High-Performance Computing, Simulation, and Data Science

Addressing national security challenges through innovative computational and predictive solutions on world-class computing resources.

Introduction

The goal of high-performance computing (HPC), simulation, and data science at Lawrence Livermore National Laboratory (LLNL) is to transform theories that explain physical phenomena into models that can reliably predict outcomes.

State-of-the-art simulations running efficiently on the world's most advanced computers are the integrating element of science-based stockpile stewardship and are critical to other national security needs. Our scientists use HPC to simulate the behavior of matter under extreme conditions of temperature and pressure, which are characteristic of nuclear detonations.

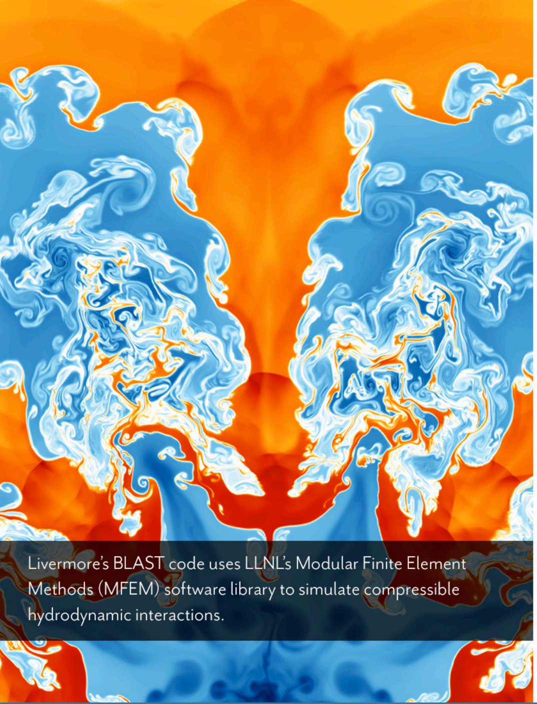
The expanding scale and complexity of the Laboratory's mission require new data-driven and artificial intelligence (AI)–augmented approaches to scientific discovery and engineering design. These techniques applied to massive data sets can help Livermore researchers better understand and predict the behavior of complex systems.

Applications

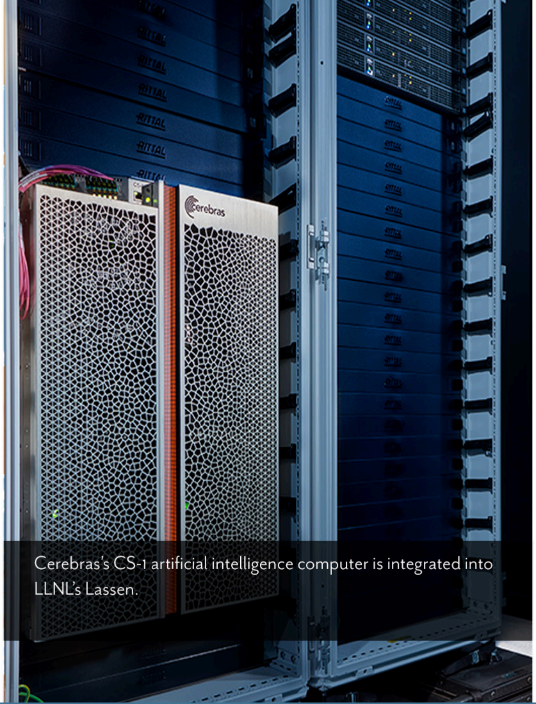
HPC at Livermore has a long history of success in close association with the Laboratory's nuclear deterrence mission. Computational scientists, computer scientists, data scientists, statisticians and mathematicians develop and use HPC to support nuclear deterrence, national security and basic scientific research. HPC capabilities remain critical to the Laboratory's science-based stockpile stewardship, ensuring the nation's existing nuclear weapons systems are safe and reliable. LLNL also uses HPC to continuously improve the scientific underpinnings of this deterrent, such as in studying the effects of material aging. Likewise, HPC facilitates stockpile modernization with newly designed and manufactured systems— like the W80-4 life extension and the W87-1 modernization programs, representing the first significantly redesigned systems to enter the stockpile since the cessation of underground nuclear testing.

LLNL's national security mission relies on simulation codes that investigate a range of physical processes. These highly specialized codes must be able to run on a variety of advanced HPC architectures, incorporate efficient solvers and numerical algorithms, and enhance researchers' predictive capabilities. Further illustrations of HPC expertise at LLNL include the following:

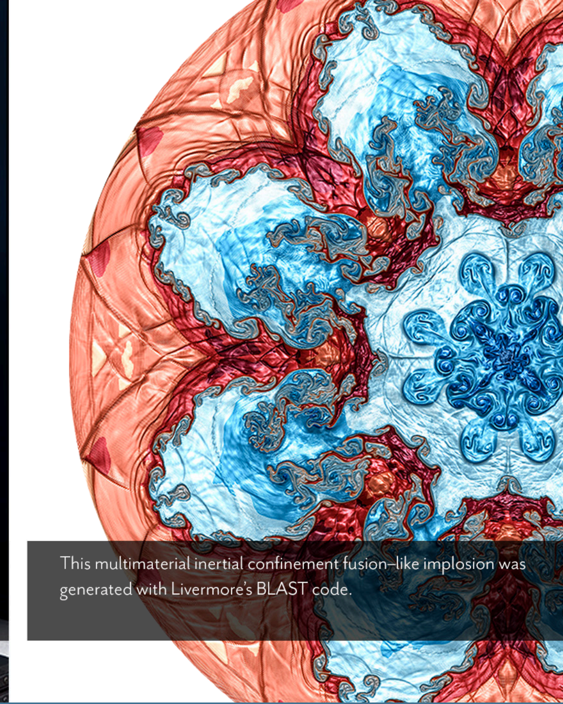
- Livermore Computing houses some of the world's most powerful computers, which use tens of thousands of processors (central and graphics processing units) running at the same time—known as parallel processing.
- El Capitan, NNSA's first exascale computing system—able to process more than a quintillion (10^{18}) calculations per second—will come online in 2024 to aid the nation's effort in a significant, time-critical weapons modernization project.
- Advances in HPC enable the use of 3D modeling in design and uncertainty quantification ensembles, which improves the accuracy of our codes instead of using outdated approximations developed during the nuclear test era.
- Innovative HPC systems and codes improve predictive understanding in complex, data-rich application areas such as advanced manufacturing, climate change, bioscience and biotechnology, energy security, nuclear science, and emerging national security threats.



Livermore's BLAST code uses LLNL's Modular Finite Element Methods (MFEM) software library to simulate compressible hydrodynamic interactions.



Cerebras's CS-1 artificial intelligence computer is integrated into LLNL's Lassen.



This multimaterial inertial confinement fusion–like implosion was generated with Livermore's BLAST code.

Accomplishments

Livermore is a leader in developing and using HPC, simulation, and data science to carry out mission-driven work in strategic deterrence, national security, and fundamental scientific research. Incredible computational capabilities make LLNL a premier destination for HPC researchers, whether their expertise is artificial intelligence, simulation or data science. LLNL scientists, researchers, and technicians often collaborate with government, academic, and industry colleagues to tackle pressing challenges using Livermore's formidable HPC resources. Some of the Laboratory's significant recent accomplishments include:

- Developing exascale-ready simulation tools that continue to both assure the safety, security, and reliability of the nation's enduring nuclear deterrent during the NNSA's annual stockpile assessment process, and also allow for new designs to enter the stockpile through multiple modernization programs in-progress and planned.
- Co-leading the Department of Energy's Exascale Computing Project and delivering algorithms, libraries, and codes that are foundational to the success of exascale-class systems.
- Integrating machine learning and other AI methods into the feedback cycle of experimentation and computer modeling to accelerate scientific discovery. These "cognitive simulation" tools helped LLNL scientists achieve fusion ignition by providing new views of inertial confinement fusion implosions as well as more accurate predictions that consider experimental parameters (e.g., laser energy, target-design specifications).
- Developing a machine learning model that can quickly and accurately predict 3D crystalline properties (e.g., density) of molecules based on their 2D chemical structures. Researchers use the model to search for new insensitive high-explosive materials.
- Using numerical simulations, powerful supercomputers, and new techniques to understand the life and death of a neutron, providing scientists a window into the subatomic world and insight into how the universe has evolved.

The Future

As LLNL's mission continues to expand in scale and complexity, so too must our computational and predictive capabilities. A computational ecosystem capable of exascale—and beyond—performance will enable new data-driven and AI-augmented approaches to scientific discovery and engineering design. We continue to build our expertise in computing hardware, software, codes, and the physical sciences to simulate these phenomena with higher fidelity and more realism.

Livermore is also pushing the frontiers of:

- Computing beyond exascale: heterogeneous, neural, and quantum architectures.
- Novel paradigms for science enabled by large-scale data analytics, machine learning, and cognitive simulation.
- New simulation technologies and algorithms, specifically in design optimization and decision support
- The interplay between HPC and cloud computing paradigms.

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