U.S. DEPARTMENT OF ENERGY | Office of Science

Shaping the Future of Manufacturing using HPC

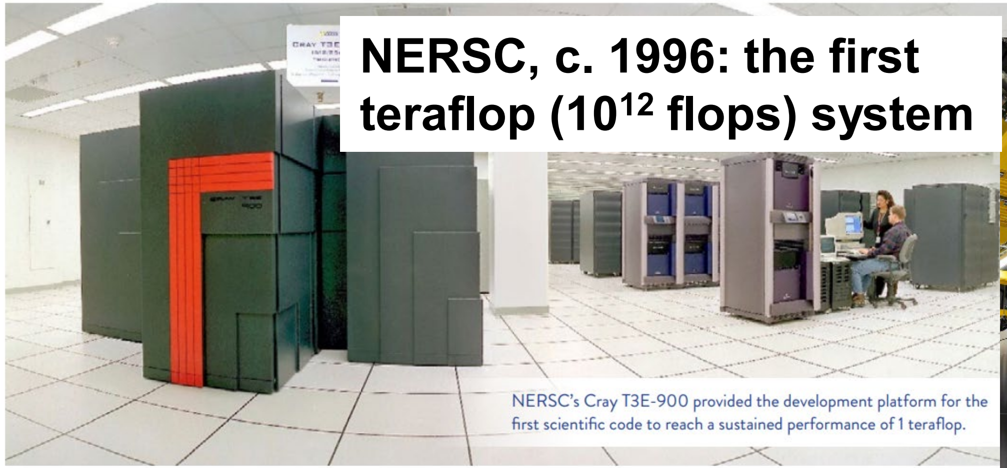
Advanced Scientific Computing Research

Dr. Steven Lee, DOE/SC

ASCR – Over 70 years of Advancing Computational Science

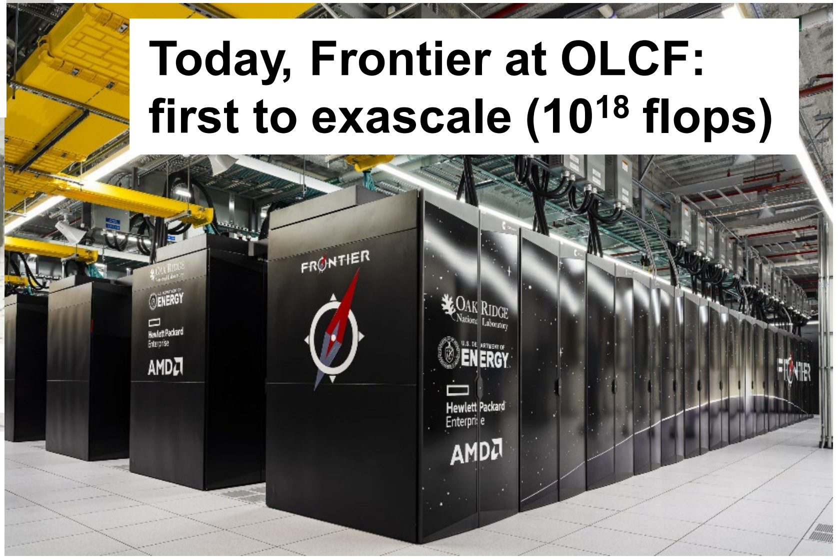
Beginnings: During the Manhattan Project, John Von Neumann advocated for the creation of a Mathematics program to support the continued development of applications of digital computing

ASCR has a rich history of investment in computational science and applied mathematics research, and revolutionary computational and network infrastructure.



NERSC, c. 1996: the first teraflop (10^{12} flops) system

NERSC's Cray T3E-900 provided the development platform for the first scientific code to reach a sustained performance of 1 teraflop.



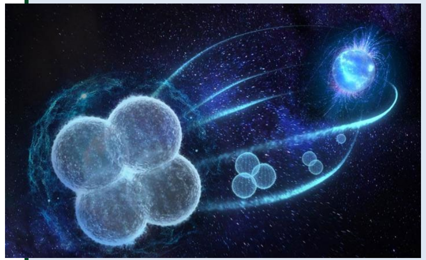
Today, Frontier at OLCF: first to exascale (10^{18} flops)

WHY COMPUTATIONAL SCIENCE?

- Computational science added a third pillar to researcher's toolkit along side theory and experiments
- Valuable when experiments are too expensive, dangerous, time-consuming or impossible
- Facilitates idea-to-discovery that leads from equations to algorithms
- Virtually every discipline in science and engineering has benefited from DOE's sustained investments in computational science

ASCR Research: Key To Enabling DOE and SC Scientific Enterprise

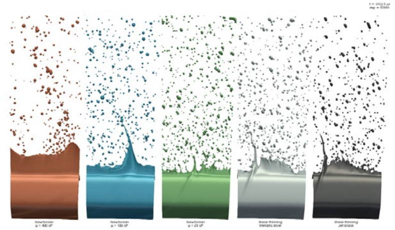
Capitalizing on decades of basic research investments in applied math, computer science and computational partnerships, the ASCR community is well-equipped to tackle scientific and societal crises.



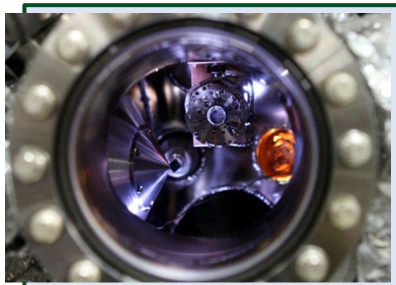
Discovery Science

ASCR's 20+ year SciDAC partnership with NP confirmed the prediction of the existence of tetraneutrons.

Lowering Energy Costs



Multi-scale mathematics algorithms and models led to insights to reduce cost in applications from electric grid to automotive industry.

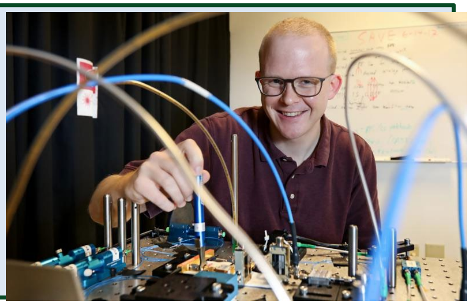


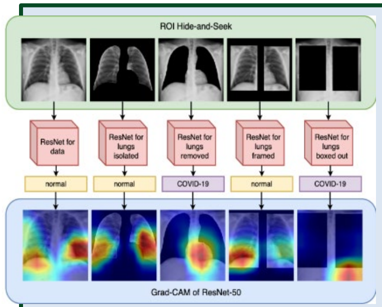
Optimizing Experiments

Optimization and machine learning methods provided real-time experiment steering at beamlines.

Foundations For the Future

Design and demonstration of the first ever Bell state analyzer enabled new quantum communication protocols.



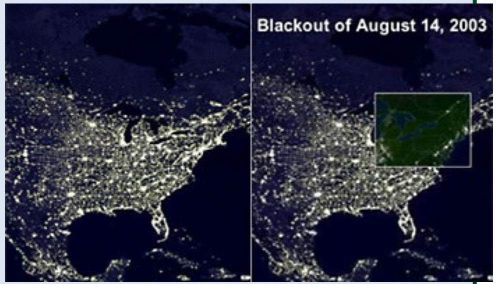


Emergency Response

ASCR CS community's expertise propelled the application of deep learning methods for pandemic response.

Decision Support

The first-ever physics based predictive models constrained the probability of cascading blackouts in power grid operations.



Exascale Computing Project (ECP)

DOE's Exascale Computing Initiative: A partnership between SC and NNSA/ASC to accelerate R&D, acquisition, and deployment to deliver exascale computing capability to DOE national labs by the early- to mid-2020s

6 Core DOE Labs
100 R&D Teams
1000 Researchers

Exascale System deployment
Frontier, Aurora, El Capitan

APPLICATION DEVELOPMENT

Develop and enhance the predictive capability of applications critical to DOE

SOFTWARE TECHNOLOGY

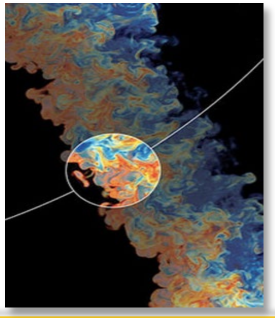
Expanded & vertically integrated software stack for capable exascale computing

HARDWARE AND INTEGRATION

Integrated delivery of ECP products on targeted systems at leading DOE HPC facilities

National security

- Stockpile Stewardship
- Reentry-vehicles
- High-energy density physics



Energy security

- Wind farms
- Small Modular Reactors
- Nuclear materials
- Subsurface Science
- Combustion
- Clean fossil fuels
- Biofuel catalysts

Economic security

- Additive manufacturing
- Power grid
- Seismic risk

Scientific discovery

- Astrophysics
- Lattice QCD
- Accelerators
- Materials
- Chemistry
- Fusion
- Standard Model

Earth system

- Earth system models
- Biomass
- Metagenomics (DOE applications)

Health care

- Cancer

On track for CD-4 in FY24

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ECP Software Technology works on products that apps need now & in future

Key themes:
- Focus: GPU node architectures and advanced memory & storage technologies
- Create: New high-concurrency, latency tolerant algorithms
- Develop: New portable (Nvidia, Intel, AMD GPUs) software product
- Enable: Access and use via standard APIs

Software categories:
- **Next generation established products:** Widely used HPC products (e.g., MPICH, OpenMPI, PETSc)
- **Robust ~~emerging~~ products:** Address key new requirements (e.g., Kokkos, RAJA, Spack)
- **New products:** Enable exploration of emerging HPC requirements (e.g., zfp, Variorum)

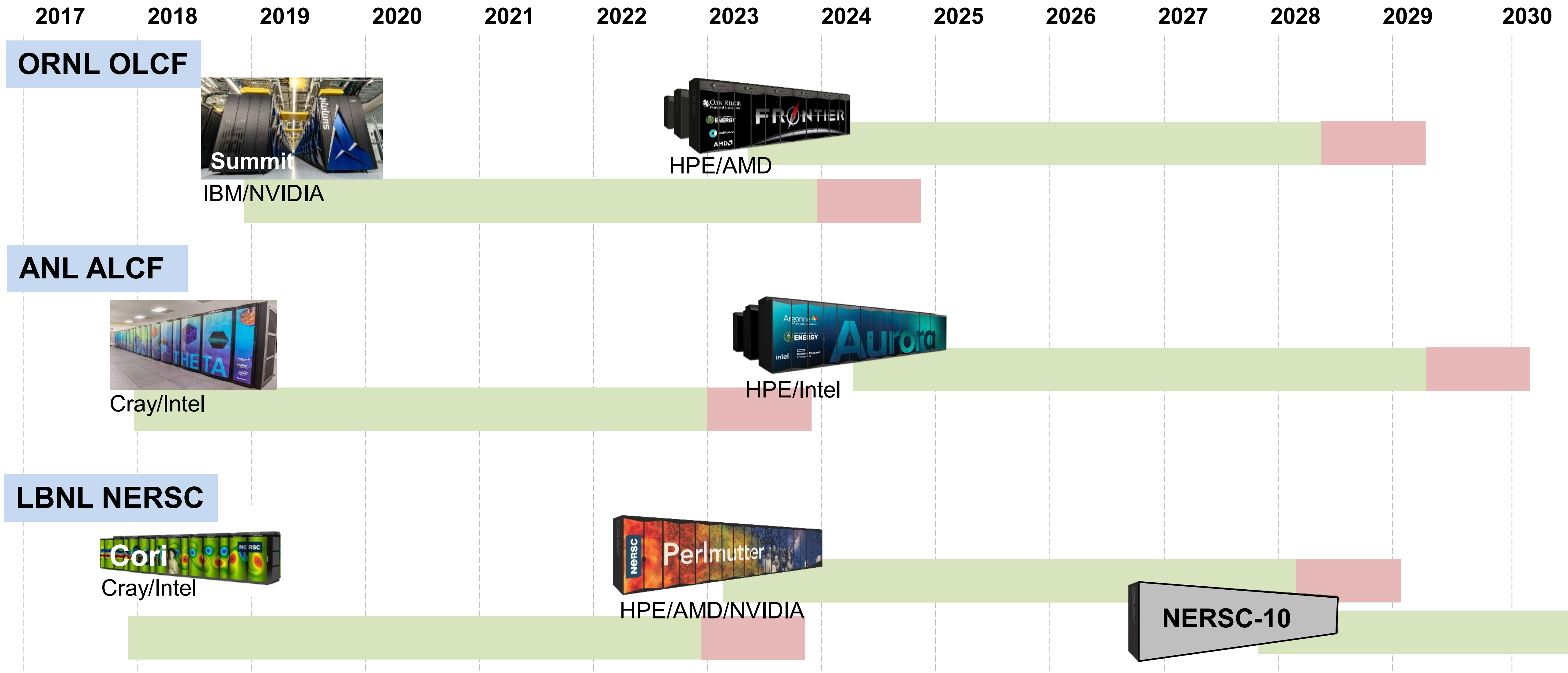
2023 R&D 100 WINNER

Legacy: A stack that enables performance portable application development on leadership platforms

Example Products	Engagement
MPI – Backbone of HPC apps	Explore/develop MPICH and OpenMPI new features & standards
OpenMP/OpenACC –On-node parallelism	Explore/develop new features and standards
Performance Portability Libraries	Lightweight APIs for compile-time polymorphisms
LLVM/Vendor compilers	Injecting HPC features, testing/feedback to vendors
Perf Tools - PAPI, TAU, HPCToolkit	Explore/develop new features
Math Libraries: BLAS, sparse solvers, etc.	Scalable algorithms and software, critical enabling technologies
IO: HDF5, MPI-IO, ADIOS	Standard and next-gen IO, leveraging non-volatile storage
Viz/Data Analysis	ParaView-related product development, node concurrency

ASCR HPC system lifecycle timeline of current and planned systems

When "accepted," a system enters a five-year operations window; the red bar indicates a possible 6th year life extension.

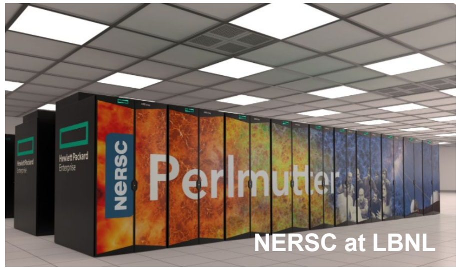


ASCR Facilities provide world-leading computing, data, and networking infrastructure for extreme-scale science while advancing U.S. competitiveness

High Performance Computing Facilities: ALCF, OLCF, NERSC

Argonne Leadership Computing Facility

Oak Ridge Leadership Computing Facility

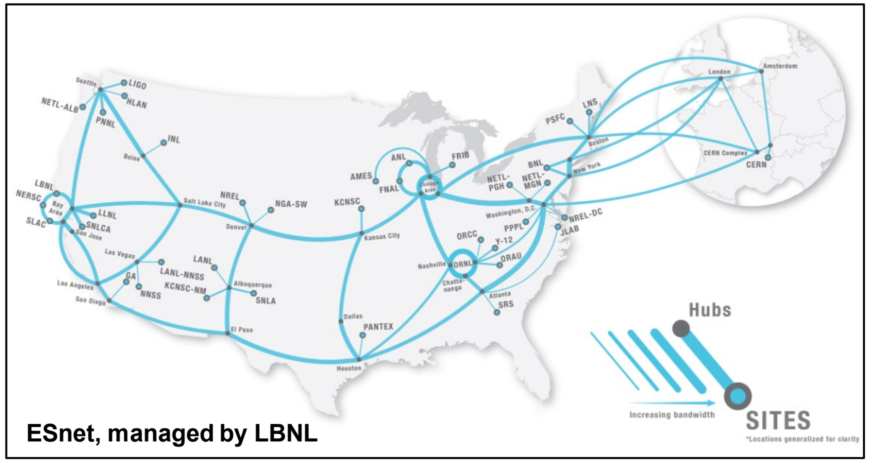


NERSC at LBNL

Leadership Computing Facilities (ALCF, OLCF):
Unique national HPC resources for extreme-scale applications, delivering the exascale (10^{18}) era of supercomputing

High Performance Production Computing Facility (NERSC):
Dedicated HPC resource for the Office of Science research community, serving many thousands of users annually

High Performance Network Facility: ESnet



ESnet, managed by LBNL

Energy Sciences Network (ESnet):
Connects all DOE national labs and dozens of other DOE sites to 150+ global research networks, commercial cloud providers, and the internet

Engineered for lossless transmission of huge data flows

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Examples of HPC4EI Projects using Exascale Computing Project software

Project Title	Company	National Lab	Codes
Additive Manufactured Composite Phase-Change Material for Thermal EnergyStorage Applications	Siemens Corporation, Technology	**ORNL**	MEUMAPPS-SL
HPC-enabled digital twin manufacturing for sustainable metalworking	ATI (Allegheny Technologies Inc)	**LLNL**	Serac/MFEM
Bioreactor Optimization through Multi-Phase Flow Models	Capra Biosciences, Inc	**LBL**	MFIX-Exa / AMReX
Multiphysics CFD simulations of CO2 solidification in a turboexpander unit-operation for the purpose of carbon-capture and sequestration	Carbon America	**NREL**	PeleC
Modeling solid electrolyte interphase formation and growth in Li-ion batteries using reactive molecular dynamics simulations.	Ford Motor Company	**ANL**	LAMMPS

DOE High Performance Computing Allocation Programs

	INCITE	ALCC	ERCAP	Director's Discretionary
Allocation Program Mission	Advance science and engineering	Advance DOE mission priorities; respond to national emergencies	Advance DOE Office of Science and SBIR/STTR research	Advance science and engineering
Allocatable Time	ALCF, OLCF: 60% NERSC: N/A	ALCF, OLCF: 30% NERSC: 10%	ALCF, OLCF: N/A NERSC: 80%	ALCF, OLCF: 10% NERSC: 10%
Managing Office	ALCF/OLCF	ASCR	DOE Office of Science Programs, SBIR/STTR	Each Facility
Award Duration	One year	One year (offset 6 months relative to INCITE)	One year	One year
Project Size (2022)	Avg: 0.8M node-hours Max: 2M node-hours	Avg: 0.4M node-hours Max: 1.68M node-hours	Avg: 20K node-hours Max: 0.7M node-hours	--

ASCR Shapes the Future of Manufacturing through HPC …

- **ASCR Research**: Applied Mathematics, Computer Science, Computational Science Partnerships
- **ASCR Facilities**: Leadership Class and High-End Computing Facilities, Energy Sciences Network
- **Exascale** Computing Facilities and Software Technology
- **DOE National Laboratory** Resources: Expertise, Software, High-Performance Computing Allocations, …

THANK YOU