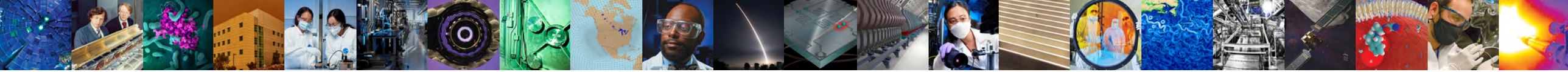


SCIENCE AND TECHNOLOGY

Expanding the boundaries of scientific knowledge and advancing the technological state of the art to solve problems of national and global importance

In addition to LLNL's extensive use of high-performance computing to support response to the COVID-19 pandemic, experiments at the Laboratory showed that thermal inactivation is a potential widely deployable method for reuse of N95 respirators.

THROUGH ITS SCIENCE AND technology capabilities, Livermore makes fundamental discoveries about nature, develops innovative technologies that improve life and drive the economy, and carries out its mission to improve national security.

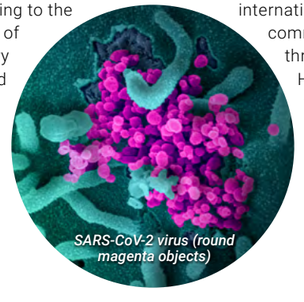
ADVANCES IN MACHINE LEARNING

Machine learning (ML) is finding wide-ranging applications at LLNL, with many focused on accelerating scientific discovery. For example, Laboratory materials and computer scientists developed an ML model that can quickly and accurately predict 3D crystalline properties of molecules (e.g., density) from their 2D chemical structures. Researchers are using the model to search for new insensitive high-explosive materials. Crystalline density is closely correlated with an energetic's potential performance. LLNL researchers are also pioneering the application of neural networks to study ion acceleration from targets impacted with a high-intensity short laser pulse. The space of experimental parameters of interest is extremely large. The neural network was trained by an ensemble of more than 1,000 simulations, which only sparsely filled the space. The network acted as a surrogate physics model to explore and discover intriguing features in regions of scientific interest. This approach is widely applicable. LLNL researchers co-authored a paper—in the May 21, 2021, issue of the journal *Nature*—that discusses future directions and challenges in similarly applying ML to accelerate nuclear fusion research.

In December 2020, two LLNL scientists presented papers at the 34th Conference on Neural Information Processing Systems, the world's most prestigious ML conference. They addressed issues pertaining to the reliability and robustness of ML algorithms. Laboratory researchers also presented a paper in May 2021 at the International Conference on Learning Representations. They developed a novel framework for a type of discrete optimization called symbolic regression. It outperforms several common benchmarks, including commercial software gold standards. At LLNL, the framework is being used to find short mathematical expressions that fit large data sets gathered from experiments.

RESPONDING TO COVID-19

LLNL provided high-performance computing (HPC) resources to the international research community in FY 2021 through the COVID-19 HPC Consortium and the National Virtual Biotechnology Laboratory formed by DOE. Among the Laboratory's many contributions to the overall HPC effort, a team of biologists and computer scientists developed an ML-training capability that greatly assists the search for therapeutics (e.g., small molecule antivirals). They trained a novel, high-quality molecular design model on 1.6 billion compounds in 23 minutes. The previous state-of-the-art solution required a day for only 1 million compounds. A complementary computational pipeline focused on developing therapeutic antibodies. Promising candidates from both efforts were screened for antiviral properties using a suite of in-vitro and in-vivo assays.



SARS-CoV-2 virus (round magenta objects)

Experimental activities also supported our nation's COVID-19 response. LLNL scientists determined that heating N95 respirators up to 75°C for 30 minutes deactivates a surrogate coronavirus without compromising the device's fit and its ability to filter airborne particles. This type of thermal inactivation offers a widely deployable method for reuse of N95 respirators in emergency situations. Other LLNL research teams leveraged their extensive experience studying the dispersion of airborne hazards to better understand the movement of virus-like particles, supporting efforts to identify countermeasures. A Laboratory-developed tool, DNATrax, allows scientists to study the movement of low concentrations of airborne particles.

MOVING TO EXASCALE COMPUTING

With the future delivery of El Capitan (see p. 7), LLNL is fully engaged in the next phase of supercomputing. Exascale machines will be able to process an exaflop—a quintillion (10^{18}) calculations per second. This technological leap offers DOE exciting opportunities to advance its national security, science, and technology-transfer missions; but it also presents enormous challenges. Funded by NNSA and DOE's Office of Science, DOE's Exascale Computing Project (ECP) is focused on application development, software technologies, and hardware and integration, with the goal of providing a comprehensive and reliable exascale computing ecosystem.

Livermore staff hold key leadership positions in ECP and participate in many projects. ECP coordinates development activities through six co-design centers that draw on multidisplinary expertise from across the DOE laboratories. An LLNL computer scientist leads the co-design Center for Efficient Exascale Discretizations, and LLNL researchers are engaged in two other centers.

An important focus within the Laboratory is the development and usage of sustainable software—ensuring that it is interoperable across computer architectures, maintainable, and dependable. LLNL's RADIUSS project is deploying and encouraging use across the institution of a common base of foundational scientific software consisting largely of open-source products, many of which have been developed at the Laboratory.

The exascale El Capitan supercomputer (depicted here) is scheduled to arrive at LLNL in 2023.

This strategy will reduce long-term software costs and increase Livermore's ability to respond rapidly to emerging programmatic needs. LLNL is a global leader in the development of open-source scientific software solutions that attract collaborators and benefit from their contributions. RADIUSS parallels similar efforts within ECP, in which a Livermore computer scientist heads the project's Extreme-Scale Scientific Software Development Kit effort.

PLANETARY DEFENSE STUDIES

In April 2021, LLNL researchers took part in the seventh International Academy of Astronautics Planetary Defense Conference (PDC). The virtual conference brought together an international group of experts, with Laboratory participants giving presentations on a wide range of topics. The scenario featured at PDC was asteroid disintegration into well-dispersed fragments, which would be necessary if there is little warning and if deflection (the preferred method) is not feasible. Livermore scientists have performed detailed simulations of high-yield nuclear device detonations a few meters from a 100-meter-diameter asteroid two months before expected impact. The fraction of impacting mass would be reduced by a factor of 1,000. Livermore researchers are conducting modeling studies in support of the National Aeronautics and Space Administration's upcoming planetary defense test, which is targeted at an asteroid called Dimorphos.