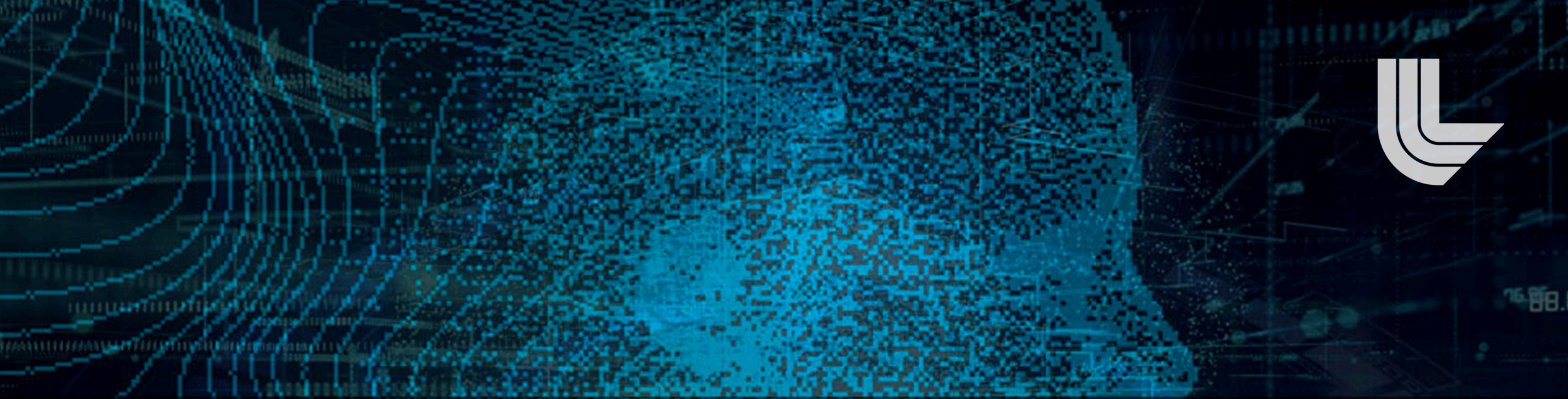


Cognitive Simulation at LLNL

Integrating artificial intelligence with high-performance computing and experiments for science and security missions.

Introduction

Institutional Initiatives reflect Lawrence Livermore National Laboratory's (LLNL's) "team science" approach and support the Laboratory's institutional mission by anticipating issues of national importance. LLNL's Cognitive Simulation Institutional Initiative aims to accelerate the integration of AI, high-performance computing, and empirical data for a range of scientific applications. Our researchers focus on inertial confinement fusion and high-energy-density (HED) projects crucial to stewardship of the nation's nuclear stockpile, then use these results to seed new opportunities across other mission areas, including climate studies, AI-driven manufacturing, and biosecurity projects modeling disease spread and drug design.

Cognitive simulation (CogSim) models use artificial intelligence (AI) to combine our simulation capabilities with high-quality experimental datasets.

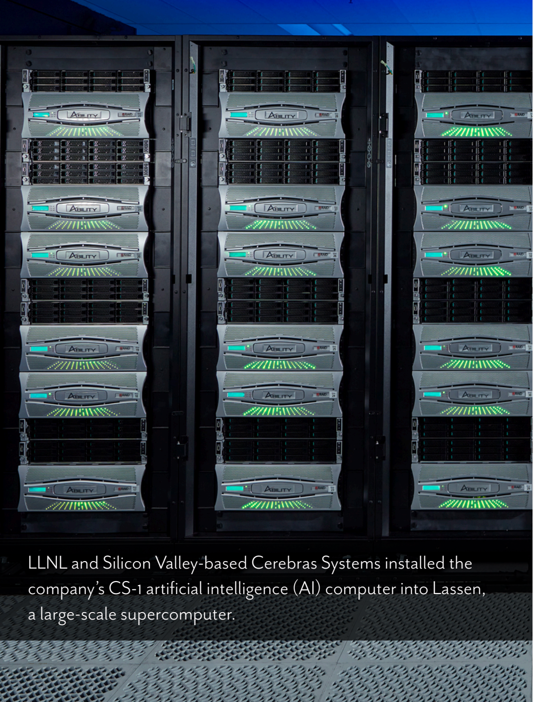
These new models improve scientific predictions by coupling large ensembles of simulations with limited quantities of experimental data—a process that enables AI to incorporate, adapt to, and guide experimental observations. The improved models deliver highly detailed uncertainty quantification and quantitative measures of the value of past and future experiments.

Applications

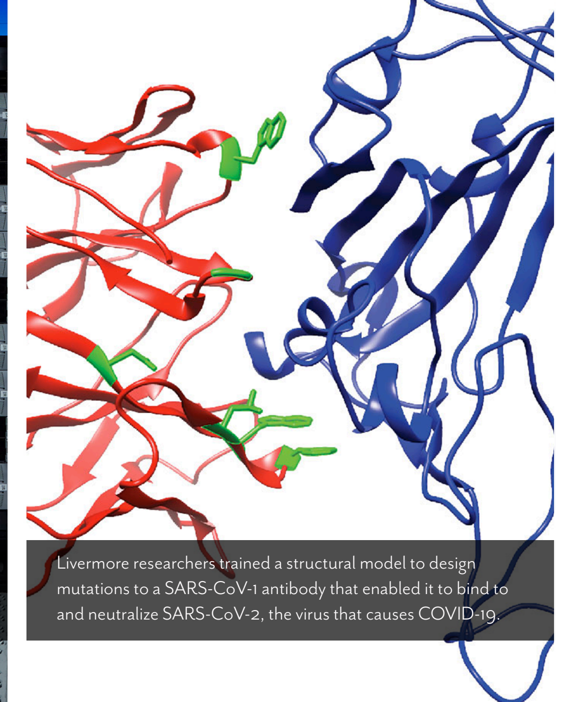
CogSim transforms the ways we apply computational capabilities to experiments and mission-driven science. LLNL's CogSim investments harness AI to accelerate scientific discovery and progress in strategic deterrence, bio-resilience, space security, and other areas. Our Discover, Design, Manufacture, Deploy (DDMD) strategy employs AI and CogSim at key points throughout the scientific lifecycle to greatly shorten the time to innovation. Additionally, world leadership in high-performance computing, simulation, experimentation, and advanced manufacturing are foundational components of this strategy for revolutionizing mission solutions.

LLNL is applying CogSim methods across its national security missions:

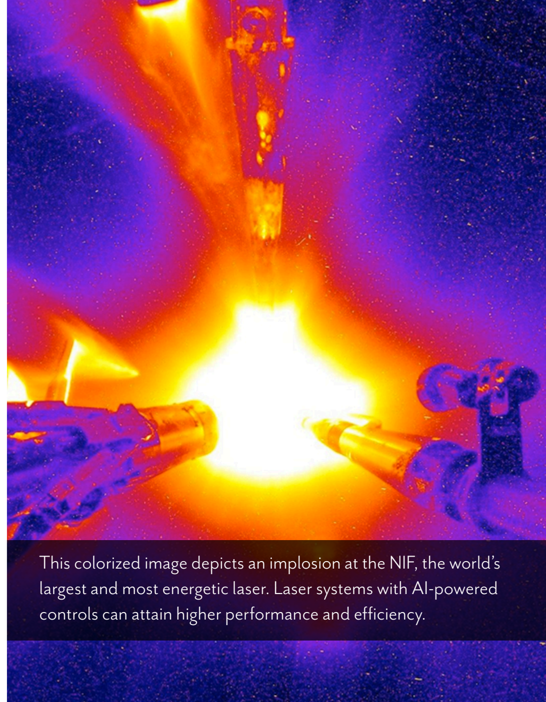
- Inertial confinement fusion: The ICF program in LLNL's Strategic Deterrence (SD) Directorate uses AI surrogate models of advanced simulations to integrate exceptionally precise, yet sparse, experimental data. These models help us better predict fusion experiment performance and optimize shot design using the world's most capable supercomputers.
- High-energy-density physics: teams from the SD and NIF&PS directorates couple edge computing (real-time computing in the experimental space itself) and AI algorithms that steer high-repetition-rate lasers (multiple experiments per second) to greatly accelerate data collection and discovery for national security missions as well as inertial fusion energy.
- Material design: SD and PLS teams use generative AI models to develop new molecular structures for critical nuclear weapons materials, such as high explosives and their polymeric binders.
- Advanced manufacturing: SD and Engineering Directorate teams design digital twins of critical manufacturing and 3D printing processes to increase throughput and prevent defects in components for the nuclear stockpile.
- Drug design: Teams in Global Security and PLS Directorates develop molecular models that propose novel therapies for emerging disease agents.
- Global security and space applications: Teams drawn from across the Laboratory perform CogSim-accelerated verification, validation, and calibration of simulation models for orbital debris impacts as part of the Space Force's new Digital Test Range.



LLNL and Silicon Valley-based Cerebras Systems installed the company's CS-1 artificial intelligence (AI) computer into Lassen, a large-scale supercomputer.



Livermore researchers trained a structural model to design mutations to a SARS-CoV-1 antibody that enabled it to bind to and neutralize SARS-CoV-2, the virus that causes COVID-19.



This colorized image depicts an implosion at the NIF, the world's largest and most energetic laser. Laser systems with AI-powered controls can attain higher performance and efficiency.

Accomplishments

CogSim provides solutions to key problems across LLNL's national security missions. While many techniques are pioneered entirely inside the Laboratory, several CogSim methods are expanded through public/private partnerships steered by the AI Innovation Incubator (AI3). This enables LLNL to share compelling interdisciplinary science challenges with AI and computing industry leaders. Demand is high for engagement with LLNL's unique CogSim research ecosystem; and new techniques and approaches that benefit both national security and national economic competitiveness can be accomplished.

- ICF predictions for fusion ignition. CogSim techniques help predict shots at LLNL's National Ignition Facility (NIF) by measuring variability across multiple shots, updating the variability distribution for future shots, and propagating variations through ICF simulations to predict critical performance—like the first-ever ignition of a laboratory fusion target.
- Generative molecular design for drug optimization. With the Accelerating Therapeutics for Opportunities in Medicine (ATOM) consortium, LLNL has developed a unique CogSim system that evaluates molecular structures for their potential as disease-fighting drugs. The system combines powerful supercomputers with AI techniques and a dataset of more than a billion molecules.
- Self-driving high-repetition-rate laser experiments. LLNL is working with computer chip manufacturer NVIDIA to develop a CogSim-based automated control system for high-energy laser experiments, leveraging the latter's research on self-driving cars and GPU hardware. Laser systems with AI-powered controls can attain higher performance and efficiency than traditional systems.
- Predictive tools for stockpile materials. CogSim techniques accelerate stockpile modernization by predicting physical properties of new materials and enabling the rapid discovery of high explosives, polymers, alloys, and more. These AI-driven tools provide predictive capabilities—such as the chemical structure of a new polymer—and shorten material development times compared with traditional optimization methods. Working together with IBM, these material discovery workflows are being joined with robotic chemistry to synthesize materials in record time.
- Digital twins for weapons manufacturing. Machine learning methods have accelerated the capture of important part metrology and its digital representation for detailed simulation evaluation. In partnership with Aerotech, we are developing these detailed models by combining software innovation with key hardware.

The Future

AI already plays an important role in how scientific experiments are conducted, how supercomputers run simulations, and how large datasets are analyzed to make predictions. As computing systems evolve past exascale capabilities toward zettascale and beyond, so too will AI technologies.

Large language models will influence scientific discovery processes, including hypothesis investigation. AI-driven automation will become more routine in laboratories and experimental facilities, producing data at unprecedented rates. Advanced manufacturing techniques augmented with AI will enable adaptive design processes and smarter production operations.

The Cognitive Simulation Institutional Initiative will ensure LLNL upholds a deliberate, focused vision for AI development and execution in addressing national security priorities. As part of this effort, AI3 will continue to coordinate multi-partner expertise focused on applications while nurturing the Laboratory's visibility and influence with sponsors and government partners.

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