AEED

Atmospheric, Earth, & Energy Division

SCIENCE VISION

of the Atmospheric, Earth, and Energy Division

Providing unique and enduring contributions to national security, energy security, and environmental resilience

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INTRODUCTION

The Atmospheric, Earth, and Energy Division (AEED) at Lawrence Livermore National Laboratory (LLNL) contributes to the success of the Laboratory's vital national security missions by providing scientific expertise, facilities, and capabilities in the areas of energy research and atmospheric and earth science. We are largely a computational organization, but our models and simulations are guided and validated by well-planned fieldwork and laboratory experiments. We have expertise in a wide variety of fields, but we also regularly collaborate with chemists, materials scientists, engineers, physicists, computer scientists, statisticians, and other experts in other divisions, directorates, and institutions to accomplish our goals.

Not only do we deliver timely and practical solutions and advice in response to national security needs, we perform leading-edge fundamental science. Our fundamental science research provides an excellent training ground for talented researchers who often go on to work in more mission-focused areas. We also excel at applying approaches and technologies developed for national security projects to fundamental atmospheric and earth science research, and vice versa. Further, we are stewards for and users of essential Livermore research facilities such as the Center for Accelerator Mass Spectrometry.

This document highlights some past and present research efforts within our division, and how those will provide a foundation for growth and expansion in the coming years, as we work to enhance our support of ongoing mission needs and anticipate future national and global challenges. The world is facing both acute and enduring climate and energy security threats. Our division has an opportunity to make unique and lasting contributions to our nation's security and thereby cultivate a more resilient planet, with a cleaner environment and more sustainable energy resources. Our strategy will enable us to realize this goal.

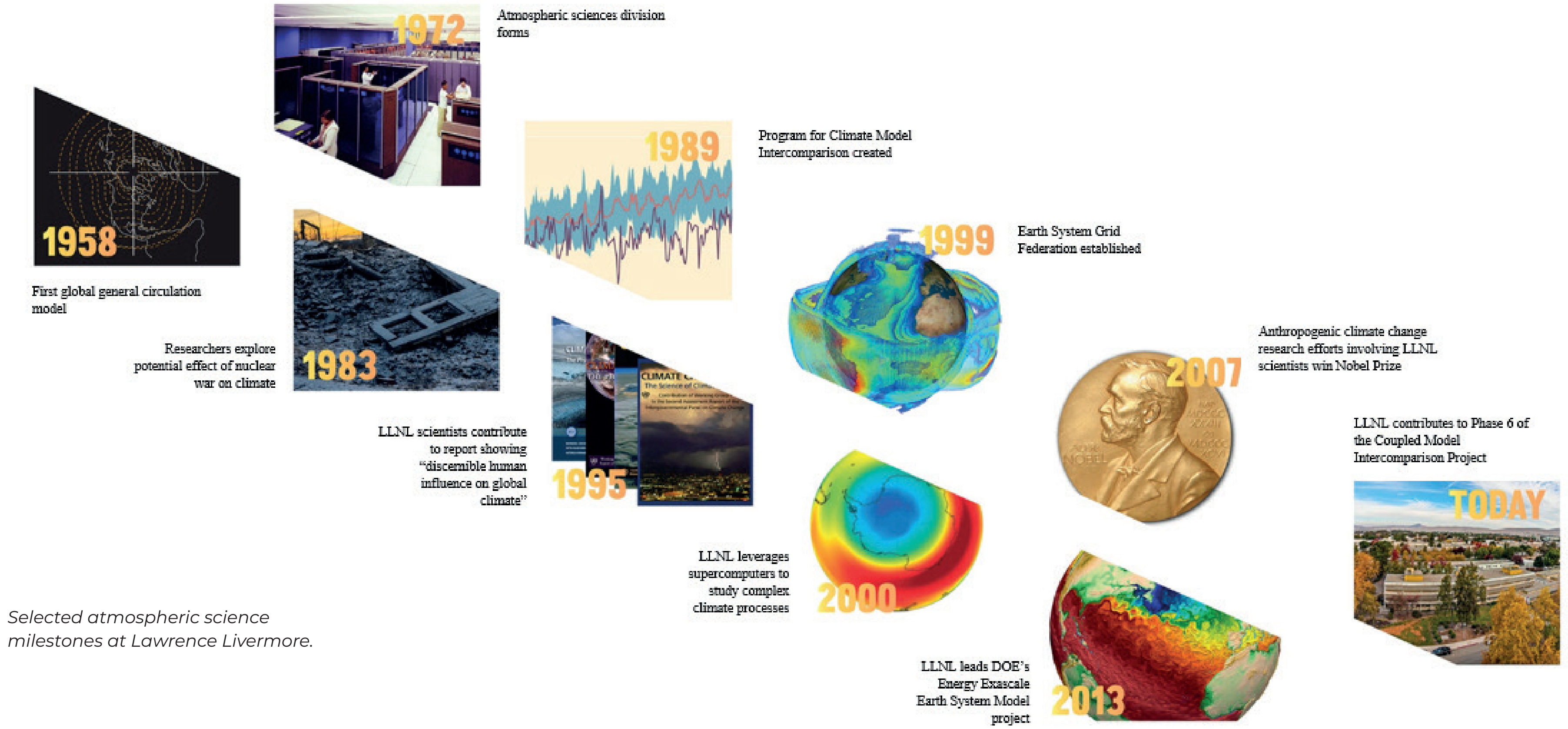
ATMOSPHERIC SCIENCE RESEARCH AT LLNL

Our atmospheric programs were stood up in the early 1960s to model the Earth's atmosphere and provide risk assessment advisories. These programs were an outgrowth of the Lab's simulations of the potential release of radionuclides from nuclear blasts at the height of the Cold War. The new Atmospheric Release Advisory Center (ARAC) received its first operational call in response to the accident at the Three Mile Island nuclear power plant in 1979 and went on to monitor and respond to countless atmospheric emergencies over the next four decades. Our mission expanded as our scientists developed some of the first regional air quality and wind field metrics, calculated the climatic impact of supersonic aircraft, and encouraged the federal government to organize the nation's first dedicated research efforts on the potential effects of carbon dioxide and other greenhouse gases on the Earth's climate.

We secured our reputation in atmospheric and global climate science by leveraging emergent high-performance computer modeling, real-time monitoring, and exceptional simulation capabilities to establish the Program for Climate Model Diagnosis & Intercomparison (PCMDI) in 1989, leading the first Coupled Model Intercomparison Project (CMIP) in 1995. Lab scientists took bold stands on climate research throughout the 1990s, publishing ground-breaking, award-winning research that identified the human "fingerprints" affecting atmospheric temperatures and other climate variables.

ARAC became the National Atmospheric Release Advisory Center (NARAC) in the 1990s, expanding its scope to include emergency preparedness, risk assessment, consequence management, forensics, and recovery for regional, national, and global atmospheric events including toxic chemical spills, industrial fires, and natural disasters. In the 2000s, after the September 11, 2001, terrorist attacks, NARAC's work incorporated homeland security concerns, providing the Interagency Modeling and Atmospheric Assessment Center with contaminant plume modeling and analysis to equip emergency responders and protect the public and the environment.

The following decade, atmospheric scientists at the Lab leveraged advances in Department of Energy supercomputing resources at Livermore and other national labs to lead development of the Energy Exascale



Selected atmospheric science milestones at Lawrence Livermore.

Earth System Model, which yielded the unprecedented model resolution needed to understand the atmosphere and address energy-related questions critical to the nation, including regional air and water temperature, water availability, and extreme water-cycle events.

Since the mid-1990s, Lab atmospheric scientists have also spearheaded an international collaboration known as the Earth System Grid Federation to support climate model comparisons, with an unparalleled collection of climate simulations and global data sets for climate change research, and notably, assessments by the Intergovernmental Panel on Climate Change. This effort evolved into the international Earth System Grid Federation. More recently, our atmospheric scientists have used rigorous field and satellite observations, machine learning, and exascale statistical analyses to improve the performance of renewable energy systems, to detect and predict decadal-to-century changes in regional and global climates, and to identify trends in global precipitation, cloud processes, and drought.

Climate science: Providing tools for assessing climate change

Beginning with development of the world's first atmospheric general circulation model in 1960, Livermore's climate research continually addressed the performance of climate models, regional climate effects, and their impacts on national security and the Earth's ecosystems. Application of high-performance computing and expertise in meteorology, climatology, applied mathematics, and computational science remain essential elements in LLNL's effort to understand and predict how the Earth's atmosphere evolves on time scales from years to centuries.

Coupled with rigorous analysis of surface, atmosphere, satellite, and oceanographic measurements, Livermore climate scientists perform statistically rigorous comparisons of these data with outputs from computer simulations to analyze and improve models and identify climate patterns and processes. To fulfill its national security mission, Livermore continues to investigate how climate change might affect, and pose security threats to, the United States and its economy.

Climate science program highlights

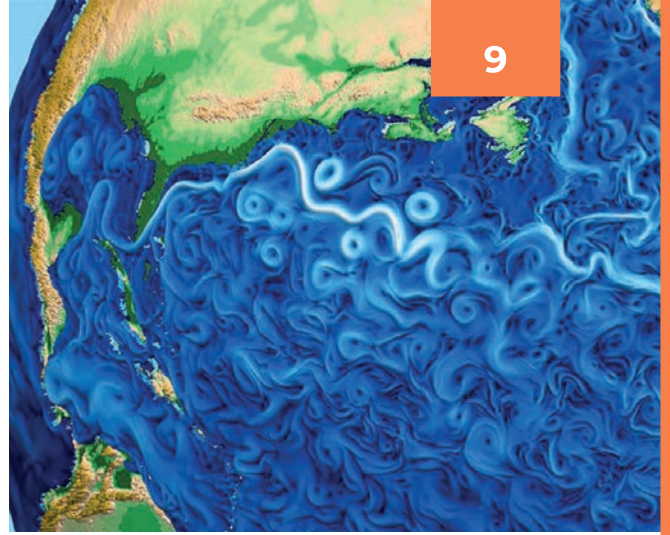
- Livermore scientists participate in the assessments of the Nobel Prize-winning Intergovernmental Panel on Climate Change, established in 1988 to provide the scientific basis for understanding climate change.
- In 1989, the Laboratory created the Program for Climate Model Diagnosis and Intercomparison, which led an international program designed to evaluate the many climate models developed by leading scientific organizations.
- The Laboratory leads the Earth System Grid Federation, an award-winning international high-volume data-management system that allows researchers from all over the world to securely store and share observational data, models, analyses, and results.
- Livermore leads the fully coupled, high-resolution Energy Exascale Earth System Model program (see next section).
- Lawrence Livermore scientists are recognized leaders in cloud processes research, including observation, diagnosis, parameterization, and evaluation in climate models and response to changing climates.

Comparing detailed, rigorous observations from surface, atmosphere, satellite, and oceanographic measurements with outputs from computer models, climate scientists improve models and identify climate patterns and causes.

Energy Exascale Earth System Model: Producing results at unprecedented resolution

The Energy Exascale Earth System Model (E3SM) is a fully coupled, high-resolution earth system and climate model. It was launched in 2014 as a multi-laboratory effort, submitted simulations to the international Coupled Model Intercomparison Project (CMIP6), and released to the broader scientific community in 2018. A multi-phase project, E3SM will ultimately leverage Department of Energy exascale computing resources—which will be delivered to Lawrence Livermore and Oak Ridge national laboratories around 2021–2022—to advance the simulation of various aspects of earth system variability and constrain decadal-scale climate changes that critically impact the U.S. energy sector. These include regional air and water temperatures, which can strain energy grids; water availability, which affects power plant operations; extreme water cycle events such as floods and droughts, which impact infrastructure and bioenergy outputs; and rising sea levels and coastal flooding, which threaten coastal infrastructure.

In 2019, for the first time, AEED scientists succeeded in generating a high-resolution modeling of the ocean's most energetic movements and the largest storms in Earth's atmosphere, which had been poorly portrayed in prior, standard resolution models. By examining the discrepancies between the higher and the standard resolutions, the scientists gained unprecedented insights into how and why resolution affects model simulations. This research, however, also revealed that resolution does not affect climate and aerosol sensitivity in E3SM—confirming that existing coarser, low-resolution models can still work well alongside E3SM and in model intercomparison projects.



This high-resolution ocean simulation uses the Energy Exascale Earth System Model, which divides the globe into a grid down to just 15 kilometers.

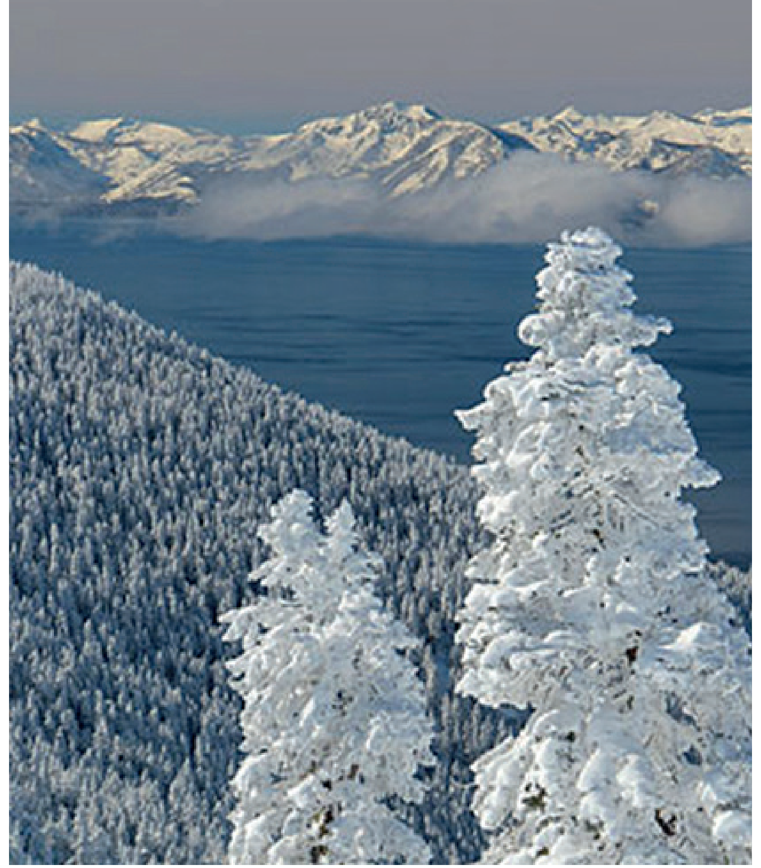
Program and research highlights

- State-of-the-science earth system model investigates energy-relevant science using code optimized for exascale computing.
- Freely available through the Earth System Grid Federation distributed archives, E3SM contributes to the CMIP6 data library.
- Recent findings indicate that combining a new evaluation technique for climate models with observations could reduce the uncertainty in predicting climate change.

Machine learning and climate prediction: Enhancing accuracy and efficiency

Machine learning is becoming an essential tool in the analysis of ever-expanding, large, multivariate observational and experimental datasets, as well as the results from computational simulations. By combining machine learning with exascale computing and earth system models, AEED scientists have uncovered extraordinary insights into global climate trends, gaining greater understanding of the past, developing more accurate contemporary models, and facilitating preparedness for future climate change. AEED scientists are currently leveraging recent advances in an area of machine learning known as "deep learning" to make season-ahead probabilistic forecasts of snowpack in the western United States. This study will help water resource managers plan for the year ahead.

Using a machine-learning algorithm, AEED scientists in 2018 determined that a combination of low-resolution simulations and a few high-resolution simulations could reduce the run time and produce reasonably accurate high-resolution predictions of the global annually averaged top-of-atmosphere energy flux and precipitation. The scientists discovered that by running an ensemble of simulations with different input values and statistical methods, they could minimize disparities between simulations and observations, and that global annually averaged precipitation is more sensitive to resolution changes than to any other model parameters. These findings constitute ground-breaking discoveries that will enhance the overall accuracy and efficiency of machine learning in climate science applications.



New computational approaches could aid water resource managers in predicting and managing snowpack in the Sierra Nevada and other mountain chains.

Project goals

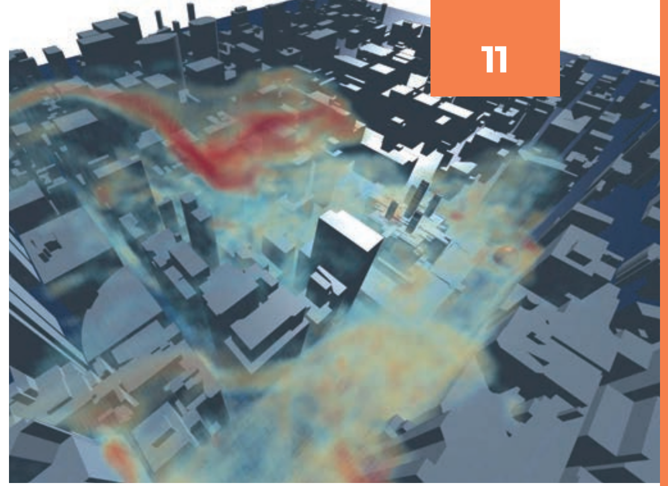
- Improved snowpack predictions six to ten months in advance.
- Reduced computational expense.
- More efficient, reasonably accurate high-resolution predictions.

NARAC: Harnessing interdisciplinary science and technology to navigate critical national security challenges

The National Atmospheric Release Advisory Center (NARAC) provides timely and accurate plume predictions and detailed studies of atmospheric releases of nuclear, radiological, chemical, biological, and hazardous materials to aid emergency preparedness, and to inform response efforts that protect the public and the environment. NARAC computer systems collect and store global meteorological data and numerical weather prediction model results, as well as geographical and population data to analyze hazardous atmospheric releases anywhere on the planet. As part of its emergency response mission, NARAC collaborates with and supports over 300 federal, state, and local agencies; emergency response teams; operations centers; and international organizations.

NARAC continues its technological leadership with advanced computing and data processing, web-based modeling, information sharing, ground-breaking atmospheric hazard analysis, and the first operational deployment of machine-learning tools to boost Bayesian source inversion. NARAC's high-resolution atmospheric and transport models incorporate complex high-resolution terrain and meteorological data to prepare and plan for a wide range of release scenarios, including large fires or chemical spills, incidents involving weapons of mass destruction, and nuclear power plant failures. NARAC's state-of-the-science system includes advanced modeling and analysis tools, and comprehensive databases. Recently, NARAC contributed to the launch of the Improvised Nuclear Device City Planner Resource—a tool that assists local governments in determining the best actions to take following the detonation of an improvised nuclear device.

NARAC is working toward the ability to model post-detonation nuclear debris material formation, cloud rise, and fallout for all possible environments, including water and urban environments. The aim is to better incorporate measurements with models to improve predictions and estimate unknown aspects of hazardous release incidents, and to utilize uncertainty quantification and probabilistic/ensemble simulations to provide predictions of the range of possible consequences from those incidents.



NARAC modeling tools help cities prepare and plan for the potential release of hazardous materials.

Program capabilities

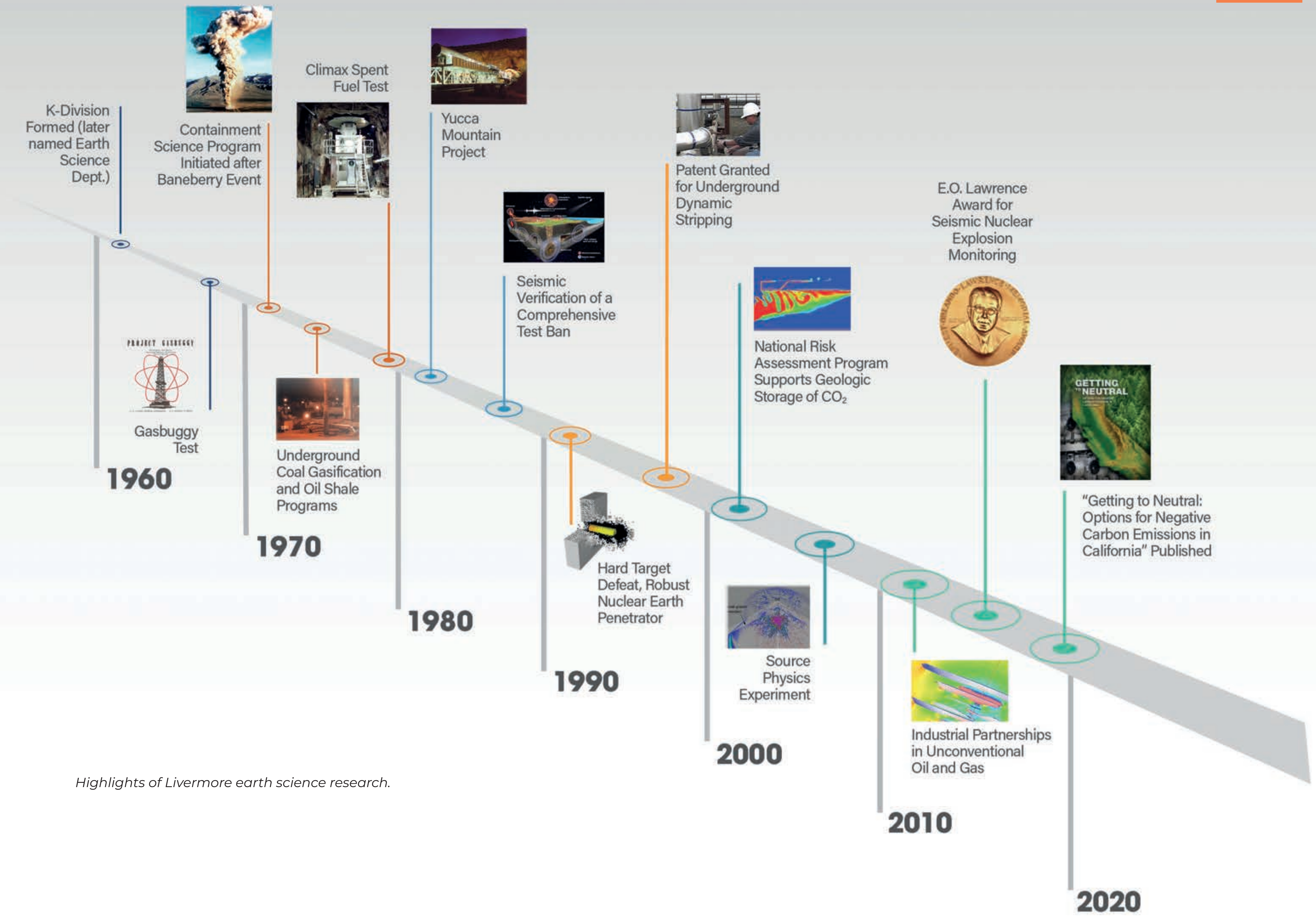
- Since 1979, NARAC has responded to hundreds of alerts, accidents, and disasters; supported thousands of exercises; and conducted numerous emergency response preparedness studies.
- NARAC's expert staff and scientists are on stand-by 24/7, 365 days a year to respond to emergencies anywhere in the world—and have done so continuously for more than 40 years.
- NARAC expert staff can provide quality-assured reports based on field data in as little as 30 minutes.
- NARAC's authorized users can perform fully automated, 3D model simulations in 5 to 15 minutes.
- NARAC responded to the nuclear power plant failures of Chernobyl (1986) and Fukushima (2011), airborne hazards in the wake of Hurricane Katrina (2005), the Deep Water Horizon oil spill fire (2010), and the spread of ruthenium across central Europe (2017).

EARTH SCIENCE RESEARCH AT LLNL

Just as Livermore's atmospheric science program was shaped by the institution's above-ground nuclear testing efforts, Livermore's geoscience program traces its origins to underground nuclear tests. By the 1970s, LLNL's extensive research into how rock responds to an underground explosion garnered our reputation as a world-leading rock mechanics and rock physics research organization. Seismic research to support international nuclear explosive testing treaties, which date back to the 1960s, led to the development of sophisticated computer models that have advanced nuclear nonproliferation, nuclear forensics, energy security, and earthquake hazards research. The close collaborations among a broad range of experts, along with state-of-the-art experimental and computational resources, has long been the foundational hallmark of earth science research at the Laboratory.

National and energy security missions continued to drive the subsequent evolution of the program's endeavors. Efforts to analyze the geological viability of sites for long-term nuclear fuel storage provided the impetus to form a robust geochemistry and reactive transport research capability. The pursuit of national energy security drove research in hydrocarbon recovery and geothermal exploitation that expanded to encompass the potential environmental consequences of these and other activities, such as analyzing the effects of accidental spills of liquefied natural gas and designing innovative methods for modeling, tracking, and cleaning up groundwater contaminants.

With a signature pairing of powerful computer models and field and laboratory experiments, Livermore geoscientists continue to support a wide range of efforts to keep the nation secure and the environment healthy. Researchers partner with industry experts, bringing high-performance computing and state-of-the-art simulation tools to bear on multiple unconventional energy recovery projects. They also investigate methods for efficiently capturing, storing, and repurposing greenhouse gases, along with operational risk assessment. Continually refining computational tools and honing observational methods fortifies our national security mission of discriminating between nuclear explosions—even small ones—and naturally occurring phenomena, and reporting them to authorities. Access to unique capabilities such as the Center for Accelerator Mass Spectrometry, the nuclear magnetic resonance facility, and Livermore's stable of world-class supercomputers ensures that the Laboratory's skilled geologists, geophysicists, geochemists, and geoengineers will be well equipped to tackle future research challenges.

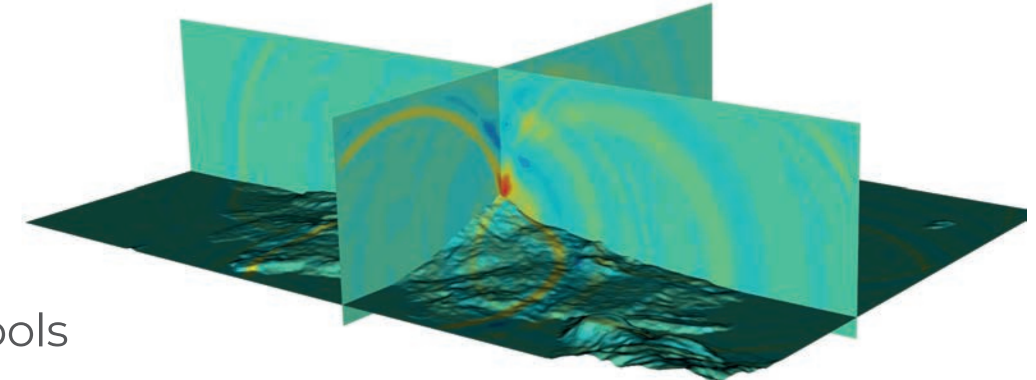


Highlights of Livermore earth science research.

Nuclear explosion monitoring: Developing tools for global security and seismic hazard assessment

The identification and location of rare, possibly covert nuclear tests, among a cacophony of natural and industrial background seismic noise, presents a major national security and scientific challenge. To meet that challenge, LLNL's nuclear explosion monitoring experts have developed a unique suite of advanced, interdisciplinary tools to monitor the planet for nuclear tests, and shed light on Earth's geologic structures and seismic hazards.

One of these groundbreaking tools, the Regional Seismic Travel Time (RSTT) model and computing code, improves the accuracy of locating and classifying seismic events by calculating seismic-wave travel time in less than one millisecond using a 3D model of the Earth's crust, upper mantle, and regional topography. Another recently developed tool, the Elastic and Acoustic code (ElAc), simulates seismic waves in the ground, acoustic waves in the atmosphere, and the fluid, energetic interaction between the two. ElAc's coupled seismoacoustic simulations have proven invaluable for nuclear forensics, nuclear nonproliferation, and global explosion monitoring. Prior to ElAc, no computational tool provided realistic modeling of seismic and acoustic signals and their interactions. These innovative tools not only improve the nation's ability to monitor nuclear explosions but also allow researchers to better identify and define seismically active faults around the planet.



Using high-performance computers, the Elastic and Acoustic Code can model mechanical waves—acoustic and seismic—as they move from the atmosphere into the earth and vice versa, enabling simulations to realistically depict energy as it propagates across complex topography.

Program advances and capabilities

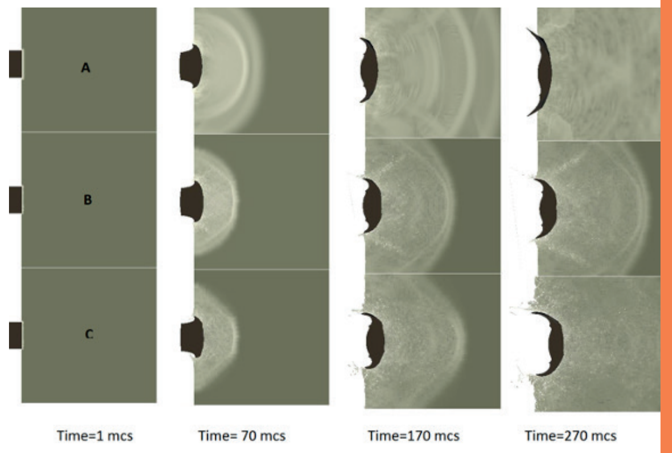
- Source modeling—Seismic events can be grouped based on their remotely observed signals. By analyzing the seismic waves produced, LLNL seismologists have been able to reliably identify and distinguish an explosion, an earthquake, or a mine collapse.
- Location—Bayesian Hierarchical Seismic Event Locator (BayesLoc) is a reliable tool that locates seismic events and stochastically considers uncertainties in arrival time, seismic phase, and velocity.
- External collaborations—Nuclear explosion monitoring researchers have worked with teams around the world to install seismic monitoring stations and establish seismic building codes.
- The Geophysical Monitoring Program at LLNL generates global-scale tomographic images of the Earth's interior for the advancement of seismic event monitoring capabilities and scientific discoveries, such as the previously unidentified southeast Indian Ocean slab.

Geomaterials modeling in the absence of nuclear testing

The GEODYN material library (gmlib) is one of the most advanced and complete geomaterials modeling libraries available for national security applications—and a core capability for AEED. Since the cessation of nuclear testing, LLNL scientists have made tremendous strides in advancing the library's capabilities, and enhancements continue to the present day. The constitutive models within the library incorporate the complex phenomena related to impact and explosions into hard rock and brittle materials. Recent additions include elements for studying fluid saturation, anisotropic properties, and granular materials. The Weapons and Complex Integration (WCI) Directorate relies heavily on the library, and its materials models have been incorporated into WCI codes that simulate the behavior of geologic materials.

Library advances and capabilities

- Source modeling—Fully anisotropic damage models have been incorporated, alleviating the demands on the host code to handle frictional contact between joint and fault planes.
- Exascale-ready—Gmlib has recently been fully upgraded to run on central processing units or graphics processing units, utilizing the tools developed in the RADIUSS project at LLNL.
- Modularity—Gmlib incorporates a function parser so that analysts may explore functional forms without recompilation. Model components such as equation of state, strength, and compaction are combined to form a complete constitutive description for a material.

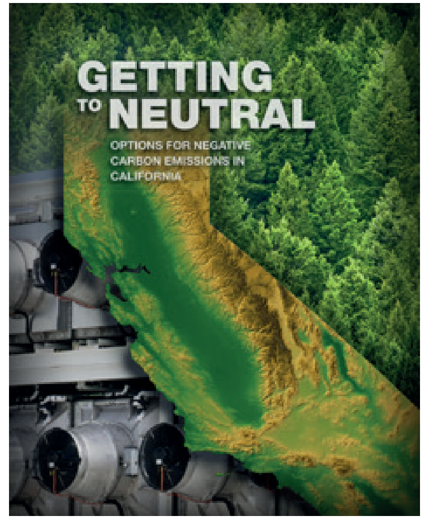


As a massively parallel physics code run on supercomputing systems, GEODYN-L has the capability to simulate nonlinear wave propagation through solid rock and ceramics. In the simulation shown, the wave-front shape and damage distribution behind a wave done from the impact of a steel projectile into borosilicate glass represented by >10K clusters of deformable finite elements interacting through interfacial contact. Different model forms for interfacial friction between the broken pieces are used in the bottom two rows resulting in observable differences in the Mescal zone.

Negative carbon: Exploring revolutionary technologies

Climate scientists calculate that even after converting to 100% renewable power sources, such as wind and solar, and emission-free cars and trucks, the world will still need to remove 10 billion metric tons of CO_2 from the atmosphere each year beginning in 2050 to avoid significant increases in global temperature. Global-scale atmospheric CO_2 removal, or "negative emissions," will be an unprecedented endeavor requiring enhanced scientific understanding, new technologies, collaborations, and companies dedicated to "cleaning" the atmosphere through CO_2 capture, sequestration, and conversion to alternative products and fuels. It will also require collaboration between technical experts and government organizations to provide the technologically feasible and effective financial incentives required to motivate this endeavor. The Lawrence Livermore Director's Initiative for "Engineering the Carbon Economy" was conceived in 2018 to help support global-scale CO_2 and methane removal. The effort comprises several research areas at the Laboratory that include manufacturing carbon-based products from CO_2, returning carbon to CO_2-depleted soil, sequestering CO_2 deep underground, and performing systems analysis to predict the costs and benefits of different carbon management approaches.

In a first-of-its-kind study published in January 2020, LLNL and external collaborators detailed which negative emissions approaches hold the most potential to help California achieve its ambitious goal of reaching carbon neutrality by 2045. The report, funded by the Livermore Lab Foundation with grant support from the Climate Works Foundation, focused on three specific pillars of negative emissions: natural and working lands, carbon capture from waste biomass utilization, and direct air capture. The report provides a thorough assessment of advanced carbon reduction technologies, their costs, as well as necessary tradeoffs required to reach the state's decarbonization goal. The report also reaffirmed significant conclusions by climate scientists, and will serve as an important resource for policymakers, government, academia, and industry partners.



"Getting to Neutral: Options for Negative Carbon Emissions in California" was conducted to identify solutions to enable global-scale CO_2 removal from the atmosphere and hit global temperature targets.

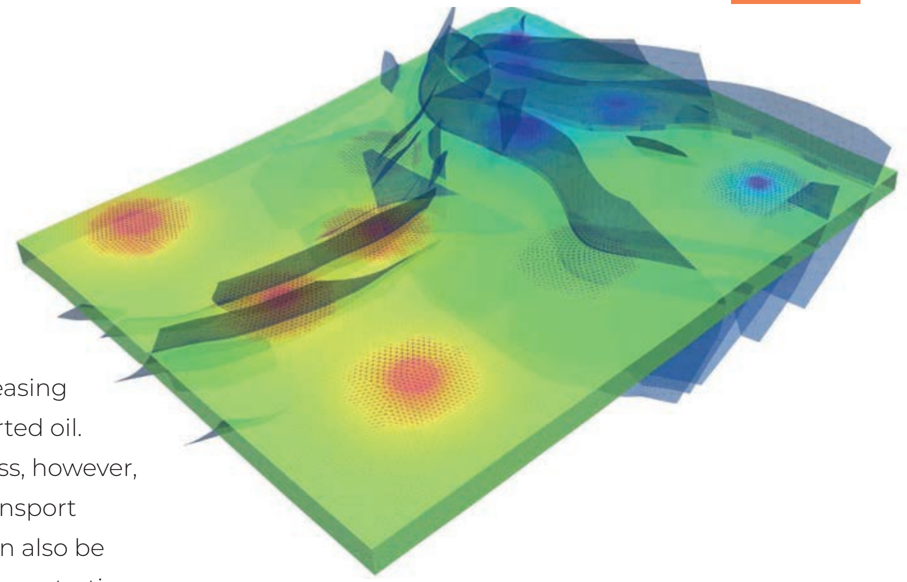
Study highlights

- Carbon neutrality is possible.
- California could become carbon neutral sooner than anticipated, at a lower cost than expected, while boosting California's economy and creating quality jobs.
- Carbon neutrality will also bring important additional benefits to air quality and wildfire prevention.
- Achieving carbon neutrality by 2045 and maintaining net negative emissions thereafter would complete a chain of other ambitious targets for reducing greenhouse gas emissions.
- By getting to neutral, California would set a precedent and demonstrate to other states how to successfully remove significant amounts of CO_2 from the atmosphere.

GEOSX: From modeling oil and gas extraction to carbon storage

Hydraulic fracturing has driven the oil and gas boom over the last decade, increasing affordable domestic energy, and making the United States less dependent on imported oil. A comprehensive understanding of the physical mechanisms that govern the process, however, remains elusive. GEOS, an advanced 3D rock mechanics, fluid flow, and proppant transport computer code, offers hydrofracturing planners a practical, yet flexible tool. GEOS can also be applied to geothermal energy analysis, nuclear explosion monitoring, and carbon sequestration, and has been the basis for many collaborations with industry partners, the State of California, and the Department of Energy.

In June 2020, LLNL, in collaboration with Total S.A. and Stanford University, publicly released GEOSX, an exascale-compatible simulator for large-scale geological CO_2 storage. The simulator, the first of its kind, uses field and engineering data to predict the behavior and impact of CO_2 stored in geological repositories. New technological developments in numerical algorithms and high-performance computing make its unrivalled resolution and speed possible. It will be used to improve the management and security of geological CO_2 repositories and support the widespread implementation, organization, and management of CO_2 sequestration at an industrial scale.



Modeling CO_2 sequestration in a Gulf of Mexico storage reservoir.

GEOSX advance

- GEOSX simulates processes that occur on both micro- and macro-scale resolutions, from nanometers to kilometers.
- GEOSX models complex thermo-hydro-mechanical-chemical processes and their resulting geophysical signatures.
- GEOSX leverages GPU computing and massively parallel algorithms to run on LLNL's world-class HPC systems.
- GEOSX combines a range of disciplines including reservoir engineering, seismology, hydrology, and computational science, along with industry expertise.

Experimental geochemistry: Generating data and applying predictive models to field operations

Understanding the role of rock–water interaction in constraining the influence of reactive chemical transport associated with subsurface operations is an enduring element of LLNL's efforts in experimental geochemistry. Experimental constraints on phase equilibria, solubility, and the kinetics of mineral dissolution and precipitation have contributed to the development of more accurate predictive models applied to the safe disposal of radioactive waste, sustained production of geothermal energy, and geologic storage of greenhouse gases. In particular, geologic carbon storage promises to be a critical technology for mitigating climate change as the world strives towards a carbon-free economy.

Experimental geochemists at LLNL are exploring the impact of rock–water interactions on geologic CO_2 storage to optimize carbon storage operations and reduce the risks of CO_2 leakage. These experiments mimic conditions typical of carbon storage reservoirs deep below the Earth's surface, allowing sampling of fluid chemistry, interrogation of rock properties, and control of temperature and pressure. Using techniques such as 3D x-ray computed tomography to image fluid transport pathways within the experimental cores, 2D scanning electron microscopy to confirm chemical compositions, and nuclear magnetic resonance to reveal molecular structures and interactions, experimental geochemists shed light on the interdependencies between chemistry, material structure, and transport.

Integration of detailed observations of chemical reactivity, structure and mechanical properties, and fluid transport through subsurface materials, with state-of-the-art reactive flow models, enables processes that occur at mineral surfaces to be scaled to engineered systems, such as repositories for radioactive waste *and* greenhouse gases.

A researcher prepares a rock sample for a core-flooding experiment to test its response to carbon dioxide exposure under reservoir temperature and pressure conditions.

Additional research highlights

- Identification of a unique aluminosilicate network structure leading to the development of a new class of cement materials with reduced CO_2 emissions.
- Provision of key kinetic rates to better inform operations of enhanced geothermal energy production.
- Enhanced wellbore integrity prediction via the development of coupled mechanical and chemical process-based models derived from calibrated experiments illustrating when, where, and under what conditions fracture pathways may seal in CO_2 storage wells, reducing risks to groundwater resources.
- Development of improved protocols for reducing corrosion of radioactive waste cannisters.

Tracking the carbon cycle with radiocarbon measurements and modeling

An important element of the carbon cycle is the constant exchange of carbon between the atmosphere and solid earth. Due to human activity—burning fossil fuels, land development, agriculture, etc.—the amount of carbon in the atmosphere has risen, impacting the planet's climate and the carbon cycle itself. How carbon is stored in the soil is a complex and poorly understood interaction between leaf litter, woody debris, and plant roots, the microbes that eat or metabolize this plant matter, and the minerals in soil that sequester carbon from decades to millennia. By examining the factors that influence the amount and age of carbon stored in soil, how plants deposit carbon into soil, and the source of carbon (new or old) released back into the atmosphere, AEED scientists hope to improve our understanding of this complex earth system and its impact on the planet's climate.

Tropical forests account for over half of the global terrestrial carbon sink and 29% of global soil carbon. A recent, ground-breaking, cross-site field study on below-ground carbon dynamics spanned the entire range of moisture regimes in tropical forests. For this study, AEED scientists gathered thousands of tropical soil samples and examined them at the Center for Accelerator Mass Spectrometry at Lawrence Livermore to radiocarbon date soil samples and assess and compare data models, yielding important discoveries about the carbon cycle.

Study findings

- Conversion of primary forest into oil palm plantations in the lowland tropical forests of Peru causes a soil carbon loss of up to 50%.
- 10- to 20-year-old oil palm plantations show some recovery of lost soil carbon.
- Young secondary forests and plantation forests retain a legacy of lost carbon.
- Cooler and wetter sites have more soil carbon.
- Drier sites have younger soil carbon.

Soil yields crucial information about the carbon cycle and climate change.

CENTER FOR ACCELERATOR MASS SPECTROMETRY

Accelerating science at atomic precision

Over the past 30 years, the Center for Accelerator Mass Spectrometry (CAMS) has established itself as a signature capability and user facility at LLNL. CAMS scientists invented the field of biological AMS, and CAMS is an officially recognized user facility for the National Institutes of Health. CAMS has a unique capability for high-energy ion implantation for materials research and is a DOE Nuclear Energy Nuclear Science User facility. CAMS has evolved to provide increasing material science, isotope production, isotopic chemistry, and forensic signature support to the weapons program, the National Ignition Facility, and the Global Security organization. CAMS also has a terrestrial carbon cycle research program focused on elucidating pathways and residence times of carbon in subsurface environments to inform climate models and is one of the primary cosmogenic isotope laboratories serving academia and National Science Foundation communities.

Through the application of both radiocarbon dating and cosmic-ray exposure dating, CAMS has played an important role in revolutionizing the fields of process geomorphology and active tectonics, providing heretofore unobtainable temporal constraints. The ability to date landscape features that are offset due to tectonic activity allows the quantification of millennial slip-rates on active faults, extending the observational range beyond that which can be sampled by land surveying measurements. Further, since the climate influences landscape formation, surface exposure dating—estimating the length of time that a rock has been exposed at or near Earth's surface—enhances the acquisition of terrestrial climate data to complement investigations of ocean sediments.

Researchers from Livermore and institutions worldwide have applied AMS to answer questions in fundamental biology, metabolism, nutrition, toxicology, pharmacology, and more recently, drug development. We have used the ultra sensitivity of AMS to measure metabolites following environmental-level exposures to toxic compounds in humans. In 2019, CAMS researchers used AMS to detect carbon-14 in in vivo testing to develop a potential antidote to the nerve agent sarin by examining how the compound penetrates the blood–brain barrier. The combined scientific capabilities provided by LLNL's supercomputers, AMS instruments, and in vivo testing resources uniquely equip researchers to conduct work relevant to antidote development.

The Center for Accelerator Mass Spectrometry uses state-of-the-art instrumentation to identify and measure trace amounts of various isotopes in samples.

CAMS highlights

- CAMS hosts a 10-MV FN tandem Van de Graaff accelerator, a NEC 1-MV tandem accelerator, and a 250KV single stage AMS deck, as well as a NEC 1.7-MV tandem accelerator for ion beam analysis and microscopy.
- CAMS performs up to 25,000 measurements per year.
- CAMS has collaborated on 1,000+ commercial and academic projects.
- CAMS has hosted 1,300+ faculty and student visitors resulting in 300+ PhD and master's degrees over the past 30 years; 30+ CAMS students and postdocs have become LLNL employees.
- CAMS facilities were used to determine the first millennial slip-rate determinations on the San Andreas Fault and to constrain earthquake recurrence intervals through first-of-its-kind direct dating of exposed bedrock fault scarps.

Solving crimes by analyzing isotopic signatures

LLNL scientists take advantage of the pulse of carbon-14 produced from the atmospheric testing of nuclear weapons from 1955 to 1963 to not only study storage of greenhouse gases in soils and date archeological specimens but also to explore key biological processes as well. Since aboveground testing was banned in 1963, atmospheric carbon-14 levels have been dropping due to diffusion, as carbon dioxide is incorporated into plants by photosynthesis and mixed with marine and terrestrial carbon reservoirs. Increased combustion of fossil fuels further contributes to the increase of carbon dioxide levels and the decline of carbon-14 in the atmosphere. Because humans eat plants, and animals that feed on plants, the concentration of carbon-14 in the human body closely parallels atmospheric concentrations. Thus, the rapid rise, sharp peak, and exponential decline of atmospheric carbon provides new opportunities to date biological samples more precisely.

At LLNL, our scientists leveraged the parallel trends between atmospheric and human carbon-14 levels, along with our expertise in isotope forensics, to develop a unique technique known as radiocarbon bomb-pulse dating. Using LLNL's powerful accelerator mass spectrometry instruments, researchers analyze isotopic signatures in biological material generated in recent decades. They measure molecular or cellular turnover with high precision and estimate the age of bio-based material. The capability expands carbon-14 dating from an archeological tool to a forensic science tool that can help law enforcement agencies solve crimes.

At LLNL's Center for Accelerator Mass Spectrometry, a suite of unique instrumentation enables scientists to analyze radioactive isotopes in bio-based samples, providing insight regarding the age of unknown biological material.

Forensics research highlights

- LLNL scientists use carbon-14 dating to help identify human remains and solve cold cases. By measuring the presence of carbon-14 in bones, teeth, or hair, they can determine an approximate date of birth and death. Investigators use this information to rule out potential victims and limit the possibilities to a smaller group of missing persons.
- LLNL scientists assist in investigations of illegal trafficking of bio-based material. They analyzed elephant tusks confiscated by law enforcement officials and determined that the elephants were killed after an international ban on ivory trading was put into effect—providing evidence needed to prosecute poachers.

FUTURE EARTH SCIENCE RESEARCH

Geophysical monitoring

The Geophysical Monitoring Program at LLNL continues to maintain strong sponsor support for a combination of numerical modeling, earth models development, Nevada National Security Site fieldwork, and detonation source physics research. Planned near-term efforts include the Phase 3 Source Physics Experiments (SPE); integration of seismology, geophysics, geomechanics, hydrology, and atmospheric transport with advanced data fusion methods for the Low-Yield Nuclear Monitoring (LYNM) effort (our fastest-growing activity); and surface experiments in support of the Defense Threat Reduction Agency.

Nonproliferation stewardship and nuclear-testing-policy-related work, such as nuclear test limitations and seismic cooperation, will be our biggest potential growth areas. The former affords us a chance to incorporate data science methods into our seismic monitoring work and the latter an opportunity for greater interaction with the international community. Leveraging our division's expertise in both energy and national security, we will also increase our work at the intersection of these two application areas by performing fundamental research to understand and measure changes in the Earth's subsurface. For instance, reservoir modeling, detonation aftershocks, and induced seismicity related to energy production all operate at scales relevant to monitoring energy and national security applications.

The monitoring program relies on the availability of data science experts to analyze large data sets. We need to redouble efforts to hire, train, and retain data geoscientists and other experts in advanced applied computational methods to solid earth geophysics. Training our current geoscientist staff on basic data science and machine-learning concepts through workshops would also enhance collaboration with computational experts. We encourage staff to work on both energy and national security problems to ensure the transfer of relevant expertise and techniques across applications.

The availability of high-performance computing resources, particularly resources that support data science research, is a continuing programmatic requirement. We anticipate that the new LLNL Nonproliferation Stewardship Program will stand up hardware and software resources that will benefit our work. As our programs grow, we ultimately envision a "monitoring program in the cloud," with the appropriate infrastructure in place to enable access in near-real time to software and tools that the sponsor and user community can employ.

Workers at the Nevada Nuclear Security Site lower the 25-foot-long Source Physics Experiment cannister into the borehole to its center depth of 76.5 meters in preparation for a shot in 2016.

Fossil fuel and geothermal energy

AEED researchers maintain a broad portfolio of fossil fuel and geothermal energy projects to support industry partners and government agencies. While the bulk of our energy research involves computer simulation, we also perform experiments with our state-of-the-art hydrothermal laboratory and nuclear magnetic resonance facility. Much of our work has focused on oil and gas stimulation, carbon sequestration, and geothermal energy, leveraging our extensive experience with subsurface science, reactive transport, fracture mechanics, and induced seismicity. Going forward, we will continue to combine expertise across all subsurface, chemical, and physical disciplines.

Efficient, environmentally sustainable subsurface energy production depends on optimal characterization and monitoring of subsurface reservoirs—a challenging proposition because the subsurface is highly heterogeneous and no one monitoring technique provides a true image of what is below ground. A range of approaches for improvement exist, but we expect the most effective approach will combine field measurements with computer modeling. Our earth science expertise and strengths in computer modeling, data analysis, and signal processing provide solid foundations for growth in this area. We will focus our efforts on how best to employ new tools and techniques to analyze and exploit the vast quantities of data from field experiments and models to better understand the subsurface at all scales. Emerging machine-learning algorithms allow us to combine and analyze data in unique ways to customize multimodal data fusion for a broad range of subsurface energy applications.

Our hardware and software resources position us to diversify the scope of applications. Leveraging recent investments in GEOSX, we will support efforts in conventional oil and gas production, assisting industry in avoiding problematic sites for these production operations. We will also perform next-generation, reservoir-scale simulations, using our strength in geomechanics, flow, and transport. This capability will also benefit carbon sequestration, environmental management, nuclear monitoring, nuclear waste storage, and even weapons applications. By applying techniques developed for national security applications, we will study induced seismicity from source to sink.

Other opportunities include the development of new monitoring instruments. This is particularly true for fiber-based sensors that build on recent investments and will be tested in geothermal field demonstrations as part of ongoing research collaborations, such as the EGS-Collab and FORGE. EGS-Collab and FORGE are two Department of Energy field research facilities dedicated to enhanced geothermal energy production. Other nonintrusive measurement technologies are greatly needed. For instance, development of a sensor capability for measuring subsurface strains and displacements obviates the need for drilling through a fault. Such a system will allow us to refine earthquake locations and reduce uncertainty without deploying time-consuming and expensive seismic instrumentation and active source work. Any sensor development efforts will be done in collaboration with Engineering and other relevant staff, such as the Fiber Laser Group, where appropriate.

Growth opportunities are numerous, but to realize them, we need to initiate a strategic, coordinated effort to expand our interdisciplinary modeling capabilities. Where feasible, we will also ensure that any significant new capabilities we develop are code agnostic for broadest utility. A modular approach will work best. We will also address staffing. We need researchers who can add reactive transport model capabilities and couple them to flow and mechanics, organic chemists to work on oil and gas geochemistry problems, new seismology staff to tackle energy-related problems, and computational scientists with experience in applied geoscience machine learning.

LLNL reservoir engineers, hydrologists, and geochemists couple modeling and analysis with field studies to quantify fluid movements in the subsurface and important rock–water interactions that control water composition and transport of contaminants.

Carbon management

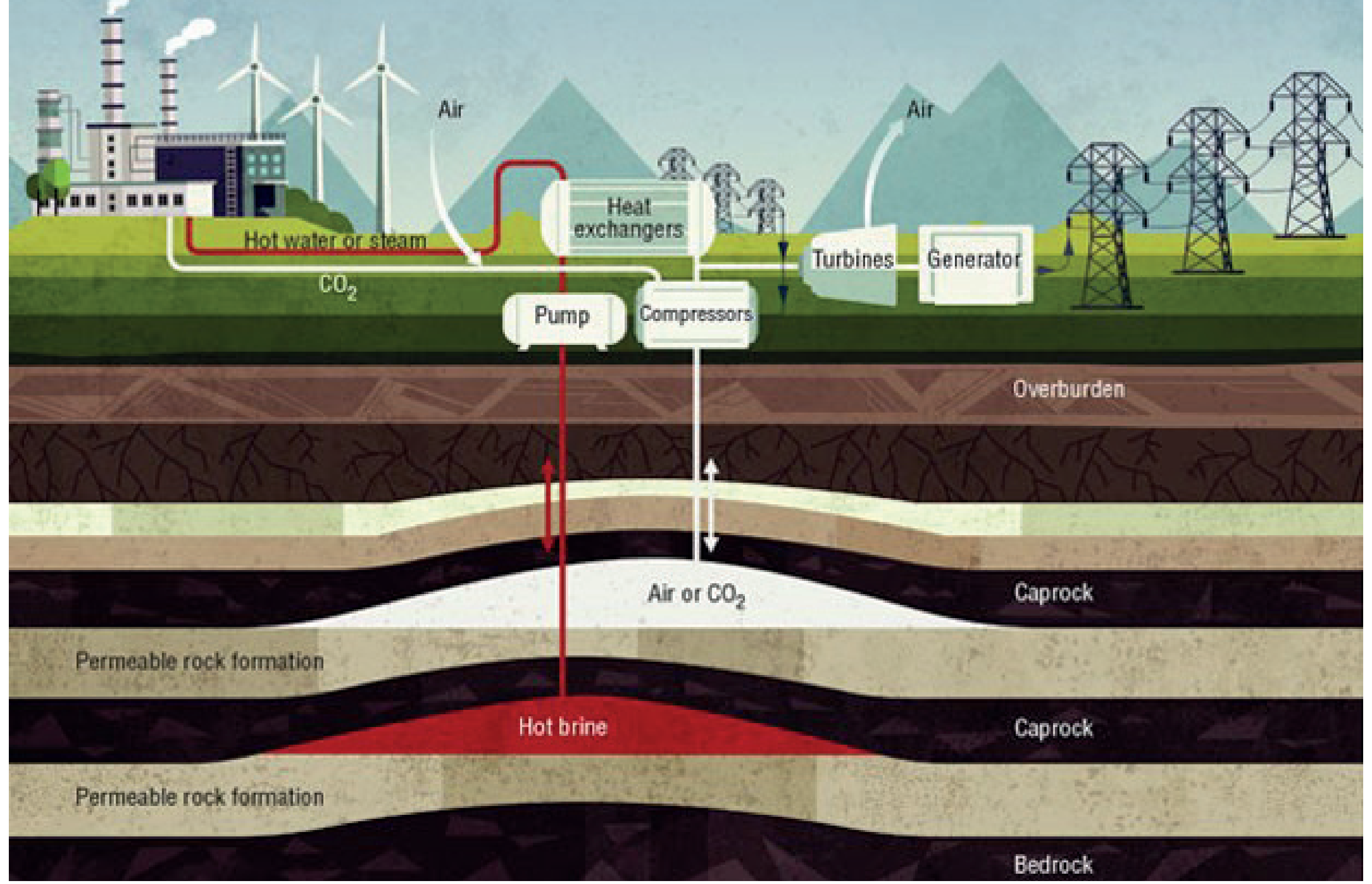
Our current understanding of the climate problem shows that permanent removal of CO_2 from the air will be necessary to reach our climate goals—most of that removed CO_2 will have to be stored in either deep geologic formations or soils. AEED will continue to pursue research relevant to these issues, which will require the establishment of multidisciplinary teams with expertise in reservoir processes, biogeochemistry, reactive transport, seismology, and engineering along with techno-economic analysis of proposed solutions.

In the area of geologic carbon storage, we have advanced the science in challenging areas such as how to limit physical and chemical damage to cap rocks and wellbores needed to securely store carbon in geologic formations and how to monitor and quickly detect leaks to limit impacts to drinking water. Now that the risks are understood and can be managed, we will turn our focus to the implementation of geologic carbon storage on the industrial scale necessary to meet climate goals. This is a topic of growing interest in California and sits at the intersection of science, engineering, public policy, and environmental concern. LLNL is already working with a number of private and public entities in pursuit of these goals and is well positioned to serve as an advisor with the capability and credibility to provide geological information as part of project screening and permit review stages, and to assist with project oversight. With staff that possess a solid grounding in policy, in addition to technical expertise, we will navigate and facilitate the practical steps necessary to work with partners to launch new carbon storage projects, including site selection.

The inherent uncertainty of properties and structure of the subsurface and their influence on the performance of energy production and storage operations can be refined by iterative application of simulation and reservoir monitoring, which may include the evolution of fluid pressure and stress, induced seismicity, chemical evolution of formation waters, and hydrocarbon production. To accomplish this kind of iterative improvement of subsurface characterization and response, our models must simulate the relevant geophysical and hydrologic observables. Our ongoing collaboration with industrial and university partners will allow us to combine the GEOSX computational framework and geomechanical capabilities with our partners' reservoir simulation expertise. The result will be a new code that can be made accessible to a broad base of collaborators.

Our goal in reservoir modeling is to develop models that use LLNL's cutting-edge computational capabilities and to integrate reservoir processes and geophysical and hydrologic response in a unified framework. For us to grow this capability we need to increase the number of staff with skills that intersect geomechanics, geophysics, and seismology. Similarly, geologic carbon storage is more than a technical issue and will involve collaboration between technical experts within the Laboratory and industry, navigation of the evolving regulatory framework, techno-economic feasibility, and public outreach. We will need to hire additional staff with broad-based skills in carbon management, policy, and systems research, who will work closely with subsurface subject-matter experts.

Most terrestrial carbon is stored in soils, and the preservation and enhancement of carbon storage in soils can play an important role in influencing the evolution of carbon in the atmosphere. Given our existing strengths in AEED and the Nuclear and Chemical Sciences division, including the Center for Accelerator Mass Spectrometry, we are poised



Livermore's Earth Battery concept stores compressed air or CO_2 underground as a renewable energy resource.

to apply a combination of large-scale modeling, field measurements, and carbon-14 analysis to a range of soil carbon monitoring efforts. Carbon-14 remains a gold standard for making detailed measurements of how carbon behaves in soil. As with weather modeling, hundreds or thousands of geographically dispersed measurements will be paired with a robust model to provide accurate predictions of the evolving soil carbon inventory, which will be integrated with earth systems models, such as E3SM, to provide a platform for unifying existing data, planning future experiments, and ultimately, constraining the role of carbon storage in soils on the evolution of carbon in the atmosphere.

Understanding the processes that control soil carbon may require the development of additional compound-specific carbon-14 capabilities to track mechanisms of soil carbon accumulation, or even acquisition of a field-deployable carbon-14 measurement system. Partnerships with organizations outside LLNL will also be beneficial. For instance, the Department of Agriculture would be a key partner for soil carbon work and the National Renewable Energy Laboratory for systems analysis. Importantly, we will also establish strategic partnerships with universities with strong programs in soil science and energy policy to build a pipeline for new staff in carbon management.

FUTURE ATMOSPHERIC SCIENCE RESEARCH

Climate impacts

Many of the observed and predicted impacts of climate change, such as sea level rise, shrinking ice sheets, and glacial retreat, can be linked to the rise of average global temperature. The occurrence of extreme climate events, including heat waves, droughts, floods, cyclones, and wildfires, result in the alteration of ecosystems, disruption of food production and water supply, and damage to infrastructure and settlements. How well our current climate models predict the frequency, severity, and regional distribution of such extreme events is of critical concern.

LLNL is in a unique position to combine our strengths in climate and computer science with our national security mission to address climate impacts and vulnerability. We envision a future where climate change analyses are regarded as an essential consideration for many existing research efforts the Laboratory undertakes, rather than independent projects, because climate change can act as an accelerant to existing stresses.

Fundamentally, we are still focused on understanding the relationships between changing greenhouse gas concentrations and their impact on the water cycle. The challenge arises from the fact that global phenomena affect local weather, calling for global models with very fine resolution. Our climate scientists are already addressing climate impacts using the power of E3SM to understand the ocean's most energetic movements and the largest storms in Earth's atmosphere. Exploring climate impacts and vulnerabilities should also involve rigorous statistical analysis of existing models and comparison with observations, similar to those performed in the Program for Climate Model Diagnosis and Intercomparison project, to plan future mitigation and adaptation strategies. The statistical analysis in this case necessarily involves extreme value analysis, a branch of statistics dealing with radical, remarkable deviations from the median of probability distributions, an expertise increasingly in demand at LLNL, and likely beneficial in subsurface analysis and life sciences disciplines as well.

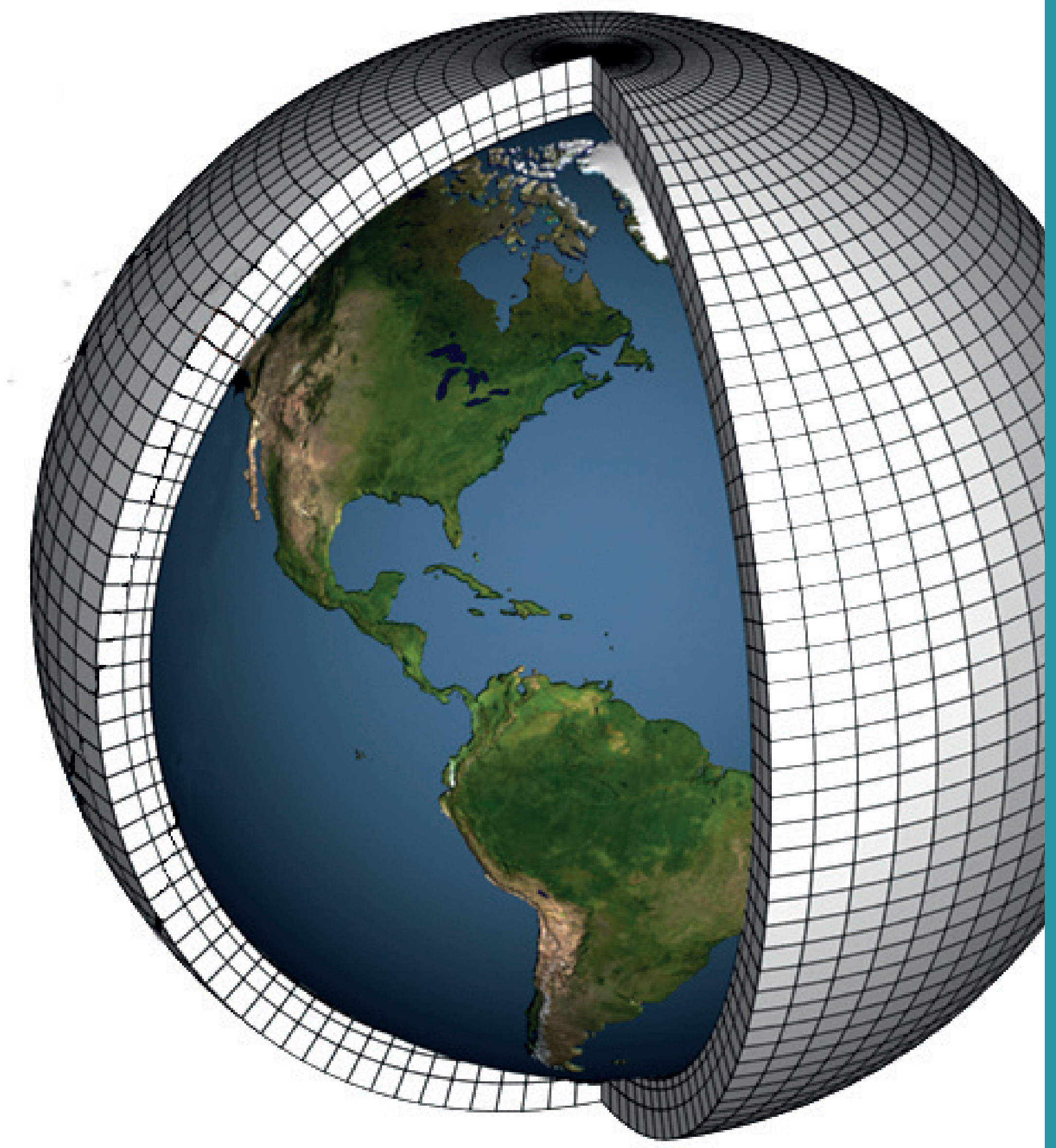
As mentioned, climate change will accelerate changes to existing conditions that will impact how the nation invests in energy and hydrologic infrastructure, and how we respond to emerging areas of unrest caused by drought, food scarcity, and sea level rise. AEED researchers have developed and refined global models to feature increasingly finer resolution and greater accuracy. Model capability has progressed to the point that we can downscale model output and use it to explore the impacts of various aspects of climate change on a local level to inform investments and policies important to energy and national security.

With our climate science capabilities and national security focus, we will make useful, timely contributions, especially by employing the latest machine-learning (ML) tools. One such ML approach being developed for a Laboratory Directed Research and Development project on regional snowpack prediction will be applied to a wide range of climate impact problems, such as wildfires, drought, streamflow, wind/solar resources, and coastal flooding. If done thoughtfully, an ML-based workflow will allow us to leverage much of our existing simulation and observational data to solve new challenges faster and more efficiently. It will also help ensure that existing efforts that draw on historical climate data, such as National Atmospheric Advisory Center operations, maintain their accuracy despite ever-evolving regional atmospheric conditions.

Geoengineering, a proposal to mitigate climate change by modifying the atmosphere's aerosol content, also sits at the intersection of climate change and national security. We will leverage our climate modeling expertise in collaboration with the Laboratory's Z program in Global Security to explore the desirable and undesirable global and regional consequences of geoengineering projects other countries might consider.

Climate impacts will be a growth area for AEED and E and Z programs at LLNL. We will expand our research to energy and national security by hiring atmospheric scientists motivated to use climate models to make the world more resilient to climate change.

Climate models divide Earth into a grid with vertical and horizontal intervals. The smaller the intervals, the finer the grid, and the better the resolution of the model—that is, the greater detail the model can produce.



High-altitude atmospheric science

The Departments of Defense and Energy want to characterize the stratosphere to understand what causes turbulence to better enable hypersonic or supersonic aircraft or reentry vehicles. This requires studying the stratosphere over small temporal and spatial scales to capture a phenomenon called boundary-layer transition. At hypersonic or supersonic speeds, a very thin boundary layer forms around the vehicle. Any small-scale disturbance mode in the atmosphere (centimeter- to millimeter-scale turbulence or an aerosol particle impact) entering the vehicle's boundary layer will create unexpected heating and aerodynamic loads on the vehicle, negatively impacting flight performance. There is a critical need for observations across length and time scales relevant to boost–glide vehicles and payloads that travel through or fly at these higher altitudes (30–60 kilometers).

Atmospheric researchers, including those in AEED, study the stratospheric ozone, stratospheric large-scale circulations, tropospheric/stratospheric interactions, and other climate-related phenomena. The primary approach uses atmospheric tracers such as aerosols or long-lived gases to quantify and understand transport and vertical exchange characteristics. In the future, AEED's unique modeling and measurement expertise will be used to address issues of importance for hypersonic or supersonic flight.

Our aim is to use observational data in the stratosphere, to validate whole atmospheric models, and to gain a better mechanistic understanding of high-altitude dynamics. In situ measurements of atmospheric motion, turbulence, aerosols, and other disturbance modes in the stratosphere are relatively rare. These data are difficult to come by because most commercial aircraft fly too low, stratospheric balloons are rarely deployed and have short flight paths, and satellite sensors currently cannot diagnose turbulent structures on fine enough length scales. It is important to resolve this gap, as the number of flight vehicles or reentry vehicles that fly or pass through the stratosphere increases and affects national security. One such effort at LLNL involving AEED scientists is the design and development of a new satellite instrument to make in situ measurements at the appropriate length scales. Another effort involves the collaboration between atmospheric and CAMS scientists and cross-country balloon deployment.

CAMS facilities can precisely measure very small quantities of stratospheric isotopes like ^{14}C, ^{10}Be, and ^{7}Be found in aerosols collected with stratospheric balloons. We will collaborate with space and weapon programs across LLNL, other national laboratories, the Department of Defense, the National Aeronautics and Space Administration, the National Oceanic and Atmospheric Administration, the National Center for Atmospheric Research, and universities to expand AEED's hypersonic–stratospheric science research efforts and to build a new capability within the Director's Hypersonic Initiative. AEED will need to allocate laboratory space and equipment to design, build, and test instrumentation and sensors. Collaborations with the Engineering Directorate will allow for laboratory access, and just as importantly, provide the engineers and technicians to help design, fabricate, and maintain samplers and sensors. Site 300 will provide an ideal test bed location for conducting balloon launches.

In previous studies, LLNL scientists collected air by high-altitude balloon flights and measured the carbon-14 content of carbon dioxide in the air.

CENTER FOR ACCELERATOR MASS SPECTROMETRY

Users come to CAMS for its combination of accessibility and unique capabilities. As accelerators shrink and more institutions have the option for in-house analysis, we will develop new capabilities to grow and maintain our user base. Additionally, expanding the center's capabilities beyond mass spectrometry will also increase its relevance to Laboratory programs. One such capability under consideration uses two ion beams to simultaneously implant ions onto a single target. A promising technique for studying materials aging for weapons applications, it allows us to faithfully mimic the natural aging process. The same technology could create targets for other national security platforms, such as the National Ignition Facility, to study radiation effects. Another unique capability under development involves a new method for measuring nuclear cross sections of short-lived radioactive targets by installing a gas-filled magnet to open up the range of ultra-trace isotopes detected. Such a capability will have relevance to ongoing and future Weapons and Complex Integration and nuclear forensics work.

Looking ahead, we seek to capitalize on existing strengths in CAMS research in the areas of geology and biology. We have a small but long-running carbon cycle research program that focuses on understanding the residence times and paths of carbon in soil in support of global climate mitigation. We will build on these efforts and explore some related questions, such as, "What elements are crucial to maintaining soil productivity?" By partnering with our geoscience systems expertise, we will transition fundamental science to models that inform and impact land use policies. We will also combine radioactive carbon dating, seismology, and high-performance computing to measure the recurrence interval for large earthquakes at resolutions fine enough to inform building codes and reliability of critical infrastructure. LLNL will expand our impact by furthering collaboration with the U.S. Geological Survey and organizations like the Southern California Earthquake Center. Many isotopes CAMS measures for geosciences projects also hold national security interest.

CAMS provides reliable and respected tools for carbon management research. The laser-based, carbon-14 spectrometer we constructed to supplement LLNL's AMS capabilities opens up new collaboration opportunities, particularly in the field of natural radiocarbon. We are currently partnering with industry to quantify carbon-14 in various batches of petroleum products, for instance, as an accounting metric for novel protocols such as California's Low Carbon Fuel Standard, intended to reduce the carbon intensity of transportation fuels. Such work will evolve into broader emissions monitoring efforts in collaboration with regulatory agencies once we demonstrate our value as objective scientific evaluators. Further hardware development will likely be needed as this work expands.

Now that CAMS has successfully established the BioAMS User Facility, we need to find ways to grow sponsor support for fundamental research and development work. We will grow the user base within and beyond the Laboratory through a combination of forensic science projects, university collaborations, and National Institutes of Health center collaborations. To do so, we plan to focus on two specific areas where we have built a reputation for expertise and excellence: pharmacological toxicology and cancer prevention. We are currently gathering approvals to perform human micro-dosing studies that will help us understand biomarkers of exposure and the efficacy of countermeasures. In time, we will develop a technique for determining if an individual has been exposed to a specific toxin.

Since it began operations in 1987, CAMS has been a cornerstone facility for LLNL. Ensuring its vitality and ability to meet future mission needs will require facility renovation. We therefore envision a "CAMS 2.0," with an enlarged building footprint that will provide much-needed space for new instrumentation and capabilities as well as refurbished infrastructure.

Lawrence Livermore's Center for Accelerator Mass Spectrometry encompasses a dozen experimental and preparation laboratories. The FN tandem Van de Graaff accelerator is the center's principal instrument and can run a single radiocarbon sample in about 15 minutes.

CROSS-CUTTING CAPABILITIES

AEED computational strategy

Computing plays an essential role in the science we do in AEED. Planning for future computing resources and capabilities is complicated, however, because computing hardware is presently undergoing dramatic and disruptive changes. The push for scalable platforms at a reasonable energy budget is driving a dramatic hardware evolution, and these new platforms require application developers to heavily modify or rewrite their codes to achieve good performance. With these challenges, though, come opportunities. For instance, specialized hardware platforms such as data science-centered architectures are becoming more readily available, as are machine-learning (ML) approaches and technology.

AEED will develop a comprehensive strategy for ensuring that significant hardware and software advances are integrated into the division's diverse research efforts. The Laboratory has committed significant resources to ensuring LLNL applications are reliable and scalable. Where possible, AEED will take advantage of existing code upgrade efforts and tools, such as RAJA and similar RADIUSS tools, to support such efforts. RAJA enables applications to be portable across diverse hardware architectures without major source code disruption. In the instances where AEED's code modernization needs diverge from those of the Advanced Simulation and Computing Program, AEED will advocate for customization so that our code developers have the tools and resources they need to make codes ready for exascale, and subsequent architectures.

At this stage of the evolution of computing architectures, pursuing an independent path for code modernization grows less and less practical. As much as possible, we want to take a modular approach to code modernization, selecting general-purpose code components created and maintained by LLNL and other national laboratories that are likely to be enduring and widely used. This solution ensures that our codes are kept up to date without requiring extensive maintenance, so our teams can focus on the science.

We are starting to see ML adopted within AEED, and it has tremendous potential for wider adoption over the next few years. We envision a computing future that is less focused on running heroic-scale calculations and more on running large ensembles of calculations simultaneously. Large ensembles, however, are computationally expensive. By incorporating ML approaches, we will be able to run less-demanding "smarter" ensembles—using a tool that launches simulations, monitors them, stops those that are redundant or useless, and chooses new runs to fill gaps in sampling as needed—that achieve the same results as running a full ensemble. Broad adoption of these techniques will necessitate the development of a flexible ML framework that we can deploy across the full range of AEED applications.

Heterogeneity is ubiquitous in earth and atmospheric science, and it is an area where, with the right tools and techniques, we will demonstrate scientific leadership. Part of the challenge is capturing the micro-scale physics that manifest in reservoir- or global-scale phenomena. This challenge will be addressed, in part, by developing embedded multiscale modeling—on demand within a large calculation. The other challenge involves capturing the Earth's variability and will be addressed by combining embedded multi-scale modeling with ML to run large-ensemble calculations to capture the range of outcomes, often referred to as uncertainty quantification (UQ). We will develop methods for using UQ for autotuning—choosing the parameter settings that optimize agreement with observations. UQ techniques will also be applied to related problems, such as source reconstruction in earth and atmospheric science. Making UQ a routine part of problem solving in AEED will have a tremendous impact on our research, but it will require gaining access to relevant hardware, modifying workflows to smoothly incorporate UQ processes, and training staff on UQ methods.

Fundamentally, realization of our vision for AEED computing will require access to the right hardware resources, tools for enabling optimal software performance on cutting-edge architectures, and the availability of computational experts committed to supporting atmospheric and earth science.

Modeling and simulation drive much of the earth and atmospheric science research in AEED.

AEED experimental strategy

Sustaining and growing a robust experimental portfolio to balance and complement AEED's strengths in computation and simulation is a priority for AEED. To do so will require a combination of strategic experimentalist hires and equipment investments, as well as a thoughtful strategy to ensure that the research pursued aligns with division strengths, strategic growth areas, and national needs.

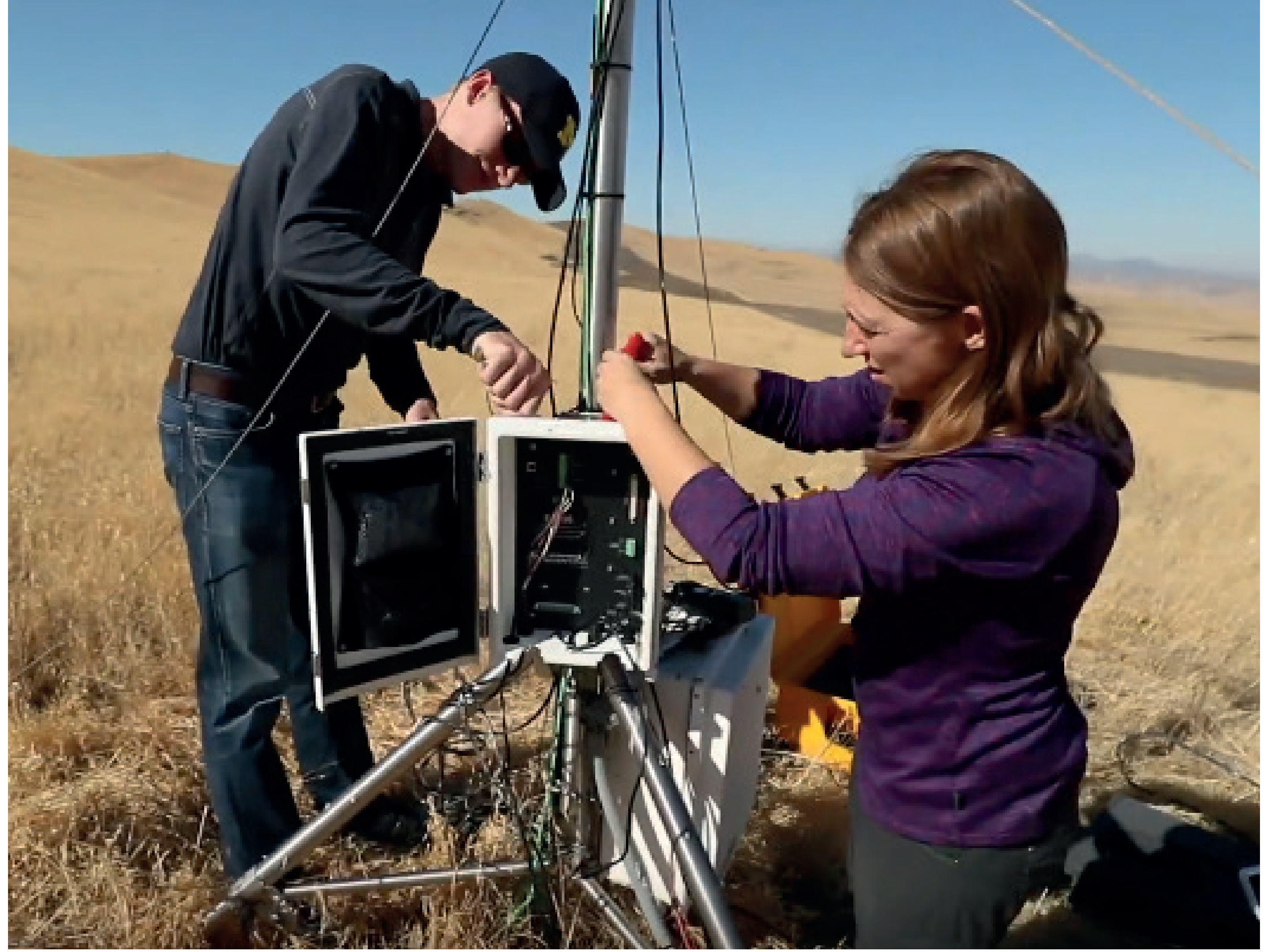
AEED experimentalists will leverage their experience in performing science at the extremes to a wide range of mission-directed research efforts. High pressures, high temperatures, high ionic strengths, and long timescales are commonplace in geology, but often considered extreme in the realm of materials science and chemistry and can be critically important for understanding failure modes and designing resilient systems. AEED researchers will also apply notable expertise in coupling mechanical and chemical reactions across physical and temporal scales, coupling high-quality data observation with newly developed coupled codes—effects often considered independently in LLNL research.

If carefully planned and coordinated to support the LLNL missions, research investments in chemo-mechanical effects on corrosion, material degradation, and even synthesis will also drive innovation in the geosciences and increase our competitiveness in these areas. We currently have the capability to investigate chemical reactions under hydrostatic conditions, but investment in equipment to look at material reactions under shear, high temperatures, and tension will enhance our capabilities.

AEED experimental efforts will add value to a wide range of Laboratory research efforts. Carbon capture and storage, hydrogen storage, and natural gas storage are all areas where the experimentalists in AEED will have a much larger footprint by exploring, through experiments and field work, the effects of rock and mineral weathering (either engineered or natural). We will also pursue greater engagement with the Laboratory for Energy Applications for the Future on mechanical and chemical characterization of new materials. Areas such as high-temperature and flow battery development will benefit from in situ measurement techniques developed by AEED. For Weapons and Complex Integration programs, there are opportunities to increase AEED experimentalist involvement in studying material aging and degradation and coupled chemical and mechanical experiments. Stratospheric research to support national security is also an area ripe for further exploration. Further discussion with Global Security and Forensic Science Center staff will generate further ideas for potential experimental collaboration in support of Livermore's mission.

With some strategic investments and collaborations, AEED's experimental facilities and capabilities will be well positioned to support experimental program growth. Our geochemistry lab, renovated a decade ago, will support LLNL's carbon capture and storage and materials at extreme conditions research. With some investments in automation for in-line sampling and analysis, we will expand into new areas, such as monitoring in situ degradation mechanisms. The 400-ton press in the geomechanics lab is used to support N Program but will also benefit additive manufacturing work. Additionally, this press can easily be converted to different types of anvils for pressures greater than 5 gigapascals with small investments in anvil, flow, and temperature control or resistive measurements. The Center for Accelerator Mass Spectrometry is another key AEED asset.

By more tightly integrating geoscience and atmospheric experimental and field efforts with some of Livermore's major programs and initiatives, we will expand our experimental capabilities, staff, and expertise and impact a broader range of research at the Laboratory.



AEED atmospheric scientists perform maintenance on wind measurement equipment at Site 300.

OUR PEOPLE

Our scientific and technical accomplishments over the past 60 years set the stage for our future. We will apply our expertise, technologies, and facilities to new challenges that will maintain our division's vitality and relevance in the years ahead. Our organization is far more than its scientific and technical achievements. We are team of 160 people, most of whom are Ph.D. scientists, and all of whom are committed to working together to solve the nation's and the world's most pressing energy, climate, and national security problems.

Our division thrives because we take the time to listen to each other's ideas, and just as we leverage our different areas of technical expertise, we draw on each other's differences to form even better working relationships. We are committed to creating a diverse workforce to capitalize on the benefits that can come from a range of backgrounds, experiences, and perspectives. To build a workforce that mirrors the U.S. population, we have implemented a comprehensive set of recruiting and hiring practices to foster a more effective, fair, and objective process based on current best practices.

We are proud of our previous successes and look forward to the next 60 years.

Photo of the division, taken in front of Building 170, home to most of AEED's atmospheric scientists.

Our division thrives because we take the time to listen to each other's ideas

AEED
Atmospheric, Earth, & Energy Division

pls.llnl.gov/aeed