required for improved discrimination of signatures associated with hydrodynamic tests related to weapons development vs. other types of high-explosive test activities. Field experiments do not allow for direct viewing of aspects of shock-contained particulate clouds, are costly, and separation of innumerate variables from observed signatures is difficult.

This work provides a lab-scale platform, diagnostics and software to reproduce, record and allow for analysis of essential hydrodynamic and electrostatic phenomena. It will improve insight into, and provide direct validation of, shock phenomena models associated with high-explosive tests. During FY 2021, controlled tests with carbonaceous detonation soots will help to further identify and validate underlying physics mechanisms associated with electromagnetic emissions and particulate evolution.

A paper describing this project—Von der Linden, J., C. Kimblin, I. McKenna, et al., submitted 2021, "Standing shock regulates sparks in explosive flows"—was submitted to *Nature Research's: Communications Earth and Environment* and is under review. *(DOE/NV/03624--1038)*



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-21-23340)*

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