Tying it all Together: The Software Stack

The Extreme-scale Scientific Software Stack (E4S) is the first and only open-source scientific software stack that provides portable high-performance tools and libraries across all GPU and CPU architectures. No other software stack plays a similar role in the high-performance scientific and AI ecosystem.

LEARN MORE

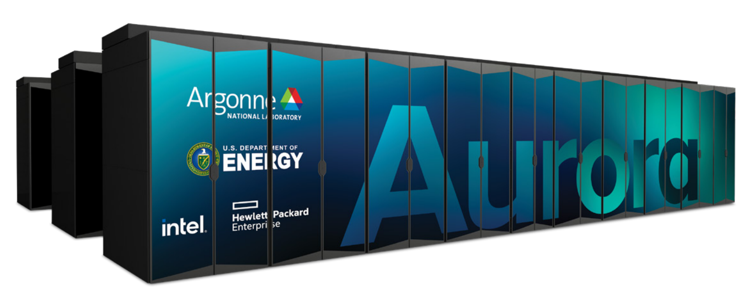
E4S is:

- Key to transforming the U.S. scientific software infrastructure to utilize modern GPU platforms to accelerate industrial, commercial and scientific advanced computing;
- Readily available for all HPC platforms and major cloud environments, including AWS and Google Cloud;
- Robust with most of the commonly used AI libraries and tools and less commonly available AI products that target scientific applications;
- Foundational to accelerating code transformations toward using GPUs effectively, key to advancing scientific progress and industrial competitiveness;
- Ready for the future. It is already available in cloud environments, provides AI capabilities, supports desktop to supercomputing performance needs, is reliable and robust through rigorous testing, and is committed to provenance and software security;
- The launching pad to further accelerate U.S. advanced computing capabilities in the future with an infrastructure that supports the use of specialized devices, including next-generation AI and quantum processors.

HPE Cray EX Frontier

Oak Ridge National Laboratory
DOE Office of Science

- Broke the exascale barrier in 2022
- First exascale supercomputer and world's fastest from 2022 to 2024
- High-temperature water cooling and GPU accelerators make Frontier incredibly energy efficient: <30MW



Intel HPE Cray EX Aurora

Argonne National Laboratory
DOE Office of Science

- Broke the exascale barrier in 2024
- World's fastest for AI at 10.6 mixed-precision exaflops on the HPL-MxP benchmark
- Highly optimized across multiple dimensions key for AI and ML

HPE Cray EX El Capitan

Lawrence Livermore National Laboratory
NNSA Advanced Simulation and Computing

- Coming online in 2025
- Classified computing for stockpile stewardship
- >2 Exaflops

ECP EXASCALE COMPUTING PROJECT

Foundations to National Progress: The Impact of Exascale Computing

June 2024

The Department of Energy made a strategic investment in high-performance computing in 2016 to sustain U.S. leadership in technology and address future challenges in energy assurance, economic competitiveness, healthcare, and scientific discovery, as well as growing security threats. Thus, the Exascale Computing Project, or ECP—a seven-year, $1.8 billion software research, development, and deployment project—was launched.

ECP is a grand convergence of advances in modeling and simulation, software tools and libraries, data analytics, machine learning, and artificial intelligence in support of delivering the world's first capable exascale ecosystem.

The payoff is here: exascale computing is revolutionizing nearly every domain of science.

DOE has three exascale systems: Frontier (2022), Aurora (2024), and El Capitan (coming online in 2025) at Oak Ridge, Argonne, and Lawrence Livermore National Laboratories, respectively.

These core resources are foundational to the progress of the nation. They can perform more than a billion billion calculations—or floating point operations—per second, referred to as exaflops.

But what can scientists do when they get their hands on exascale-level computing power?

The Exascale Computing Project Impact: by the Numbers

Created to develop the nation's first capable exascale computing ecosystem, this unprecedented DOE research, development, and deployment project has already made a huge impact on computational science:

2,800 collaborators funded to develop exascale applications, software, and hardware

Game-changing results in a broad spectrum of science and engineering application areas

2 different GPU architectures now proven to work with exascale environments

First and only open-source scientific software stack developed for scalability and available across all HPC platforms, including cloud computing

National Security: Grid Resilience

The nation's power grid is vulnerable to disruption by extreme weather events and cyberattacks. Previous simplified models relied on heuristics from past events.

16

An ECP team outperformed the North American Electric Reliability Corporation's operating standard of a 30-minute short-term response with a short-term response of 16 minutes.

Exascale computing is enabling accurate modeling of the grid under numerous potential, never encountered, scenarios to address challenges associated with decarbonization, energy justice, reliability, and resilience.

Renewable Energy: Wind Power

The U.S. is investing heavily and quickly in wind power as a source of clean and renewable energy. However, past efforts to increase turbine efficiency and to design wind farms have been limited by computer processing speed.

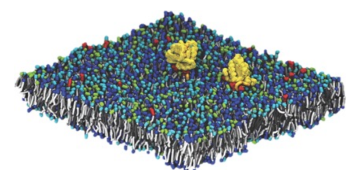
Exascale computing is optimizing wind energy production with new turbine and wind farm designs.

Results of a high-fidelity wind farm simulation artifact from the ExaWind solver suite. Credit: National Renewable Energy Laboratory

Health: Cancer

Potential breakthroughs in cancer research could be realized through automated complex data analysis and modeling, but previous generations of computers were not up to the task.

Exascale computing and machine learning are helping create and train large numbers of computational models for new insights into cancer, improving treatment options.



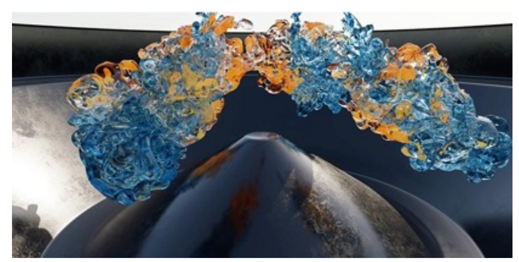
12X

Up to 12 times reduction in drug discovery design periods, going from 5-10 years to 6-9 months.

Combustion: Clean Energy

Combustion processes have historically dominated electrical power production and transportation systems. Despite significant advances in improving the efficiency and reducing the costs of alternative energy sources, combustion-based systems are projected to dominate the marketplace for decades, especially for hard-to-electrify sectors including aviation. Consequently, these systems must be optimized for energy efficiency and reduced emissions.

Exascale computing is helping design more efficient combustion processes for clean energy and transportation while mitigating climate change.

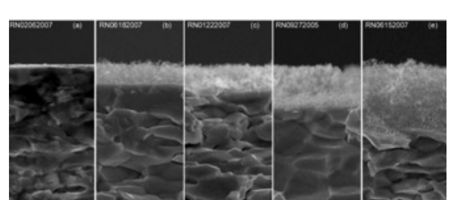


A highly reactive diesel fuel (dodecane) is injected into a turbulent methane-air mixture at extremely high pressure inside the compression-ignition combustion chamber above a shaped piston head. Credit: the Pele team with PeleLMeX

Fusion Power: Energy Materials

Fusion reactors will require advanced structural materials that can resist very high temperatures and extremely hot plasmas. Researchers are exploring at the atomic scale how the structures of different materials will evolve in the harsh conditions typical of these reactors. Tracking every atom in a system over long timescales and at quantum levels of accuracy requires incredible supercomputing power.

Exascale computing is enabling unprecedented simulation of materials under extreme conditions, such as plasma-facing components in fusion reactors.



Advanced structural tungsten materials interacting with plasmas: exploring radiation tolerance in fusion reactors.

Fission Power: Small Modular Reactors

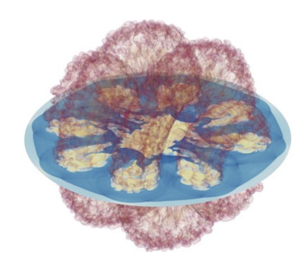
Small modular reactors (SMR) represent a new generation of fission power plants that have reduced construction costs and time to production. Researchers need computer simulations to predict the viability of proposed SMR designs but the models are computationally demanding and expensive, limiting their usage by industry.

Exascale computing is delivering experiment-quality simulations of reactor behavior to enable the design and commercialization of advanced nuclear reactors and fuels at significant savings in time (from years to months) and money.

> *"By accurately predicting the nuclear reactor fuel cycle, ExaSMR reduces the number of physical experiments that reactor designers would perform to justify the fuel use, which are enormously expensive."*
> *—Steven Hamilton, Oak Ridge National Laboratory*

National Security: Stockpile Stewardship

The focus of the National Security applications is to deliver comprehensive science-based, computational weapons applications, able to provide, through effective exploitation of exascale HPC technologies, breakthrough modeling and simulation solutions that yield high-confidence insights into problems of interest to the NNSA Stockpile Stewardship Program (SSP).



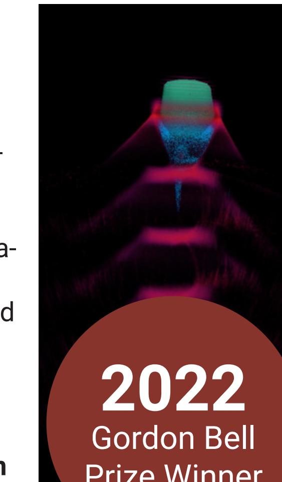
MARBL Code for Inertial Confinement Fusion and pulsed power applications. Credit: LLNL

Exascale computing is helping to deliver comprehensive science-based computational weapons applications to provide breakthrough modeling and simulation solutions.

Particle Accelerators: Medical Applications

Particle accelerators are vital tools in medicine and industry, from treating cancer with radiation therapy to helping manufacture semiconductors for computer chips and experiments in high-energy physics. Massive (and massively expensive) accelerators are required for these purposes, but experimental plasma-based particle accelerators with high-intensity lasers promise to be smaller and cheaper to construct than conventional radio-frequency accelerators.

Exascale computing is enabling computational design of next generation plasma-based accelerators, making their use in scientific and medical applications more practicable.



2022
Gordon Bell
Prize Winner

Prestigious HPC Award

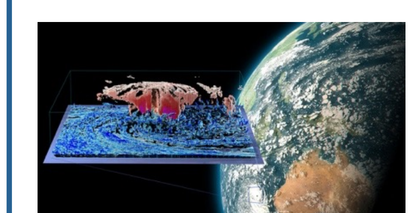
Carbon Capture and Waste Disposal: Subsurface

Modeling of reactive fluid flow through underground rock at unprecedented scale and complexity is critical to efforts to capture and store carbon dioxide below the Earth's surface and ensure that waste and other toxic materials remain sequestered away from people and the environment.

> *"The ECP effort proved GPU accelerators (and their software ecosystems) were productive across a wide variety of science, de-risking our decision [to invest in GPU HPC capabilities at ExxonMobil]."*
> *— Mike Townsley, ExxonMobil*

Exascale computing is enabling the level of fidelity and complexity needed to develop safe and reliable long-term CO_2 storage, geothermal energy, nuclear waste isolation, and petroleum extraction.

Climate: Clouds



Scientists need ensembles of increasingly accurate, detailed climate models to make useful predictions of the impact of a changing climate. But 3D models of the complicated interactions among the Earth systems, particularly the details of cloud formation, have been too computationally expensive for past supercomputers.

Exascale computing is delivering detailed insights into the possible consequences of droughts, floods and other calamities at unprecedented speed, scale, and resolution.

2023
Gordon Bell
Special Prize

Prestigious HPC Award