



# Quarterly Highlights

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FY22 Q3

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## FEATURE STORIES

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### Getting a grip on wildfire

Last year marked the 10<sup>th</sup> anniversary of the Las Conchas wildfire, which burned 150,000 acres in and around Los Alamos, blackening the sky, threatening the Laboratory, and prompting the evacuation of the town. Wildfires across the country are larger, hotter, and more frequent than in the past, in part due to climate change and in part due to mismanagement. For over a century, humans have dealt with wildfires by putting them out, but this approach, it turns out, was misguided. The exclusion of fire from the landscape results in dangerous accumulations of combustible biomass, overgrown understories, and overpopulated canopies, all of which have paradoxically led to more out-of-control wildfires, posing severe threats to people, property and ecosystems.

Fire kills diseased plants, keeps down crowding, and recycles nutrients back into the soil—it is an integral part of forest ecology. Rather than attempting to exclude fire, land managers now look for ways to trade high-intensity wildfires for low-intensity controlled fires, mimicking the natural fires of eons past. Prescribed burning, as the practice is known, is a tool being used increasingly throughout the country to keep forests healthy and productive, help manage terrestrial carbon stores, and reduce the risk of catastrophic conflagration.



*In the mountains of Northern New Mexico and throughout the West, the summer months bring plumes of smoke and the question: Is that a wildfire, or a prescribed burn? Los Alamos is intimately familiar with both. The Cerro Grande wildfire, pictured here in May of 2000, began as a prescribed burn, but it got out of control and burned 43,000 acres in and around Los Alamos, causing an estimated billion dollars in property damage. More recently, in 2011, the record-breaking Las Conchas fire was ignited by a tree falling on a power line and burned over 150,000 acres in the Los Alamos area. (Photo courtesy of LANL)*

Prescribed burning must manage smoke and ensure safety while maximizing effectiveness, so it requires robust scientific guidance. Laboratory scientists are working along three avenues to improve prescribed burning in the West: building a science-based foundation of knowledge on which to base decisions, integrating fire models with other relevant models, and including the processes of climate change in fire management.

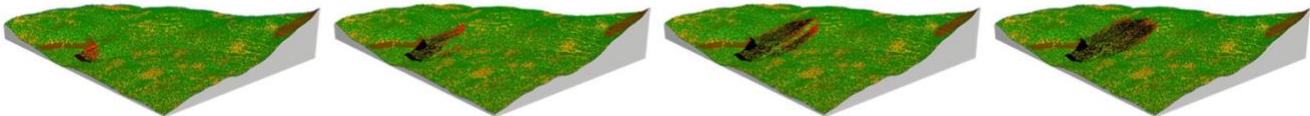
## Modeling tools

“Seasoned prescribed-burn practitioners have amazing intuition that comes from their extensive experience,” Los Alamos scientist Rod Linn explains, “but accelerating the learning curve for less experienced practitioners is important for the success of prescribed-fire practices.” Linn and his colleagues are building a science-based foundation of knowledge—a sort of database of different sets of conditions with known outcomes—that will help land managers and fire experts know what to expect in a given scenario, even if they have never seen it before. The database includes data from real fires as well as computer models—complementary sources of invaluable information that together enable the exploration of “what if” scenarios in new landscapes with evolving conditions.

### The composition of the forest affects the fire, and the fire affects the composition of the forest.

In collaboration with the United States Forest Service and Florida-based Tall Timbers Research Station, the Los Alamos team has developed a suite of computer models that are helping build the database and are being deployed in real-time fire-management situations. The first of these models was FIRETEC, which was designed to couple with a Los Alamos computational fluid-dynamics model called HIGRAD that models airflow over various terrains. The result is HIGRAD/FIRETEC, a coupled atmosphere-fire model based on physics principles such as conservation of mass, momentum, atomic species, and energy, that produces high-resolution, high-fidelity, 3D simulations of wildfires. The model has been used to explore how topography, fuel structure, and interactions between these factors drive fire behavior, and to study how fire severity is influenced by bark beetle outbreaks. HIGRAD/FIRETEC is useful not only for studying hypothetical scenarios, but also for working backwards from real-world fires to help explain their behavior and delineate cause-and-effect relationships.

However, because HIGRAD/FIRETEC runs on a Laboratory supercomputer, it’s not a field-deployable, real-time tool. To fill this niche, the scientists developed a laptop-capable, fast-running tool called QUIC-Fire. The Laboratory hosts a family of QUIC (Quick Urban & Industrial Complex) models, developed by physicist Mike Brown and his team, to model how airborne chemical, biological, and radiological agents are transported and dispersed around buildings. QUIC-Fire uses algorithms originally developed for other QUIC models, which makes it both fast and nimble.



*QUIC-Fire is the team’s field-deployable, real-time fire model designed for site-specific use by members of the fire community. This QUIC-Fire simulation, set in the Valles Caldera National Preserve near Los Alamos, illustrates how a hypothetical fire might progress under specific conditions. In the second frame, the fire splits into two paths, as a result of how the wind travels over the terrain. By the fourth frame the two paths have converged and the fire continues its spread up the hill. This kind of real-time information helps fire managers know what to expect so they can plan accordingly. (Graphic courtesy of David Robinson/LANL)*

“Careful choices were made to balance the need for accuracy and the tool’s usability by the fire community,” says Sara Brambilla, one of the lead developers of QUIC-Fire. “We now have a tool that brings in real terrain, evolving weather, and complex ignition patterns to simulate fire spread and smoke transport. And we can run it on a laptop.” Because QUIC-Fire can run hundreds or even thousands of simulations in a relatively short time, it is especially useful for exploring a wide range of outcomes for prescribed-fire scenarios and site-specific strategies.

As well as atmospheric and transport models, the team is also integrating ecology and hydrology computer models with their fire models. For example, vegetation is a strong driver of fire behavior, and accurately linking vegetation-specific effects to fire behavior is essential. Los Alamos scientists Adam Atchley and Turin Dickman are working on understanding how the moisture levels and distribution of fuels impact the spread of fire.

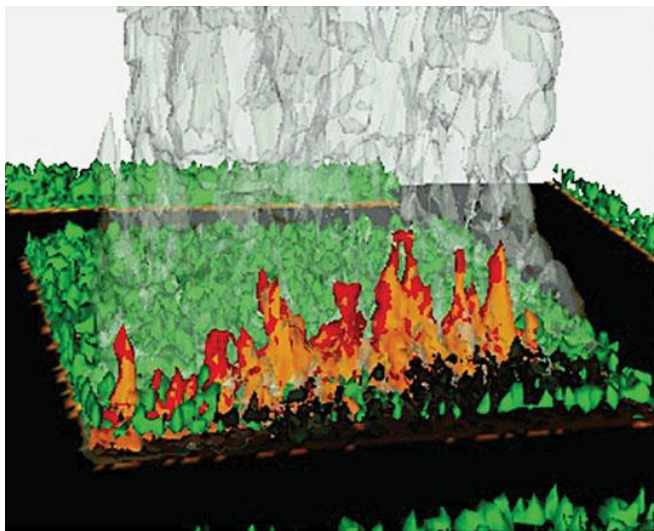
The parameters in fire models become moving targets when viewed through the lens of climate change.

“Better representations of the distribution and attributes of live vegetation will improve our ability to accurately model prescribed fires, which are more sensitive to small changes in these quantities than wildfires are,” explains Atchley. This is because wildfires typically occur under ideal conditions, when things are hottest and driest, while prescribed burns are deliberately done under marginal conditions when not everything will burn. Dickman adds, “Prescribed fire is about killing some plants to save others. The fire community is just starting to recognize the importance of plant-carbon and water cycles in fire behavior and post-fire plant survival, particularly for low-intensity burns.”

In other words, it’s not just about how the composition of the forest affects the fire, but also about how the fire affects the composition of the forest. Some plant species, like the lodgepole pine, thrive in post-fire environments and have evolved so that their seeds will only germinate after having gone through low-to-moderate intensity fire. Capturing the biophysical feedbacks between vegetation and fire means scientists can explore the influence of different forest treatments, as well as drought and other warming responses, on fire outcomes, including vegetation recovery or mortality.

### Fire forecast

But many of the parameters being included in the fire models—atmosphere, hydrology, vegetation, etc.—become moving targets when viewed through the lens of climate change. Longer summers with higher peak temperatures and lower precipitation can turn Western forests into tinderboxes. The Los Alamos team is using future climate projections to understand how climate change will impact land managers’ ability to put more low-intensity fire back onto the landscape. Atmospheric scientist Alex Jonko works with Atchley to study the climate-induced expansion and contraction of prescription windows—the range of conditions under which prescribed fires can be safely implemented.



*HIGRAD/FIRETEC is the team’s physics-based atmosphere-fire model, which runs on a supercomputer. It produces 3D simulations of fires, which are used to understand fire behavior in general. Here a HIGRAD/FIRETEC simulated fire (left) is compared to an actual experimental burn in the Northwest Territories of Canada (right). By combining simulation data with real-world data, scientists are building a foundation of knowledge that can help decision makers know what to expect in a variety of circumstances. (Graphic courtesy of LANL)*

Jonko explains, “Rising temperatures reduce the opportunities to burn during increasingly hot summers, and variable precipitation can lead to either drier or wetter fuels in the future, so we’re using information from climate models to evaluate how well current prescription windows might hold up.” Here in the West where the air is

already dry and the terrain can be treacherous, even a small change in these variables could necessitate substantial revision of current prescribed-fire practices.

The Laboratory's fire modeling team is also investing locally in wildfire-related projects. Local Native American communities have long understood that intentional fire is a way to keep the landscape resistant to extreme fire. To engage these communities, the fire modeling team set up a Wildfire Simulation and Visualization summer program and year-long internship targeted at Native American undergraduate students. Additionally, as Los Alamos itself is no stranger to wildfire, the team is working with the Laboratory's Wildland Fire Program to improve understanding and find ways to reduce fire risk across the Laboratory's 22,200 acres.

Longer fire seasons and more extreme fire behavior are the new norm. The prescription, it would seem, is to develop tools that can keep up with these changes to ensure safe communities and healthy forests. [View the article written by Eleanor Hutterer, 1663 Magazine](#)

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## Ground delivery goes green

Transportation is particularly difficult to make environmentally friendly. Electricity can be generated from dams, windmills, or solar cells instead of fossil fuels, but vehicles need a power source they can carry with them. And while charged batteries are suitable for lightweight, short-haul travel, they would be impractically heavy for larger vehicles or longer routes.



*Image of U.S. Interstate Highways courtesy of Stratosphere CC0, via Wikimedia Commons*

Fortunately, there's a promising middle ground: fuel cells. Fuel cells are essentially batteries that are refueled rather than recharged, and the fuel is clean-burning hydrogen. Los Alamos has been on the forefront of fuel-cell development since 1977, and that investment—widely recognized for its potential to replace hydrocarbon-fuel engines entirely—is paying great dividends. Already, high-efficiency fuel-cell vehicles are driving on the nation's roadways, mostly in California, where virtually all of America's 50 or so hydrogen refilling stations reside.

“Every fuel-cell vehicle in existence or under development depends on technology invented at Los Alamos,” says Laboratory scientist and fuel-cells program manager Rod Borup. The key lies in specialized, reaction-catalyzing materials for the fuel cell’s electrodes: the anode and cathode. Unlike a conventional battery, whose electrodes are relatively simple conductors with the energy stored in an ion-carrying electrolyte sandwiched between them, a fuel cell depends on porous electrodes to convey inflowing hydrogen (fuel) and oxygen (to react with) into controlled contact with the electrode catalysts and the electrolyte, while managing the outflow of the cell’s one and only waste product, water. The anode catalyzes the dissociation of H<sub>2</sub> molecules into electrons (which are sent along the circuit path to power the vehicle) and H<sup>+</sup> ions (which are routed through the chemical electrolyte). These two paths reconverge at the cathode, which catalyzes the process of making water from the hydrogen ions, oxygen, and the electrons arriving after completing the circuit.

President Biden has set a goal for the United States to reach net-zero greenhouse gas emissions by 2050 and at least a 50-percent reduction from 2005 levels by 2030. Doing this will require a substantial ramp-up of many green technologies, and Borup and his colleagues at Los Alamos and other Department of Energy (DOE) sites have teamed up to jumpstart the fuel-cell aspect. Success will require a massive investment in infrastructure for hydrogen production, transportation, and refilling stations comparable to existing gasoline-based infrastructure. How does one obtain a toehold on such a grand undertaking?

“With trucks, no question,” says Borup. “Semi-trucks have limited routes compared to passenger vehicles yet account for about a third of transportation-based emissions. So we can have a huge impact with a comparatively modest, truck-only initial investment. Besides, long-haul, heavy-duty transportation is where fuel cells really shine.” Los Alamos is contributing to the DOE’s Million Mile Fuel Cell Truck consortium to enable hydrogen fuel-cell technology to be dramatically scaled up beyond its current limited application in California, with ongoing research aimed at improving cost effectiveness and durability.

How impactful will success be, for emissions from trucks and subsequent fuel-cell vehicles, which might one day include ships and aircraft as well? Enormously impactful, it turns out. If the hydrogen is sourced using renewable power, it will cut greenhouse gas emissions to essentially zero—and this in the eco-resistant transportation sector! If the hydrogen is initially sourced from natural gas—widely recognized as a transition fuel to renewable power—the reduction would still be about 50 percent.

“If we’re serious about rising to the challenge of climate change, this is necessarily a big part of how we do it,” says Borup. “Nothing short of our future is at stake.” [View the article written by Craig Tyler, 1663 Magazine.](#)

(LA-UR-21-32363)

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## New laser-based volumetric additive manufacturing method can 3D print glass in seconds

Versatile and ubiquitous, glass is increasingly found in specialized applications such as fiber optics, consumer electronics and microfluidics for “lab-on-a-chip” devices. However, traditional glassmaking techniques can be costly and slow, and 3D-printing glass often results in rough textures, making them unsuitable for smooth lenses.

Using a new laser-based Volumetric Additive Manufacturing (VAM) [approach](#) — an emerging technology in near-instant 3D printing — researchers at [Lawrence Livermore National Laboratory](#) (LLNL) and the [University of California, Berkeley](#) have demonstrated the ability to 3D-print microscopic objects in silica glass, part of an effort

to produce delicate, layer-less optics that can be built in seconds or minutes. The results are reported in the latest edition of the journal [Science](#).

Nicknamed “the replicator” after the fictional device in “Star Trek” that can instantly fabricate nearly any object, the Computed Axial Lithography (CAL) [technology](#) developed by LLNL and UC Berkeley is inspired by computed tomography (CT) imaging methods. CAL works by computing projections from many angles through a digital model of a target object, optimizing these projections computationally and then delivering them into a rotating volume of photosensitive resin using a digital light projector. Over time, the projected [light](#) patterns reconstruct, or build up, a 3D light dose distribution in the material, curing the object at points exceeding a light threshold while the vat of resin spins. The fully formed object materializes in mere seconds — far faster than traditional layer-by-layer 3D printing techniques — and then the vat is drained to retrieve the part.



*Volumetric additive manufacturing microtubule structure demonstrating perfusibility. (Graphic courtesy of LLNL)*

Combining a new microscale VAM technique called micro-CAL, which uses a laser instead of an LED source, with a nanocomposite glass resin developed by the German company Glassomer and the University of Freiburg, UC Berkeley researchers reported the production of sturdy, complex microstructure glass objects with a surface roughness of just six nanometers with features down to a minimum of 50 microns.

UC Berkeley Associate Professor of Mechanical Engineering Hayden Taylor, the project’s principal investigator, said the micro-CAL process, which produces a higher dose of light and cures 3D objects faster and at higher resolution, combined with the nanocomposite resins characterized at LLNL proved a “perfect match for each other,” creating “striking results in the strength of the printed objects.”

“Glass objects tend to break more easily when they contain more flaws or cracks or have a rough surface,” Taylor said. “CAL’s ability to make objects with smoother surfaces than other 3D-printing processes is therefore a big potential advantage.”

The team compared the breaking strength of glass built with micro CAL against objects of the same size made by a more conventional layer-based printing process. The team found the breaking loads of CAL-printed structures were more tightly clustered together, meaning that researchers could have more confidence in the breaking load of CAL-printed components over conventional techniques.



LLNL co-author Caitlyn Krikorian Cook, a group leader and polymer engineer in the Lab's Materials Engineering Division, characterized the curing kinetics of the nanocomposite resin with light exposure. Printing higher-viscosity resins is challenging, if not impossible, with current traditional stereolithography systems at LLNL, Cook said, adding that the benefit of VAM for micro-optics is that it can produce extremely smooth surfaces without layering artifacts, resulting in faster printing without additional post-processing time.

"You can imagine trying to create these small micro-optics and complex microarchitectures using standard fabrication techniques; it's really not possible," Cook said. "And being able to print it ready-to-use without having to do polishing techniques saves a significant amount of time. If you can eliminate polishing steps after forming the optics — with low roughness — you can print a part ready for use."

*Researchers at Lawrence Livermore National Laboratory and the University of California, Berkeley demonstrated the ability to 3D-print microscopic objects in silica glass through volumetric additive manufacturing (VAM), part of an effort to produce delicate, layer-less optics that can be built in seconds or minutes. (Image courtesy of Adam Lau/Berkeley Engineering)*

Cook performed *in-situ* resin characterization with a spectrometer to measure the thresholding response of an inhibitor modifier in the material's photopolymerization kinetics. The modifier, combined with the preciseness of the laser VAM method, was the "secret sauce" to printing high-resolution optics at a microscale.

"By creating a thresholding response, we're able to significantly improve the resolution," Cook said. "We're taking advantage of the similar thresholding response reported in our previous [work](#), except we're implementing it in a different class of photopolymer chemistry. We're beginning to better understand the necessary kinetics for volumetric manufacturing."

For the past several years, the LLNL/UC Berkeley VAM collaboration has experimented with different resins and materials to create intricate objects. The latest advancement stems from a study with UC Berkeley to discover new classes of versatile materials that could expand the range of chemistries and material properties achievable through the VAM method.

Cook and the UC Berkeley researchers said VAM-printed glass could impact solid-glass devices with microscopic features, produce optical components with more geometric freedom and at higher speeds and could potentially enable new functions or lower-cost products.

Real-world applications could include micro-optics in high-quality cameras, consumer electronics, biomedical imaging, chemical sensors, virtual-reality headsets, advanced microscopes and microfluidics with challenging 3D geometries such as "lab-on-a-chip" applications (where microscopic channels are needed for medical diagnostics), fundamental scientific studies, nanomaterial manufacturing and drug screening. Plus, the benign properties of glass lend themselves well to biomaterials, or to cases with high temperature or chemical resistance, Cook added.

The Berkeley/LLNL team also is examining applications in bioprinting, such as fabricating organs or "lung-type" structures using a combination of VAM and projection micro-stereolithography.

At LLNL, Cook said she and her team will further tune the resolution of VAM and the doses required for variable range of resolutions and print speeds. Cook is continuing to support characterization and materials development, and Dominique Porcincula and Rebecca Walton, members of her Functional Architected Materials Engineering group, currently have a VAM feasibility study to advance the VAM glass printing efforts for larger optics.



“The challenge with printing glass is that the larger the part, the more significant the shrinkage stresses are when going from a green state to burning out the binder between the silica particles into a brown part to fusing the particles together into a fully dense glass part. Cracking problems typically arise in larger prints due to these shrinkage stresses,” Cook said. “Our teams at LLNL are developing custom formulations to produce larger optics and glass printed parts that will not crack during the de-binding and sintering processes.”

The latest [work](#) at LLNL was funded by the Laboratory Directed Research and Development (LDRD) [program](#).

Co-authors on the [Science](#) paper included lead author Joseph Toombs and Chi Chung Li of UC Berkeley, Manuel Luitz and Sophie Jenne of the University of Freiburg in Germany, and Bastian Rapp and Frederik Kotz-Helmer of Glassomer and the University of Freiburg.

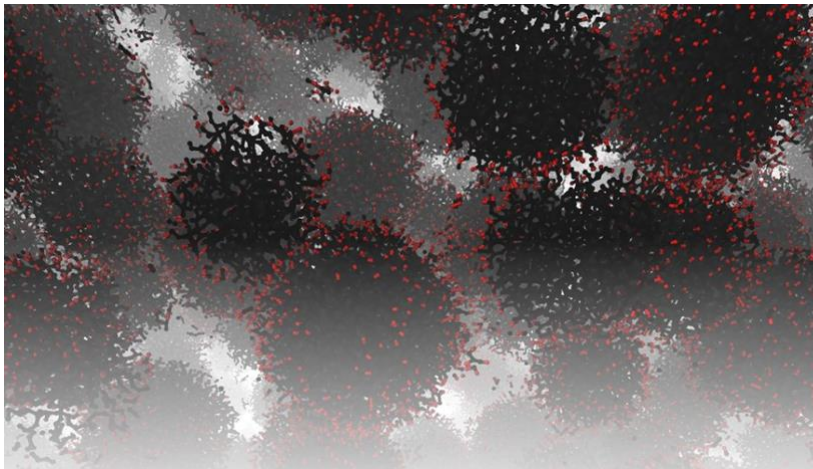
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## Paving the way to tailor-made carbon nanomaterials and more accurate energetic materials modeling at Lawrence Livermore Lab

Carbon exhibits a remarkable tendency to form nanomaterials with unusual physical and chemical properties, arising from its ability to engage in different bonding states. Many of these “next-generation” nanomaterials, which include nanodiamonds, nanographite, amorphous nanocarbon and nano-onions, are currently being studied for possible applications spanning quantum computing to bio-imaging. Ongoing research suggests that high-pressure synthesis using carbon-rich organic precursors could lead to the discovery and possibly the tailored design of many more.



To better understand how carbon nanomaterials could be tailor-made and how their formation impacts shock phenomena such as detonation, [Lawrence Livermore National Laboratory](#) (LLNL) scientists conducted machine-learning-driven atomistic simulations to provide insight into the fundamental processes controlling the formation of nanocarbon materials, which could serve as a design tool, help guide experimental efforts and enable more accurate energetic materials modeling.

*Oxygen-decorated liquid nanocarbon clusters predicted to form from shock compressed cryogenic liquid carbon monoxide. The snapshot, which is from machine-learning-driven atomistic simulations, shows only carbon (black) and oxygen (red) atoms participating in cluster formation and not the surrounding reactive fluid. (Image courtesy of Rebecca Lindsey/LLNL)*

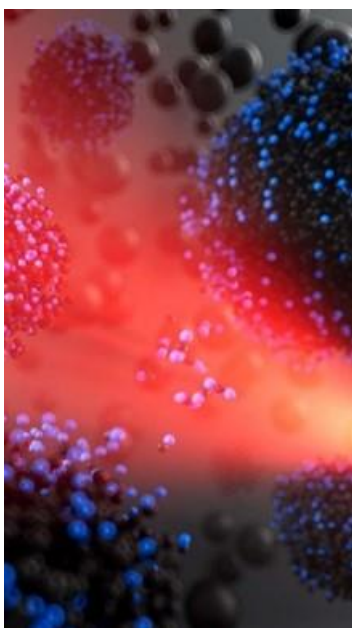
Laser-driven shock and detonation experiments can be used to drive carbon-rich materials to conditions of temperatures of the 1,000s of degrees Kelvin (K) and pressures of 10s of GPa (one GPa equals 9,869 atmospheres), under which complex processes lead to the formation of 2-10 nanometer nanocarbons within 100s of nanoseconds. However, the precise chemical and physical phenomena governing emergent nanocarbon formation under elevated pressure and temperature have not been fully explored yet, due in part to the challenges associated with studying systems at such extreme states.

Recent experiments on nanodiamond production from hydrocarbons subjected to conditions similar with those of planetary interiors offer some clues on possible carbon condensation mechanisms, but the landscape of systems and conditions under which intense compression could yield interesting nanomaterials is too vast to be explored using experiments alone.

The LLNL team found that liquid nanocarbon formation follows classical growth kinetics driven by Ostwald ripening (growth of large clusters at the expense of shrinking small ones) and obeys dynamical scaling in a process mediated by reactive carbon transport in the surrounding fluid.

“The results provide direct insight into carbon condensation in a representative system and pave the way for its exploration in higher complexity organic materials, including explosives,” said LLNL researcher Rebecca Lindsey, co-lead author of the corresponding paper appearing in [Nature Communications](#).

The team's modeling effort comprised in-depth investigation of carbon condensation (precipitation) in oxygen-deficient carbon oxide (C/O) mixtures at high pressures and temperatures, made possible by large-scale simulations using machine-learned interatomic potentials.



Carbon condensation in organic systems subject to high temperatures and pressures is a non-equilibrium process akin to phase separation in mixtures quenched from a homogenous phase into a two-phase region, yet this connection has only been partially explored; notably, phase separation concepts remain very relevant for nanoparticle synthesis.

The team's simulations of chemistry-coupled carbon condensation and accompanying analysis address longstanding questions related to high-pressure nanocarbon synthesis in organic systems. “Our simulations have yielded a comprehensive picture of carbon cluster evolution in carbon-rich systems at extreme conditions — which is surprisingly similar with canonical phase separation in fluid mixtures — but also exhibit unique features typical of reactive systems,” said LLNL physicist Sorin Bastea, principal investigator of the project and a co-lead author of the paper.

Other LLNL scientists involved in the research include Nir Goldman and Laurence Fried. The research was funded by [LLNL's Laboratory Directed Research and Development program](#).

*Artist's interpretation of reactive transport between liquid nanocarbon clusters predicted to form from shock compressed cryogenic liquid carbon monoxide. Small black and blue beads correspond to carbon and oxygen atoms respectively, and the red light is meant to evoke the laser used drive shock compression experiments. (Image courtesy of Brendan Thompson/LLNL)*

“Directly simulating ion transport across heterogenous interfaces remains technically challenging,” said LLNL materials scientist Stephen W Weitzner, lead author of the paper. “In many instances, we need to rapidly and accurately compare the effects of different environmental conditions on ion transport processes, but current simulation strategies can be too resource-intensive for high-throughput studies. So, we developed a set of dynamic metrics that provide a fast and intuitive way to compare the relevant chemical features.

“Our analysis showed that the new set of dynamic metrics not only correctly encoded key physical behavior, but also could explain trends in ion behavior that were challenging to classify using conventional static descriptors.”

Weitzner added that beyond aiding the description and discussion of ion transport kinetics, the metrics provide useful targets for the development of machine learning-based force fields that could dramatically accelerate future simulations of metal ion dissolution and transport rates without loss of accuracy.

Other Livermore researchers include Tuan Anh Pham, Christine Orme, S. Roger Qiu, and Brandon Wood. The work is funded by LLNL’s Laboratory Directed Research and Development [program](#).

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344 and was supported with Laboratory Directed Research and Development funding under Project 20-SI-004.

(LLNL-[WEB-458451](#))

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## NSS researchers advance wearable sensor technology to keep employees, partners performing optimally

The human body can know something’s awry at a cellular level up to 10 days before physical symptoms manifest.

Nevada National Security Site (NNSS) researchers are tapping into this phenomenon—through wearable sensor technology—to provide self-assessment tools to employees and partners in near real time if their bodies are in a heightened state.

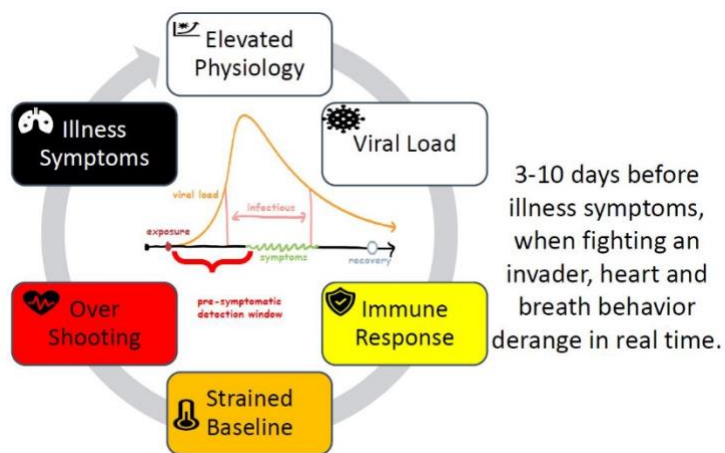


The human performance analytics program at the NNSS is advancing its capabilities in detecting fatigue and immune response to cardiorespiratory performance through the use of wearable sensors. The innovative sensors capture data at a physiological level while employees and partners are working out and sleeping and provides feedback for users to self-assess changes from individualized trend ranges of typical sleep and exercise levels.

When the rhythm variance increases in both heart and breath rates, they lose synchronization, decreasing stamina levels. This data visualization is being configured to be monitored in real time and can be measured during waking hours as well as during sleep.

*A GUI shows data collected from the sensors. (Image courtesy of NNSS project team)*

This technology could fill gaps in diagnostic capability in public hospitals, and assist where commercial off-the-shelf technology does not have the form factor or easily portrayed physiological parameters of interest. For example, NNSS researchers are exploring the technology’s potential to detect the onset of COVID-19 symptoms 72 hours before symptoms arise, and up to 10 days before.



Heart and breath behavior derange in measurable ways days before illness symptoms manifest. (Illustration courtesy of NNSS project team)

In recent months, the NNSS has strengthened its collaboration with federal partners on the implementation of the technology and is exploring other industry partnerships and commercial uses. Future development plans include research into how to make the sensors smaller, more lightweight and powerful.

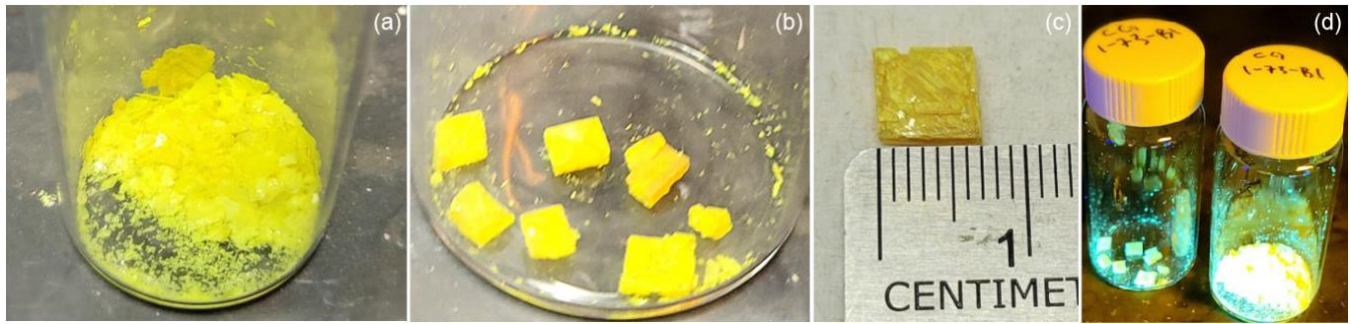
*(Per NNSS classification, this article is confirmed to be unclassified and approved for public release.)*

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## NNSS researchers create new scintillation materials with applications in both homeland security and cancer treatment

A team of researchers based in the NNSS Special Technologies Laboratory in Santa Barbara, California, is developing a dual-use technology that has the potential to contribute not only to the advancement of threat reduction science and technology but also to the development of a novel class of drugs that treat cancer. The research is funded by the SDRD program and conducted in collaboration with researchers from the Department of Chemistry at the University of California, Santa Barbara, and the Molecular Foundry at the Lawrence Berkeley National Laboratory in Berkeley, California. The objective of this research project is to develop a new class of scintillators for use as advanced materials that allow for better radiation detection and particle discrimination and as novel reagents that release antitumor agents in vivo for enhanced radiation therapy in cancer treatment.

The key to achieving this twofold objective is to create scintillation materials that can capture energy from high-energy particles and store this energy in the long-lived, lowest-energy excited molecular states via multiphoton events. In detector and imaging applications, they can be used where temporal separation methods are not practical for achieving a good neutron-gamma discrimination. With these scintillators, differences in energy deposition can be exploited for neutron-gamma differentiation, paving the way for a spectral, color-based approach for neutron-gamma discrimination. This approach could augment or replace existing methods that use digital pulse shape discrimination, requiring significant electronics for imaging applications. In cancer therapy applications, their long-lived excited molecular states make them particularly suitable for use in x-ray-induced photodynamic therapy for the treatment of deep tumors. The materials can be functionalized with organometallic compounds and used as sensitizers that drive the in vivo release of antitumor agents upon x-ray excitation in locations deep in the body.



Examples of compounds containing cuprous iodide cluster anions (a–d). They have been shown to be bright scintillators (emission efficiencies from optical excitation exceed 75%). Some of the large crystals are obtained directly from the synthesis procedure (b–d). (Photos courtesy of NNSS project team)

This two-year research project is in the second year, building on the work accomplished in FY 2021, which included developing a rational, iterative synthesis and analysis approach for creating scintillation materials suitable for use in these applications. A number of copper complex and gadolinium nanoparticle samples have been prepared and analyzed, and encouraging results have been obtained. Work planned for this year includes the investigation of two additional promising classes of compounds for their emission and scintillation properties.

*(Per NNSS classification, this article is confirmed to be unclassified and approved for public release.)*

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## LDRD Grand Challenge project could transform electronics, solve energy challenges

Like so many projects before it, this one started with some good questions. Arguably, too many.

The first question seemed simple enough: Could certain specialized fabrication techniques impact fields outside of quantum information science? But as soon as Sandia physicist Shashank Misra started to unpack it, he discovered a monster of a problem that was difficult to solve with a conventional research project.

“There were so many interwoven science questions that any regular [Laboratory Directed Research and Development](#) project might answer one or a few but wouldn’t reduce the overall risk because there wouldn’t be time to address the others,” Shashank said.

His idea was to take qubit fabrication methods originally developed by researchers in Australia, and later adopted by Sandia, for quantum computing and use these methods to make microelectronics.



The payoff could be huge — a fundamentally new way to build integrated circuits, power electronics and other semiconductor devices. New quantum microelectronics could potentially be as transformative as quantum computers and quantum sensors, and they could be a key to solving looming energy challenges.

“The power demand for electronics is going to outstrip the world’s capability for generating power, based on current trends,” said Paul Sharps, manager over Sandia advanced electronic and optoelectronic materials. “I think it’s very critical that we invest now in other sorts of electronic devices that significantly reduce power consumption.”

*Sandia’s Conrad James, left, Shashank Misra, center, and Paul Sharps present the first silicon wafer with circuits that combine devices made using atomic precision advanced manufacturing with industry-standard complimentary metal-oxide semiconductors. The wafer was produced at Sandia’s Microsystems Engineering, Science and Applications Complex. (Photo courtesy of Bret Latter/Sandia)*

## A Grand Challenge emerges

The toolkit Shashank wanted to use is called atomic precision advanced manufacturing, which he and others simply call APAM. It’s a collective term for technologies that let researchers control where individual atoms go in a device.

“The transistors involved in microelectronics for the last 40 years have used one form of physics,” said Conrad James, one of the Grand Challenge’s strategists and a former Grand Challenge principal investigator in his own right. “What APAM does is open up different physics to perform the switching in microelectronics, and that provides a wide range of opportunities for improvements in microelectronics, including reduced power consumption and new types of sensors.”

But Shashank said there were too many open questions to get the idea off the ground. Nobody was willing to fund their project ideas.

“The place where we ran into it headlong was when we would pitch application ideas where having atomic-scale control was really important. The push back was there were too many open science questions that could prevent having a significant impact. It was either that, or if we were to show in principle that having atomic-scale control opens up this opportunity space, there is no path to implement it in a way that works alongside current technologies. Up to that time nobody had shown that devices could work outside of a cryostat,” a machine that maintains ultra-low temperatures, Shashank said.

So, he changed his tack. Instead of jumping to applications, he decided to tackle some of the open science questions by pulling together a cross-disciplinary team — an approach perfectly suited for a Grand Challenge LDRD.

The FAIR DEAL Grand Challenge, short for Far-reaching Application, Implication and Realization of Digital Electronics at the Atomic Limit, ran from fiscal years 2019 through 2021.

With a team of 36 people over three years, Shashank aimed to answer three main questions: Can Sandia-developed atomic precision advanced manufacturing build a device that is compatible with CMOS, the industry-standard method of semiconductor manufacturing? Can it be accomplished in a practical environment (i.e., not at cryogenic temperatures)? Does the final product do anything special that a conventional device can’t?

Shashank never expected the answers would be yes, yes and yes.

“If somehow I had a genie grant me a wish at the beginning of the project, the truth is I would have wished for less,” he said.

“In any project this ambitious, you think about it in terms of triage,” he said. “What’s the off-ramp when A works, and B doesn’t work? What’s the off-ramp when it’s vice versa? I think the most surprising thing was, in general, there may be a lot of engineering difficulty, but there is no basic obstacle holding you back. The fact that all of those things were true was very surprising to me.”

### Creating new engineering opportunities

The FAIR DEAL team successfully built a microchip in which an APAM nanodevice worked directly in concert with a CMOS circuit built at the [Microsystems Engineering, Science and Applications Complex](#). Not only did the combined circuit work as planned, and at room temperature, but the team also demonstrated that APAM devices shouldn’t compromise the robustness of the microchip.

As FAIR DEAL began answering scientific questions, Shashank and his team were able to restart conversations about applying the manufacturing methods to specific uses. In 2021, a spin-off project began with DOE’s Advanced Manufacturing Office, aiming at developing what FAIR DEAL began for energy-efficient microelectronics.

Paul, who was a member of the Grand Challenge, said, “I saw that as a major step forward because I saw that as being recognition from an outside agency, not just Sandia, that’s willing to put money into something — that this is really key, that this is really a breakthrough. All the parts need to get put together, but enough things have been done to really tee that up for outside recognition and funding.”

Sandia has also begun several collaborations with university partners, and the team is in talks with potential sponsors about whether this new way of processing silicon could create opportunities to implement new kinds of hardware trust and security measures.

Shashank says that his team’s success has opened even more scientific questions that need to be studied.

“We have atomic-scale control over some elements in silicon,” he said. “And I think the science opportunities that other people are pursuing on the project at this point are looking at whether we can have atomic-scale control in every material. There’s a lot of thought that has to go into how you do that, but I do think that’s where the science is headed.”

(SAND2022-1967L)

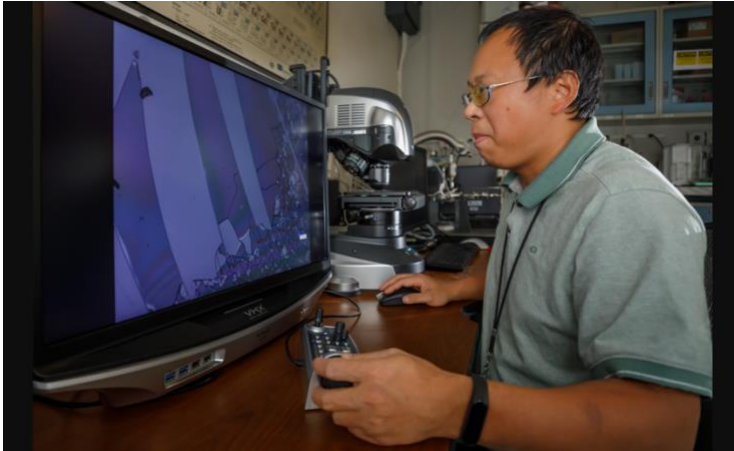
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## Seashell-inspired Sandia shield protects materials in hostile environments

Word of an extraordinarily inexpensive material, lightweight enough to protect satellites against debris in the cold of outer space, cohesive enough to strengthen the walls of pressurized vessels experiencing average conditions on

Earth and yet heat-resistant enough at 1,500 degrees Celsius or 2,732 degrees Fahrenheit to shield instruments against flying debris, raises the question: what single material could do all this?



*Sandia researcher Guangping Xu employs a digital optical microscope to examine the unusually hard coatings his lab has produced. The aim is better, cheaper protection of instruments and drivers in danger of fast-moving debris flung by Sandia's Z machine when it fires. The coatings offer many other possibilities as well. (Photo courtesy of Bret Latter/Sandia)*

The answer, found at Sandia National Laboratories, is sweet as sugar.

That's because it is, in fact, sugar — very thin layers of confectioners' sugar from the grocers, burnt to a state called carbon black, interspersed between only slightly thicker layers of silica, which is the most common material on Earth, and baked. The result resembles a fine layer cake, or more precisely, the organic and inorganic layering of a seashell, each layer helping the next to contain and mitigate shock.

“A material that can survive a variety of insults — mechanical, shock and X-ray — can be used to withstand harsh environmental conditions,” said Sandia researcher Guangping Xu, who led development of the new coating. “That material has not been readily available. We believe our layered nanocomposite, mimicking the structure of a seashell, is that answer.”

Most significantly, Xu said, “The self-assembled coating is not only lightweight and mechanically strong, but also thermally stable enough to protect instruments in experimental fusion machines against their own generated debris where temperatures may be about 1,500 C. This was the initial focus of the work.”

“And that may be only the beginning,” said consultant Rick Spielman, senior scientist and physics professor at the Laboratory for Laser Energetics at the University of Rochester, credited with leading the initial design of Sandia's Z machine, one of the destinations for which the new material is intended. “There are probably a hundred uses we haven't thought of.” He envisions possible electrode applications delaying, rather than blocking, surface electron emissions.

### Aiding the nuclear survivability mission

The coating, which can be layered on a variety of substrates without environmental problems, was the subject of a Sandia patent application in June 2021, an invited talk at a pulsed power conference in December 2021 and again in a recent [technical article](#) in MRS Advances, of which Xu is lead author.

The work was done in anticipation of the increased shielding that will be needed to protect test objects, diagnostics and drivers inside the more powerful pulsed power machines of the future. Sandia's pulsed-power Z machine — currently the most powerful producer of X-rays on Earth — and its successors will certainly require



still greater debris protection against forces that could compare to numerous sticks of dynamite exploding at close range.

“The new shielding should favorably impact our nuclear survivability mission,” said paper author and Sandia physicist Chad McCoy. “Z is the brightest X-ray source in the world, but the amount of X-rays is only a couple percent of the total energy released. The rest is shock and debris. When we try to understand how matter — such as metals and polymers — interacts with X-rays, we want to know if debris is damaging our samples, has changed its microstructure. Right now, we’re at the limit where we can protect sample materials from unwanted insults, but more powerful testing machines will require better shielding, and this new technology may enable appropriate protection.”



Other, less specialized uses remain possibilities.

*Physicist Chad McCoy at Sandia's Z machine loads sample coatings into holders. When Z fires, researchers will observe how well particular coatings protect objects stacked behind them. (Photo by Bret Latter)*

The inexpensive, environmentally friendly shield is light enough to ride into space as a protective layer on satellites because comparatively little material is needed to achieve the same resilience as heavier but less effective shielding currently in use to protect against collisions with space junk. “Satellites in space get hit constantly by debris moving at a few kilometers per second, the same velocity as debris from Z,” McCoy said. “With this coating, we can make the debris shield thinner, decreasing weight.”

Thicker shield coatings are durable enough to strengthen the walls of pressurized vessels when added ounces are not an issue.

### Dramatic cost reduction anticipated

According to Guangping, the material cost to fabricate a 2-inch diameter coating of the new protective material, 45 millionths of a meter and microns thick, is only 25 cents. In contrast, a beryllium wafer — the closest match to the thermal and mechanical properties of the new coating, and in use at Sandia’s Z machine and other fusion locations as protective shields — costs \$700 at recent market prices for a 1-inch square, 23-micron-thick wafer, which is 3,800 times more expensive than the new film of same area and thickness.

Both coatings can survive temperatures well above 1,000 C, but a further consideration is that the new coating is environmentally friendly. Only ethanol is added to facilitate the coating process. Beryllium creates toxic conditions, and its environs must be cleansed of the hazard after its use.

### How testing proceeded

The principle of alternating organic and inorganic layers, a major factor in seashell longevity, is key to strengthening the Sandia coating. The organic sugar layers burnt to carbon black act like a caulk, said Sandia manager and paper author Hongyou Fan. They also stop cracks from spreading through the inorganic silica structure and provide layers of cushioning to increase its mechanical strength, as was reported 20 years ago in an earlier Sandia attempt to mimic the seashell mode.

Greg Frye-Mason, Sandia campaign manager for the Assured Survivability and Agility with Pulsed Power, or ASAP, [Laboratory Directed Research and Development](#) mission campaign funding the research, initially had his doubts about the carbon insertion.

“I thought that the organic layers would limit applicability since most degrade by 400 to 500 C,” he said.

But when the carbon-black concept demonstrated robustness to well over 1,000 C, the positive result overcame the largest risk Frye-Mason saw as facing the project.

Seashell-like coatings initially tested at Sandia varied between a few to 13 layers. These alternating materials were pressed against each other after being heated in pairs, so their surfaces crosslinked. Tests showed that such interwoven nanocomposite layers of silica with the burnt sugar, known as carbon black after pyrolysis, are 80% stronger than silica itself and thermally stable to an estimated 1,650 C. Later sintering efforts showed that layers, self-assembled through a spin-coating process, could be batch-baked and their individual surfaces still crosslinked satisfactorily, removing the tediousness of baking each layer. The more efficient process achieved very nearly the same mechanical strength.

	Kevlar	Aluminum	Kapton	Spectra	Beryllium	Natural seashell	<u>Carbon black coating</u>
Hardness (Gpa)	N/A	1.25	0.3	7.6	1.7	3	>11
Elastic modulus (Gpa)	70-112	69	2.8	200	287	70	>120
Melting Temperature (degrees Celsius)	500*	660*	400*	150*	1,287*	600*	up to 1,650*

*Mechanical properties of representative high-strength materials versus natural seashell and Sandia-developed coating. (Graphic by Alicia Bustillos and data provided by Hongyou Fan and Guangping Xu)*

Research into the coating was funded by ASAP to develop methods to protect diagnostics and test samples on Z and on next-generation pulsed power machines from flying debris.

“This coating qualifies,” Frye-Mason said.

(SAND2022-5811E)

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## BREAKING NEWS: AMAZING LDRD HIGHLIGHTS

### LANL researchers discover that ultra-high-energy gamma rays originate from pulsar nebulae

LOS ALAMOS, N.M., April 21, 2021—The discovery that the nebulae surrounding the most powerful pulsars are pumping out ultra-high-energy gamma rays could rewrite the book about the rays’ galactic origins. Pulsars are rapidly rotating, highly magnetized collapsed stars surrounded by nebulae powered by winds generated inside the pulsars.

“We took advantage of the wide field-of-view and survey capabilities at the High-Altitude Water Cherenkov Observatory (HAWC) to search around a collection of powerful pulsars. We found significant evidence that ultra-high-energy gamma-ray emission is a universal feature found near these objects,” said Kelly Malone, an astrophysicist in the Nuclear and Particle Physics and Applications group at Los Alamos National Laboratory and lead author of the HAWC Collaboration’s [new study](#) of gamma radiation from pulsars.

The HAWC Collaboration comprises more than 100 international researchers. Malone developed the gamma-ray energy estimation algorithm that is used in the paper and led the entire analysis.

Conventional wisdom had attributed ultra-high-energy (more than 56 teraelectronvolts) gamma ray emissions to sources of neutrinos and gamma rays called PeVatrons, which are associated with this acceleration of charged cosmic rays to petaelectronvolt energies. The energies are about five times higher than those produced by accelerators on Earth. This came into question when, in 2020, the HAWC Collaboration [released a catalog](#) of nine gamma-ray sources emitting above 56 teraelectronvolts. That's the highest-energy catalog of astrophysical sources ever produced. The team was surprised to find that all of the detected sources were near the most powerful pulsars ever observed.



*After discovering nine ultra-high-energy gamma-ray sources in 2020, researchers at the High Altitude Water Cherenkov Observatory (HAWC) took advantage of the facility's wide field-of-view and survey capabilities to determine that the regions around powerful pulsars universally emit ultra-high-energy gamma rays. (Photo courtesy of Instituto Nacional de Astrofísica, Óptica y Electrónica)*

In the new paper, the team searched for ultra-high-energy gamma-ray signals near extremely powerful pulsars.

“We find that ultra-high-energy emission appears to be a generic feature for these objects. The gamma rays are likely created by interactions in the pulsar wind. This allows us to create a fuller picture of how the most energetic gamma rays ever detected are created in our galaxy,” Malone said. “Now that we know that pulsar wind nebulae emit at these energies, we can focus on detecting more of them with longer searches and more sensitive experiments.”

The HAWC Collaboration recently constructed an upgrade to the detector that is more sensitive to the highest energy gamma rays. Additionally, the planned Southern Wide-field Gamma-ray Observatory (SWGGO) experiment will be extremely sensitive above 50 teraelectronvolts and will be able to perform detailed studies of emissions associated with pulsars.

The HAWC Observatory is composed of an array of water-filled tanks high on the flanks of the Sierra Negra volcano in Puebla, Mexico, where the thin atmosphere offers better conditions for observing gamma rays. When gamma rays strike molecules in the atmosphere they produce showers of energetic particles. When some particles in cosmic ray showers travel strike the water inside the HAWC detector tanks, they produce flashes of light called Cherenkov radiation. By studying these Cherenkov flashes, researchers reconstruct the sources of the particle showers to learn about the particles that caused them.

**Paper:** “Evidence that Ultra-high-energy Gamma Rays Are a Universal Feature near Powerful Pulsars,” The Astrophysical Journal Letters. A. Albert, R Alfaro, C. Alvarez, et al.

**Funding:** The Laboratory Directed Research and Development (LDRD) program of Los Alamos National Laboratory; the US Department of Energy Office of High-Energy Physics; the National Science Foundation (NSF), Consejo Nacional de Ciencia y Tecnología (CONACyT), México; and a variety of international funders for members of this international collaboration.

Read the article by Charles Poling [here](#)

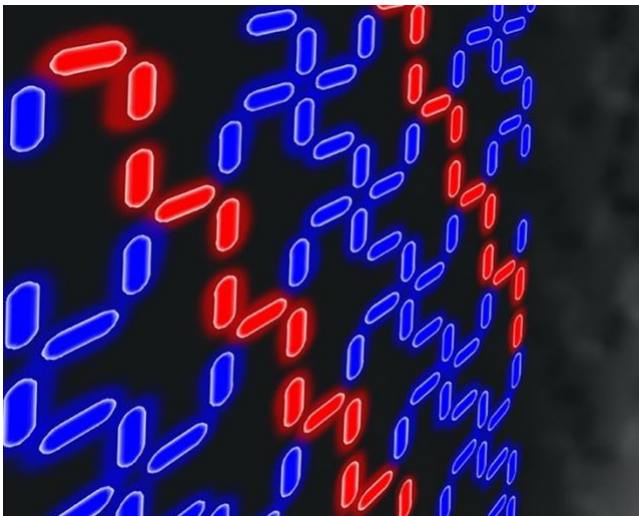
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## New ‘frustrated’ nanomagnets order themselves through disorder: LANL researchers create ‘entropy-driven order’

Extremely small arrays of magnets with strange and unusual properties can order themselves by increasing entropy, or the tendency of physical systems to disorder, a behavior that appears to contradict standard thermodynamics — but doesn’t.



“Paradoxically, the system orders because it wants to be more disordered,” said Cristiano Nisoli, a physicist at Los Alamos and coauthor of a [paper](#) about the research in Nature Physics. “Our research demonstrates entropy-driven order in a structured system of magnets at equilibrium.”

The system examined in this work, known as tetris spin ice, was studied as part of a long-standing collaboration between Nisoli and Peter Schiffer at Yale University, with theoretical analysis and simulations led at Los Alamos and experimental work led at Yale. The research team includes scientists from a number of universities and academic institutions.

*Extremely small arrays of magnets, known as tetris spin ice (shown here), can order themselves by increasing their disorder. (Photo by University of Illinois at Urbana-Champaign)*

Nanomagnet arrays, like tetris spin ice, show promise as circuits of logic gates in neuromorphic computing, a leading-edge computing architecture that closely mimics how the brain works. They also have possible applications in a number of high-frequency devices using “magnonics” that exploit the dynamics of magnetism on the nanoscale.

Entropy is the measure of the state of disorder, randomness or uncertainty in a physical system. A liquid, for instance, has high entropy because at warm temperatures — high energy — its molecules are free to move around in a random, disordered way.

But when liquids are cooled to form solids, the molecules calm down and order themselves through interactions to optimize their energy. They can arrange themselves in a crystal lattice in only a limited number of configurations. This lowers their entropy: they are highly ordered.

Some systems, however, are not so simple. Parts of the system settle in an orderly way, but others don't. These "frustrated" systems retain disorder.

Tetris spin ice, which is composed of 2D arrays of very small magnets that interact but are frustrated, is a strange mix of the two cases. The magnetic pole orientations frustrated in such way that the system retains some order while remaining disordered. At low temperature it decomposes into alternating ordered and disordered stripes.

The apparent paradox of increasing entropy with increasing order is resolved by the entropic interaction between the alternating layers. By mutual ordering of the ordered stripes, the system increases the disorder in the other stripes. Thus, order happens without any decrease in energy, but via an increase in entropy.

"No law of thermodynamics is truly broken," Nisoli said. "The concept that systems order by reducing entropy applies to most systems, but, as we show, not to all. Our system is exotic and behaves counterintuitively, with an increase of entropy, a measure of disorder, being the driver of visible order."

The research team comprised members from Lawrence Berkeley National Laboratory, Los Alamos, Seagate Technology, University of Illinois at Urbana-Champaign, University of Liverpool, University of Minnesota, Wayne State University and Yale.

**Paper:** "[Entropy-Driven Order in an Array of Nanomagnets](#)," Hilal Saglam, Ayhan Duzgun, Aikaterini Kargioti, Nikhil Harle, Xiaoyu Zhang, Nicholas S. Bingham, Yuyang Lao, Ian Gilbert, Joseph Sklenar, Justin D. Watts, Justin Ramberger, Daniel Bromley, Rajesh V. Chopdekar, Liam O'Brien, Chris Leighton, Cristiano Nisoli, and Peter Schiffer, in *Nature Physics*. DOI: 10.1038/s41567-022-01555-6

**Funding:** Laboratory Directed Research and Development at Los Alamos National Laboratory and U.S. Department of Energy Office of Basic Energy Sciences, and National Science Foundation.

Read the article by Charles Poling [here](#)

(LA-UR-22-21432)

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## Urgent questions in human health: LLNL study on tumor/immune cell interaction could impact cancer immunotherapies

[Lawrence Livermore National Laboratory](#) (LLNL) scientists exploring the interaction between cancer cells and the extracellular matrix (ECM) — the "scaffolding" of organs — found that proteins in the ECM can dramatically impact the immune system's ability to kill tumors. Researchers said the findings, [published online](#) in the journal *Biomaterials*, could represent a novel approach to studying immunosuppression found in many breast cancers and open new pathways of activating the immune system to target cancer.

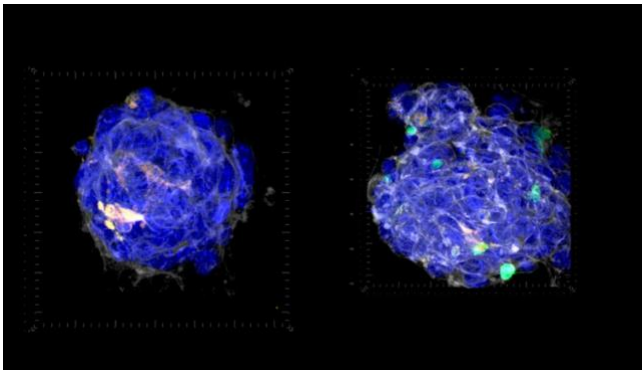
In the paper, LLNL engineers and biologists report on the development of an assay for testing the efficacy of T cells — the white blood cells that in healthy persons surveil and eliminate precancerous cells. But in most breast cancers, these T cells fail to do their job.

The researchers cultured tumor and immune cells on various compositions of ECM (the molecules and proteins that make up the structural support system surrounding cells). By screening 25,000 cells on 36 different combinations of nine ECM proteins, the team demonstrated, for the first time, the ability of immune cells to clear tumors is regulated by the makeup of the ECM substrate.

“The surprising thing was finding the ability of the immune cell to kill a tumor depends on what [scaffolding proteins] the tumor is sitting on,” said LLNL mechanical engineer Claire Robertson, who led the work. “Depending on the ECM environment, the tumor cells were either completely susceptible and died off or they remained completely resistant to T cells.”

Most notably, the team found that in the presence of Collagen IV, breast cancer cells were more likely to grow and were more resistant to T cells, whereas T cells were more likely to die off. “The T cells that were touching Collagen IV were just not doing their job,” Robertson said. “In fact, we found that any time Collagen IV was in the mix, the T cells were dying instead of the tumor cells — exactly what you don't want to happen if you have a tumor.”

Researchers also discovered that in Collagen IV, T cells turned off gene signatures related to killing harmful cells, whereas tumor cells turned on signatures of cytokines that send messages to T cells that there is no tumor present.



*This image shows tumor and immune cells (blue for all nuclei) grown on Collagen IV. The orange spots show T-cells (immune cells) in the process of dying. Right: This image depicts tumor cells combined with living T-cells growing on a scaffolding of proteins. (Image courtesy of Monica Moya/LLNL)*

Robertson said the experimental results provide clues as to why immune checkpoint therapies like Programmed death-ligand 1 (PD-L1) inhibitors, which have improved the prognosis of various cancers, have been largely ineffective in treating breast cancer. Breast cancers rarely express PD-L1 development as biomarkers, making patients ineligible for such therapies, she explained. Importantly, tumor cells cultured on Collagen IV turned PD-L1 off, but still showed profound immunosuppression, mimicking what happens in human breast tumors, Robertson added.

“The question is, what can we do to activate the immune system in these patients? The thing that's really exciting is the fact that we’ve found a completely unique mechanism of immunosuppression. It means we have a whole new way of targeting cancer,” she said.

The work was funded by a Laboratory Directed Research and Development Strategic [Initiative](#) (LDRD SI) on tumors and from Robertson’s Lawrence [Fellowship](#). Researchers said the pipeline they developed could apply beyond breast cancer to nearly any form of cancer.

“This research offers a new approach to identify and tease apart the critical components for understanding the biology of tumors, which may provide novel insight for more targeted cancer treatment,” said co-author Matt Coleman, a Translational Immunobiology group leader in the Lab’s Biosciences & Biotechnology Division.

The team’s next step is to determine what drugs can target the interactions between Collagen IV, tumor cells and T cells, with an eventual goal of developing a new therapeutic candidate capable of activating the immune system in breast cancer patients.

“In our LDRD SI, we set out to develop a 3D tumor model platform with the mindset that if you can build something, you truly understand it,” said LLNL biomedical engineer Monica Moya, the Engineering lead on the project. “This work was critical to understanding both how to build systems to ensure cells behave as they would *in vivo*, but more fundamentally addresses a previously unknown element of T cell biology. We’re proud to be using bioengineering to address urgent questions in human health.”

LLNL co-authors included Aimy Sebastian, Aubree Hinckley, Naiomy Rios-Arce, Skye Edwards, Wei He, Nicholas Hum and Gabriela Loots from LLNL’s Physical & Life Sciences directorate, and William Hynes and principal investigator Elizabeth Wheeler from LLNL’s Engineering directorate.

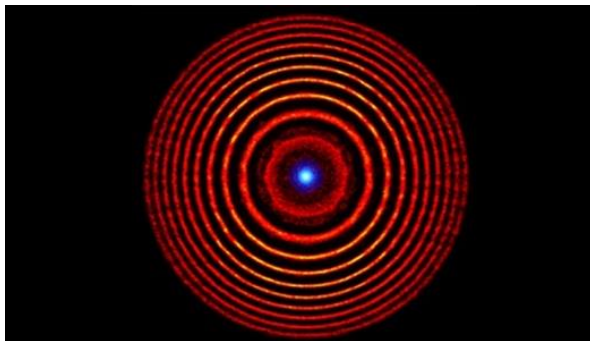
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➤ Technical Vitality

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## Building laser optics from plasma at LLNL: Holographic plasma lenses for ultra-high-power lasers

In the [National Ignition Facility](#) (NIF), the world’s highest-energy laser system, a complex series of glass optics — including amplifiers, mirrors, wavelength converters and focusing lenses — strengthens and guides the laser light to its destination. Over the years, researchers have developed and refined these optics so they can withstand the intense energies generated by NIF’s powerful laser beams.



Not even the hardest solid-state optics, however, can cope with the energies that will be produced by the next generation of ultra-intense, high-repetition-rate lasers now being developed at [Lawrence Livermore National Laboratory](#) (LLNL) and elsewhere around the world. Current state-of-the-art 10-petawatt (quadrillion-watt) lasers may soon be eclipsed by 100-petawatt and even exawatt lasers capable of generating 1,000 petawatts of peak power — more than five times the power the Earth receives from sunlight.

*Colorized illustration from a simulation of a holographic plasma lens. The red concentric circles denote alternating high- and low-density plasma rings. The blue dot at the center represents the focused light. (Image courtesy of Matthew Edwards/LLNL)*

To help enable these ultrafast, ultra-high-power lasers, Livermore researchers and their colleagues are exploring ways to build laser optics from plasma — a charged mixture of ions and free electrons — to overcome the limits on maximum fluence (energy density) imposed by conventional solid optics. A plasma optic allows a large amount of energy to be directed into a small space and time in a well-collimated (focused) beam.

Because plasma has a much higher energy density than glass, it can withstand much higher optical densities. Plasma-based replacements for a variety of standard optical components would allow the manipulation of light at extreme fluences, opening the door to higher laser intensities and energies.

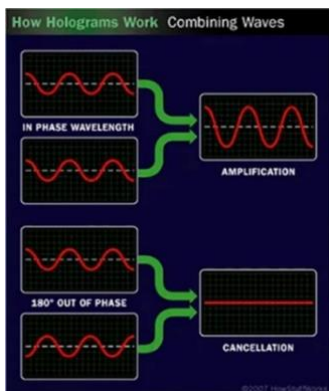
One example of this is described in a featured [Physical Review Letters paper](#) published online last month. LLNL postdoc Matthew Edwards and colleagues present an approach to building a robust holographic plasma lens “capable of focusing or collimating a probe laser at intensities several orders of magnitude higher than the limits of a nonionized (solid) optic.”

“Glass focusing optics for powerful lasers must be large to avoid damage,” Edwards said. “The laser energy is spread out to keep local intensity low. Plasma is far more resistant to light damage than any solid material, and optics built from plasma can therefore be a thousand to a million times smaller than those built from glass.”

The Laboratory’s work on plasma optics is closely related to the long-standing efforts of researchers to control cross-beam energy transfer (CBET) — the exchange of energy between overlapping laser beams as they enter the laser entrance holes of a NIF hohlraum. CBET creates a grating, or diffractive optic, in the hohlraum plasma that can be manipulated by wavelength tuning to direct the incoming laser light to where it’s needed to create a symmetrical implosion.

“Our new approach to using a plasma for focusing is based on diffraction — like a hologram or a zone plate — rather than refraction like a traditional lens design,” Edwards said. “Diffraction makes the plasma optic insensitive to imperfections in plasma density, which is important because it is, in general, difficult to create a plasma with optically precise properties.”

“The generality of holography means that holographic plasma optics can almost arbitrarily manipulate intense beams,” the researchers said in the paper. “These mechanisms are not limited to the creation of simple lenses.”



To create a holographic plasma lens, two co-propagating pump beams are fired into a gas jet. The interference pattern imprints a three-dimensional refractive index structure in the resulting plasma, inducing density variations that act as a diffractive lens capable of focusing a multi-petawatt-scale laser beam without being damaged.

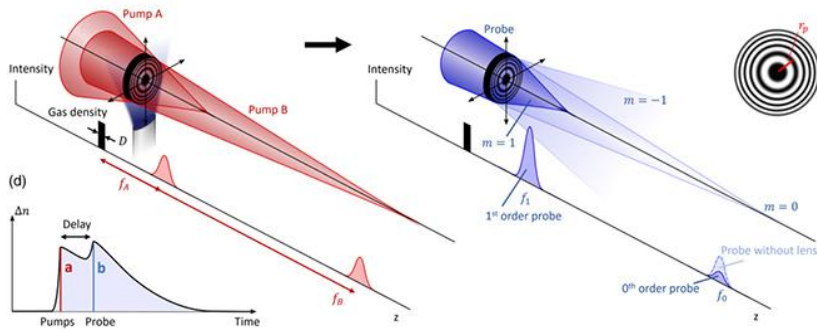
The researchers tested the concept through computer simulations of two plasma mechanisms: spatially varying ionization, in which variations in laser intensity create static regions of ionized and non-ionized gas; and ion-density fluctuations that occur in the plasma as electrons and ions are forced from areas of high laser intensity to areas of lower intensity.

*A hologram is a three-dimensional image generated by interfering light beams. In constructive interference, two overlapping light waves are in phase and reinforce each other, while in destructive interference, the waves are out of phase and cancel each other out. (Graphic by HowStuffWorks)*

Because plasma optics are transient and generated from a gas, these lenses would be particularly well-suited to high-repetition-rate laser systems, such as the LLNL-developed [L3-HAPLS laser in the Czech Republic](#) as well as potential [inertial fusion energy](#) systems.

“We have shown that plasma nonlinearities can be used to create efficient high-damage-threshold diffractive plasma lenses,” the researchers concluded. They said the simulations suggest that the intensity damage threshold of the lenses ranges from fluences of more than  $10^{14}$  (100 trillion) watts per square centimeter ( $W/cm^2$ ) for the ionization mechanism to more than  $10^{17}$  (100 quadrillion)  $W/cm^2$  for the ion-density mechanism.





*Schematic of a holographic plasma lens. Left: Two pump lasers overlap at  $D$  in a gas jet, arranged so that their interference pattern is a sinusoidal zone plate consisting of concentric alternating regions of opaque or phase-shifting material, all spaced so that transmitted light interferes constructively at the desired focal point. Center: At a delayed time, a probe laser passes through the resulting structure and is diffracted into one or more diffraction orders. Right: The intensity profile of the overlapped pumps and the resultant index modulation. (Graphic courtesy of LLNL)*

“The required plasma is similar to those that have been achieved experimentally for plasma gratings,” Edwards said, “and a lens of this design may be feasible in the near future.”

Joining Edwards on the *Physical Review Letters* paper, “[Holographic Plasma Lenses](#),” were LLNL colleagues Eugene Kur, Nuno Lemos and Laser-plasma Interactions Group Leader Pierre Michel; Vadim Munirov, Ashwin Singh and Jonathan Wurtele from U.C. Berkeley; and Nicholas Fasano and Julia Mikhailova from Princeton University.

(LLNL-WEB-458451)

➤ Mission Agility, Technical Vitality

## LLNL’s Algal Bloom Forecast Technique: With better algal forecasts comes safer water

[Lawrence Livermore National Laboratory](#) (LLNL) scientists and collaborators have used a new technique to better forecast the level of algal toxins that accumulate in Lake Erie every year.

Harmful algal blooms (HABs) are global phenomena and, in freshwater lakes and reservoirs, are caused by cyanobacteria of the genus *Microcystis* that produce microcystins, a suite of amino-acid-like toxins that are harmful to wildlife and humans. Understanding the environmental drivers that affect microcystin concentrations and developing forecasting capabilities are critical to protect human and environmental health and ultimately prevent future HABs.

The team used isotope labeling of the cyanotoxins to examine its degradation in Lake Erie. Using LLNL’s NanoSIMS instrument, they confirmed that a small but highly active component of the microbiome was responsible for the degradation of the toxin. The research appears in the journal [Limnology and Oceanography](#).

Microcystins are a potent liver toxin and possible human carcinogen. Cyanotoxins can also kill livestock and pets that drink affected waters. Fish and bird mortalities also have been reported in water bodies with persistent cyanobacteria blooms. These blooms form when cyanobacteria, which are normally found in water, start to multiply very quickly. Blooms can form in warm, slow-moving waters that are rich in nutrients from sources such as fertilizer runoff or septic-tank overflows.



*Algal blooms in Lake Erie. (Adobe Stock image)*

Cyanobacterial biomass forecasts in Lake Erie — which has a history of cyanobacterial HABs — are made possible with frequent remote sensing data and lake water mass movement. One of the more widely known forecasts is from NASA and the National Oceanic and Atmospheric Administration (NOAA) that uses satellite images of Lake Erie to forecast cyanobacteria location and biomass two to four days in advance.

However, while the biomass forecasts have aided managers in predicting when and where the cyanobacterial blooms will be located, the forecasts cannot currently predict microcystin concentrations because toxicity is not always correlated with biomass. Insights on how microcystin production and degradation change spatially and temporally in a bloom could help overcome the limitations that currently prevent microcystin concentration forecasts.

To date, there were no previous studies linking microcystin production and biodegradation in a naturally occurring *Microcystis*-dominated cyanobacterial bloom. The study's results provide evidence for *in situ* microbial degradation of microcystin. Using nitrogen-15 ( $^{15}\text{N}$ ) isotope labeling to trace the fate of an algal toxin into the bacterial community had not been done before; a major finding was that degradation appears to be limited to a small subset of the Lake Erie microbial community.

“The high spatial resolution of the NanoSIMS allowed us to identify that the isotope-labeled toxin was being incorporated into the biomass of a small fraction of the microbial population living inside the bloom, and not the cyanobacterial cells that had released it, something that could not be accomplished with any other detection method,” said LLNL scientist Xavier Mayali, a co-author of the study.

“The results of our study not only provide new insights into the dynamics of cyanotoxins in nature but also suggest a potential new direction for cyanotoxin treatment using specialized toxin-degrading bacteria,” said LLNL postdoctoral scientist Wei Li, another co-author of the paper.

The team also quantified microcystin production rates. “We found that the HABs produce microcystins the fastest during the start of the bloom, and the high production rates in the early bloom align with when we see the highest microcystin concentrations in Lake Erie. During the late bloom, we measured low production rates and low concentrations in the lake,” said Justin Chaffin from The Ohio State University, the study's lead author.

Co-author Thomas Bridgeman, from the University of Toledo's Lake Erie Center, said: “We have been measuring microcystin concentrations in Lake Erie for many years, but this study is the first to show that the toxin levels we measure on any given day are the net result of competing microcystin production and degradation processes that vary over time and space. It's a big step towards the development of models that will be able to produce microcystin forecasts for the benefit of water-treatment plants and recreational users of Lake Erie.”

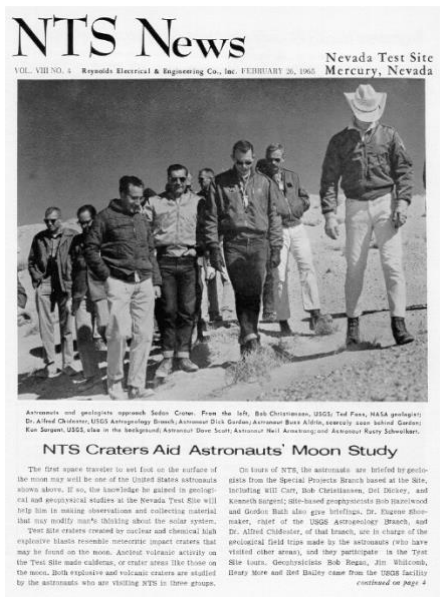
LLNL staff scientist Peter Weber, principal investigator of the NanoSIMS facility, was also part of the team. Other institutions include The Ohio State University, Wayne State University, Bowling Green State University and University of Toledo. The LLNL portion of the [research](#) was funded by the [Laboratory Directed Research and Development](#) program.

(LLNL-WEB-458451)

➤ Technical Vitality

## NNSS SDRD feasibility study: Product development to support NASA’s Artemis program and astronaut training

The Site-Directed Research and Development (SDRD) Program seeks submissions each fiscal year for feasibility study proposals in favor of initial exploration of innovative, high-risk, high-impact project concepts. Feasibility studies provide a flexible way for researchers to execute short-term and low-cost projects to evaluate the potential success of novel technical approaches to mission-relevant science and technology (S&T) challenges and to address emerging S&T needs. Bryan Eleogram at the Nevada National Security Site (NNSS) wants to develop detailed geoscience and operational training products needed for astronaut training.



The NNSS and National Aeronautics and Space Administration (NASA) will collectively work to support NASA’s Artemis program and its associated astronaut training program. The NNSS partnered with NASA and played a key role in providing a realistic training ground for the Apollo program, which ran from the early 1960s to 1972. Voice transcripts from Apollo astronauts on the Moon demonstrated that their unique training conducted at the NNSS, called the Nevada Test Site (NTS) at that time, was realistic and greatly beneficial for lunar exploration.

NASA is preparing to return to the lunar surface as part of the nation’s Artemis program. The cratered terrain and associated features found uniquely at NNSS have the potential to play a significant role in human space flight again by training the next generation of astronauts to explore the Moon.

*The front page of the February 26, 1965, edition of the NTS News with a photograph of astronauts and geologists approaching the Sedan crater in preparation for a series of*

*geological and geophysical studies at the NNSS. (Photo courtesy of Apollo Lunar Surface Journal)*

The NNSS team specifically aims to collect precursor data in high-value NNSS locations, update mapping and in situ training resources for these regions, and develop detailed geoscience and operational training products needed for astronaut training. The tasks, deliverables, and collaboration outlined in this project are anticipated to aid Artemis astronauts to return to and explore the Moon. NNSS will collect the data required for NASA, provide the updates, and help develop the training products critical to successful field training for astronauts.

The primary goal of this project is to help NASA train Artemis astronauts for the next generation of lunar exploration, equipping them with knowledge that only NNSS training and experiences can provide. To achieve this goal, the project team collects precursor data via existing NNSS drone capabilities in the near term. The data collected and products generated will be made available to other interested parties via reports, publications, and data repositories.



Astronauts examine the geology around the rim of the Schooner crater. The area was thought to be similar to the South Ray crater at the Apollo 16 target landing site on the Moon. (Photo from NNSS fact sheet “Apollo Astronauts”)

(Per NNSS classification, this article is confirmed to be unclassified and approved for public release.)

➤ Mission Agility, Technical Vitality

## Brain-based computing chips are only logical: Sandia researchers show neuromorphic computing widely applicable

With the insertion of a little math, Sandia National Laboratories researchers have shown that neuromorphic computers, which synthetically replicate the brain’s logic, can solve more complex problems than those posed by artificial intelligence and may even earn a place in high-performance computing.

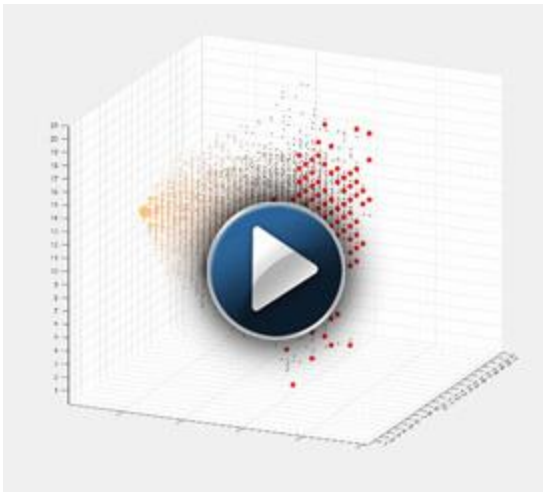
The findings, detailed in a recent article in the journal [Nature Electronics](#), show that neuromorphic simulations using the statistical method called random walks can track X-rays passing through bone and soft tissue, disease passing through a population, information flowing through social networks and the movements of financial markets, among other uses, said Sandia theoretical neuroscientist and lead researcher James Bradley Aimone.

“Basically, we have shown that neuromorphic hardware can yield computational advantages relevant to many applications, not just artificial intelligence to which it’s obviously kin,” said Aimone. “Newly discovered applications range from radiation transport and molecular simulations to computational finance, biology modeling and particle physics.”

In optimal cases, neuromorphic computers will solve problems faster and use less energy than conventional computing, he said.

The bold assertions should be of interest to the high-performance computing community because finding capabilities to solve statistical problems is of increasing concern, Aimone said.

“These problems aren’t really well-suited for GPUs [graphics processing units], which is what future exascale systems are likely going to rely on,” Aimone said. “What’s exciting is that no one really has looked at neuromorphic computing for these types of applications before.”



*A random walk diffusion model based on data from Sandia National Laboratories algorithms running on an Intel Loihi neuromorphic platform. (Graphic courtesy of Sandia)*

Sandia engineer and paper author Brian Franke said, “The natural randomness of the processes you list will make them inefficient when directly mapped onto vector processors like GPUs on next-generation computational efforts. Meanwhile, neuromorphic architectures are an intriguing and radically different alternative for particle simulation that may lead to a scalable and energy-efficient approach for solving problems of interest to us.”

Franke models photon and electron radiation to understand their effects on components.

The team successfully applied neuromorphic-computing algorithms to model random walks of gaseous molecules diffusing through a barrier, a basic chemistry problem, using the 50-million-chip Loihi platform Sandia received approximately a year and a half ago from Intel Corp., said Aimone. “Then we showed that our algorithm can be extended to more sophisticated diffusion processes useful in a range of applications.”

The claims are not meant to challenge the primacy of standard computing methods used to run utilities, desktops and phones. “There are, however, areas in which the combination of computing speed and lower energy costs may make neuromorphic computing the ultimately desirable choice,” he said.

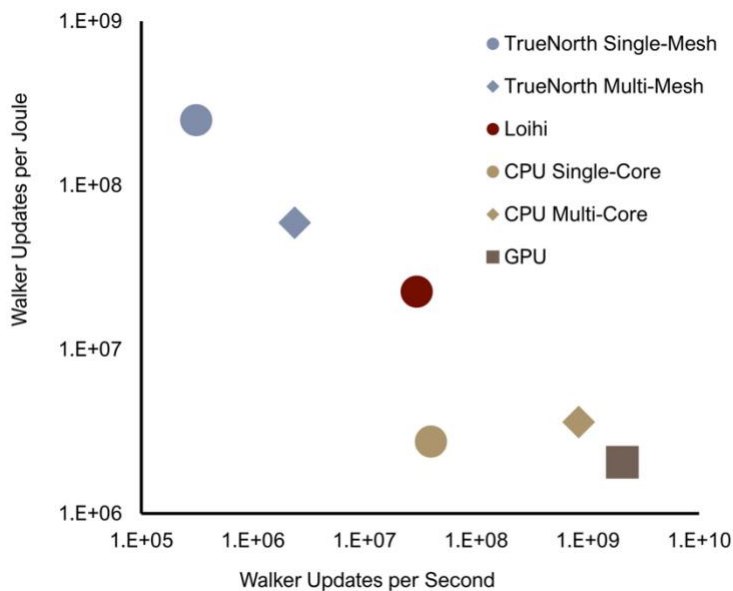
Unlike the difficulties posed by adding qubits to quantum computers — another interesting method of moving beyond the limitations of conventional computing — chips containing artificial neurons are cheap and easy to install, Aimone said.

There can still be a high cost for moving data on or off the neurochip processor. “As you collect more, it slows down the system, and eventually it won’t run at all,” said Sandia mathematician and paper author William Severa. “But we overcame this by configuring a small group of neurons that effectively computed summary statistics, and we output those summaries instead of the raw data.”

Severa wrote several of the experiment’s algorithms.

Like the brain, neuromorphic computing works by electrifying small pin-like structures, adding tiny charges emitted from surrounding sensors until a certain electrical level is reached. Then the pin, like a biological neuron, flashes a tiny electrical burst, an action known as spiking. Unlike the metronomical regularity with which information is passed along in conventional computers, said Aimone, the artificial neurons of neuromorphic computing flash irregularly, as biological ones do in the brain, and so may take longer to transmit information. But because the process only depletes energies from sensors and neurons if they contribute data, it requires less energy than formal computing, which must poll every processor whether contributing or not. The conceptually

bio-based process has another advantage: Its computing and memory components exist in the same structure, while conventional computing uses up energy by distant transfer between these two functions. The slow reaction time of the artificial neurons initially may slow down its solutions, but this factor disappears as the number of neurons is increased so more information is available in the same time period to be totaled, said Aimone.



*Showing a neuromorphic advantage, both the IBM TrueNorth and Intel Loihi neuromorphic chips observed by Sandia researchers were significantly more energy efficient than conventional computing hardware. The graph shows Loihi can perform about 10 times more calculations per unit of energy than a conventional processor. Energy is the limiting factor — more chips can be inserted to run things in parallel, thus faster, but the same electric bill occurs whether it is one computer doing everything or 10,000 computers doing the work. (Image courtesy of Sandia)*

The process begins by using a Markov chain — a mathematical construct where, like a Monopoly gameboard, the next outcome depends only on the current state and not the history of all previous states. That randomness contrasts, said Sandia mathematician and paper author Darby Smith, with most linked events. For example, he said, the number of days a patient must remain in the hospital are at least partially determined by the preceding length of stay.

Beginning with the Markov random basis, the researchers used Monte Carlo simulations, a fundamental computational tool, to run a series of random walks that attempt to cover as many routes as possible.

“Monte Carlo algorithms are a natural solution method for radiation transport problems,” said Franke. “Particles are simulated in a process that mirrors the physical process.”

The energy of each walk was recorded as a single energy spike by an artificial neuron reading the result of each walk in turn. “This neural net is more energy efficient in sum than recording each moment of each walk, as ordinary computing must do. This partially accounts for the speed and efficiency of the neuromorphic process,” said Aimone. More chips will help the process move faster using the same amount of energy, he said.

The next version of Loihi, said Sandia researcher Craig Vineyard, will increase its current chip scale from 128,000 neurons per chip to up to one million. Larger scale systems then combine multiple chips to a board.

“Perhaps it makes sense that a technology like Loihi may find its way into a future high-performance computing platform,” said Aimone. “This could help make HPC much more energy efficient, climate-friendly and just all around more affordable.”

The work was funded under the [NNSA Advanced Simulation and Computing program](#) and Sandia's [Laboratory Directed Research and Development](#) program.

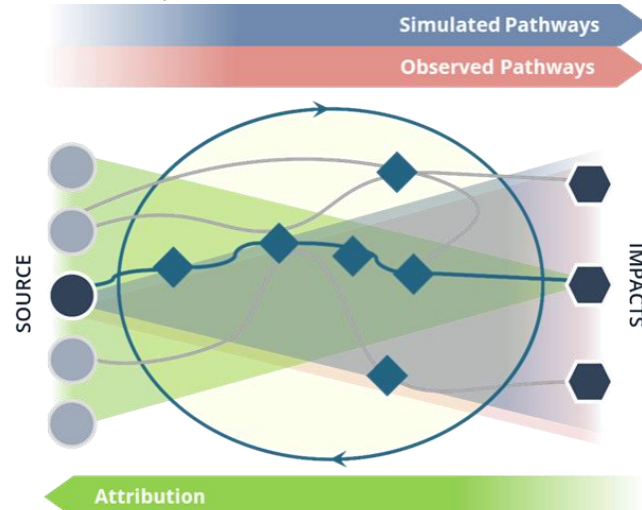
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➤ Mission Agility, Technical Vitality

## Engaging early-career researchers in critical battle: Sandia and universities partner on climate

More than 30 people from Sandia and the University of Illinois Urbana-Champaign participated in a workshop on Feb. 11 focused on climate-modeling research. The workshop was the fourth in a yearlong series centered on climate security topics and designed to create interactions between Sandia researchers and university faculty and students.

“The idea is to get people together and get them engaged, so they know what each other is doing and what expertise each is bringing to the table,” explained Brenda Wilson, microbiology professor at the university and Sandia faculty fellow for the Office of the Vice Chancellor for Research and Innovation. From there, she added, participants can identify additional perspectives and gaps that can be filled through cooperation, which often leads to new projects and funding proposals.



Mallory Stites, a University of Illinois Urbana-Champaign campus partnership manager for Sandia, along with Matt Windsor, said that for the Labs, University of Illinois Urbana-Champaign and other universities have capabilities and resources that make partnering with academia both complementary and valuable. “The more we can figure out what universities are doing to stay on the cutting edge of climate science and then bring it into our work makes it a force multiplier for achieving our missions,” Mallory said.

*Sandia's Climate impact: Determining etiology through pathways, or CLDERA, project combines simulated and observational data to understand the physical processes that connect geographically and temporally localized climate-change sources to impacts, illustrated from left to right; resulting pathways will then be used to attribute impacts back to the source, illustrated from right to left. The goal is to transform the science of attribution to improve climate risk assessments for national security and policy decision-making. (Graphic courtesy of Jason Bolles/Sandia)*

University of Illinois Urbana-Champaign is part of Sandia's [University Partnerships Network](#), which supports university partnerships to increase the Labs' impact and solve big problems. According to Amy Halloran, Sandia's University of Illinois Urbana-Champaign campus executive and director of the Nuclear Fuel Cycle and Grid Modernization Center, this relationship has been so successful because the university's strengths in engineering and applied work translate well to what we do at Sandia. Currently, more than 300 staff possess over 400 degrees from University of Illinois Urbana-Champaign.

With that successful history in mind, the workshop organizers wanted to use this series as an opportunity to expand outreach to other academic programs.

“Faculty in other areas — atmospheric sciences, biology, genomics, geology, mathematics, statistics and more — were doing exciting things in alignment with Sandia's work,” said Wilson. “We also saw a lot of interest in climate and environmental policy topics, so it made sense to engage those people, too.”

In addition to climate change being a broad topic that intersects with multiple disciplines, this issue is gaining traction as a strategic priority for Sandia because of the national and global security threats it poses. Further, the climate crisis can't be addressed by Sandia alone. "Partnerships with universities help us leverage what Sandia can do," Wilson said.

Previous workshops in this series covered the water-energy-climate nexus and geological carbon storage. This particular workshop was the second to tackle the topic of climate modeling.

Presentations by University of Illinois Urbana-Champaign researchers revealed a broad range of climate modeling activities, from advancing methods to simulate complex interactions between the atmosphere and oceans, to combining observations, numerical models and statistical tools to better predict regional impacts of extreme weather. This research not only advances the science of climate modeling but also builds awareness of potential climate change risks, such as how increasing temperatures could impact agricultural yields.

Sandia's portion of the workshop highlighted the CLDERA, or Climate impact: Determining etiology through pathways, Grand Challenge project, with presentations from Diana Bull, principal investigator, and Laura Swiler, attribution lead, as well as a presentation from Kenny Chowdhary on autotuning funded by DOE's Office of Science. CLDERA seeks to develop new methods to attribute climate impacts to source events using a novel pathways approach. Attribution of the source of an impact is needed to guide liability, policy, treaty and national security decisions, especially as climate intervention strategies are being proposed as options to reduce the negative impacts of climate change.

"Establishing connective relationships in climate is hard because of confounding characteristics like high internal variability in earth systems, limited ensemble members from earth systems models and historically limited observational data," said Diana. "We want to move beyond a correlative approach to establish connective relationships in a way that's not just about a single source and a single impact. Our novel approach is focused on tracing how a source drives the climate system to respond with varied impacts."

This collaborative project draws on Sandia's capabilities in modeling and simulation, detection and attribution, risk analysis, high-reliability engineering, as well as the expertise of four academic partners, including University of Illinois Urbana-Champaign.

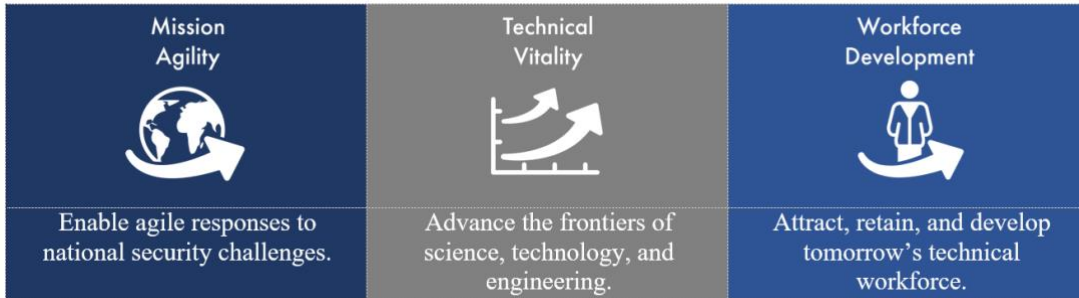
As discussion was winding down, the question of how to capitalize on all the overlapping interests discovered through the workshop revealed another goal of this partnership: to create career pathways for students from University of Illinois Urbana-Champaign to Sandia. One of the easiest ways to start collaborating is to get students involved in joint projects, such as through internships and postdoctoral appointments at Sandia.

In general, Mallory said that the workshop series has been a great way to get early-career researchers excited about Sandia's climate security-related research and to show students outside of engineering disciplines that there is room for their skills at Sandia. "We are creating a community of common researchers."

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➤ Mission Agility, Technical Vitality, Workforce Development





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 [NNSA-LDRD.lanl.gov](https://www.llnl.gov/nnsa-lldr). (Complete Newsletter Review & Release: LA-UR-22-25945)

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