

# Balancing Priorities in a Very Fast-Moving Field

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(ASCR)

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U.S. DEPARTMENT OF  
**ENERGY**

Office of  
Science

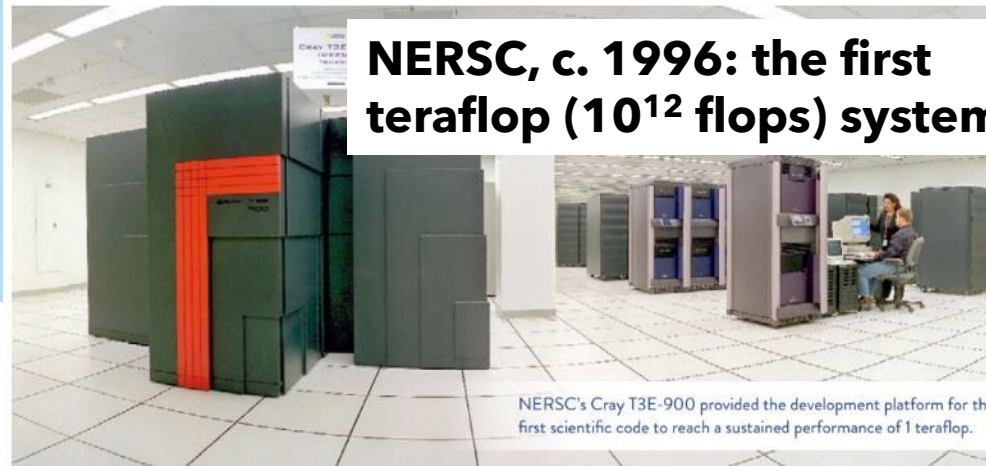
[Energy/gov/science](https://www.energy.gov/science)

# 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



Over 40+ years, ASCR has a rich history of investment in computational science and applied mathematics research, and revolutionary computational and network infrastructure.

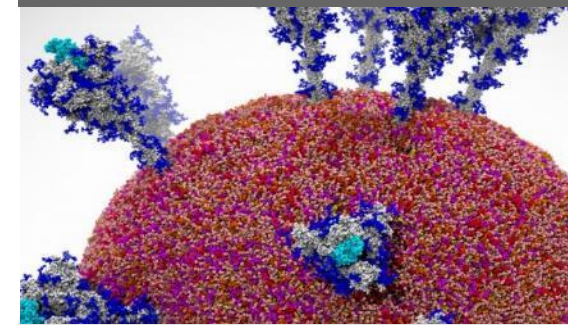


## WHY COMPUTATIONAL SCIENCE?

- ◆ 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

# Advanced Scientific Computing Research Today

- ◆ ASCR research lays the groundwork for scientific discoveries
  - **Applied Mathematics and Computer Science foundations** advance the understanding of natural and engineered systems and to reveal scientific insight from massive data.
  - **Advanced Computing** to prepare for the future of science based on emerging computing technologies and microelectronics.
- ◆ ASCR facilities drive the American global leadership in computing, data, and networking
  - As we deploy the world's first **exascale supercomputers**, we continue to build an open national research infrastructure for all.
  - Advanced network capabilities connect **DOE science** to global partners.
- ◆ ASCR's strategic partnerships enable scientific breakthroughs and advance America's economic competitiveness
  - ASCR's world-leading programs in **interdisciplinary research** to enable scientific applications to take full advantage of computing and networking capabilities that push the frontiers.
  - Unique models of partnerships advance **American vendor computing technologies**.
- ◆ ASCR invests in people
  - **Computational Science Graduate Fellowship** continues to train leaders since 1991.



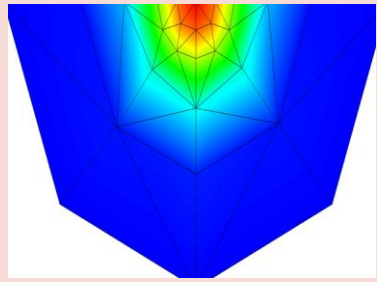
Gordon Bell Prize researchers leverage modeling and AI to understand COVID mutations



CSGF alumni work in DOE laboratories, industry and educational institutions

# ASCR Research: Key To Enabling DOE Scientific Enterprise

Simulation, modeling and data-driven discovery combined with testbeds and prototypes equip the ASCR community, big and small, to tackle scientific and societal crises.



## Discovery Science

ASCR's partnership with Fusion Energy Sciences uses exascale-ready software to understand plasma motion.

## Lowering Energy Costs

Multi-scale mathematics algorithms and models led to insights to reduce energy in industrial coating by nearly a third.

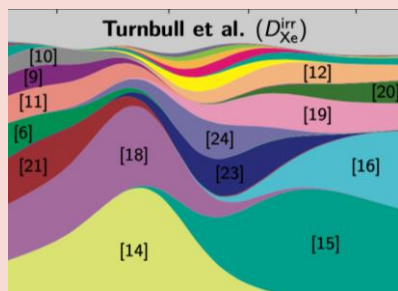
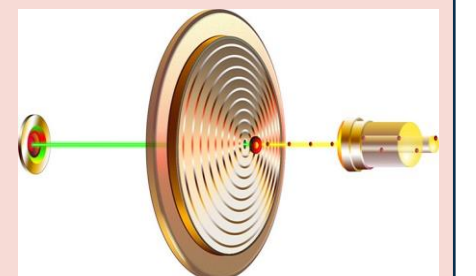


## Optimizing Experiments

Optimization and AI methods provided real-time experiment steering at beamlines and microscopes.

## Foundations For the Future

Design and demonstration of a deterministic single-photon source for quantum networking and computing.

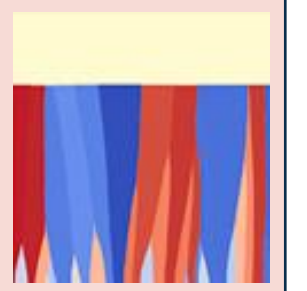


## Partnerships for Energy

ASCR's partnership with Nuclear Energy predicts diffusion of xenon under irradiation conditions.

## Insights Unlocking Technologies

AI models predict the 3D grain structures of cooling metals to enable new advanced-manufacturing technologies.



# 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



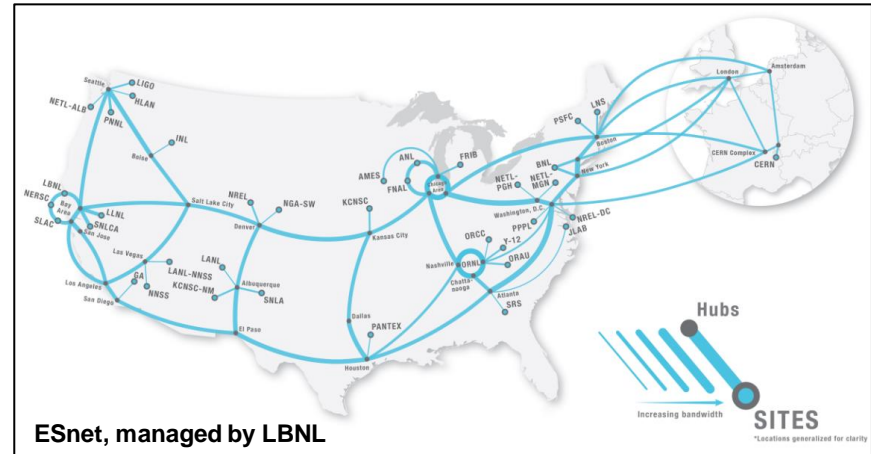
NERSC at LBNL



**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



**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

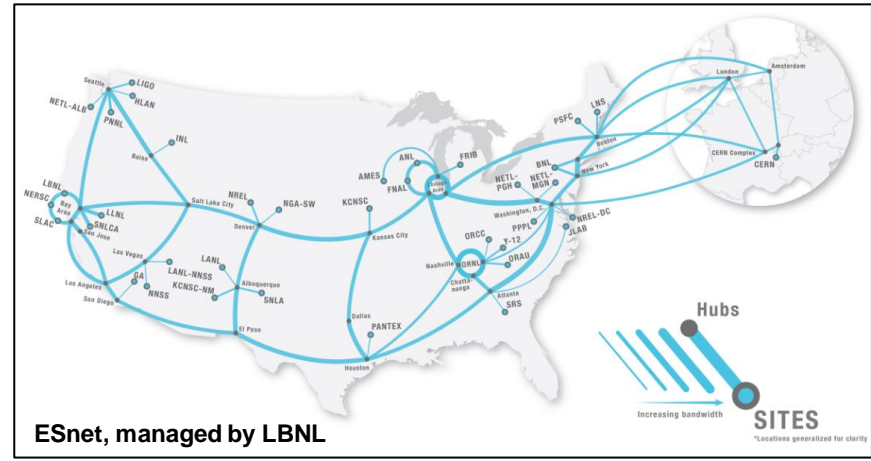
# ASCR Facilities provide world-leading computing, data, and networking infrastructure for extreme-scale science while advancing U.S. competitiveness

## High Performance Computing Facilities: ALCF, OLCF, NERSC



# Each ASCR Facility is an Innovation Engine

## High Performance Network Facility: ESnet



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Engineered for lossless transmission of huge data flows

# ASCR Launched The Exascale Era

## FRONTIER

CONGRATS TO OUR COLLEAGUES AT THE OLCF AND VENDOR PARTNERS AT HPE & AMD



- 74 HPE Cray EX cabinets
- 9,408 AMD EPYC CPUs, 37,632 AMD GPUs
- 700 petabytes of storage capacity, peak write speeds of 5 terabytes per second using Cray Clusterstor Storage System
- 90 miles of HPE Slingshot networking cables

Sources: May 30, 2022, and November 14, 2022, Top500 releases

TOP500

#1

1.1 exaflops of performance on the TOP500 List.

\*May and November 2022



GREEN500

#2

62.04 gigaflops/watt power efficiency on a single cabinet.

\*November 2022



HPL-MxP

#1

7.9 exaflops on the HPL-MxP (formerly HPL-AI) benchmark.

\*November 2022

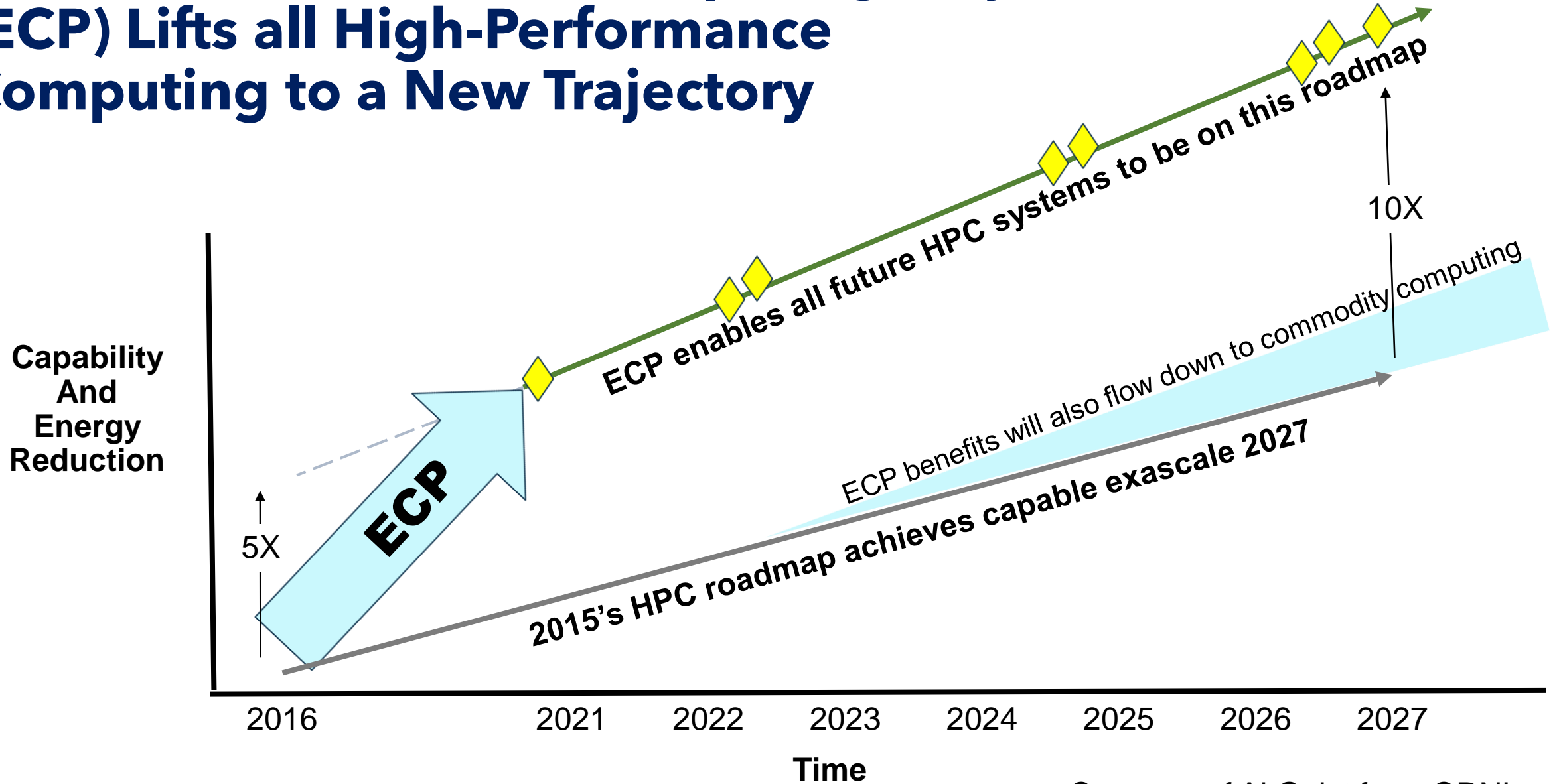


Leadership in AI capability

Leadership in computational capability

Leadership in energy efficiency

# 2015 Vision: Exascale Computing Project (ECP) Lifts all High-Performance Computing to a New Trajectory



Courtesy of AI Geist from ORNL

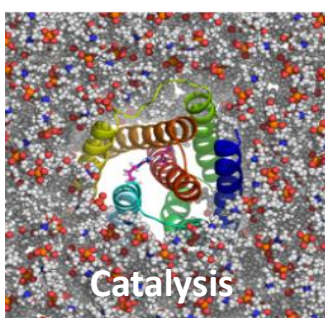
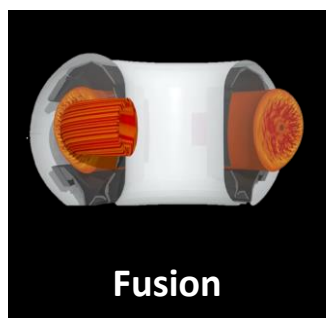
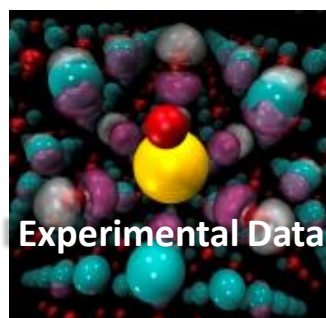
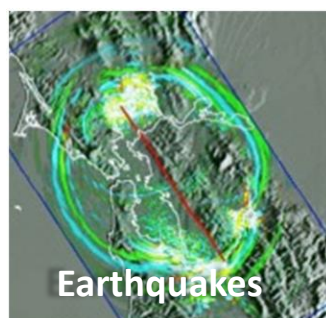
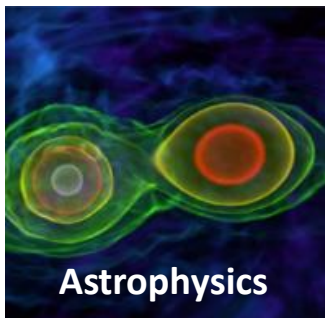
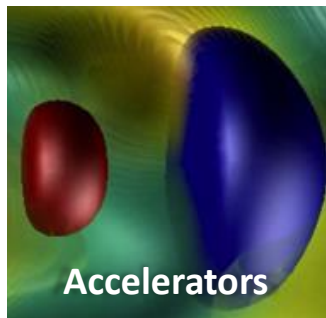
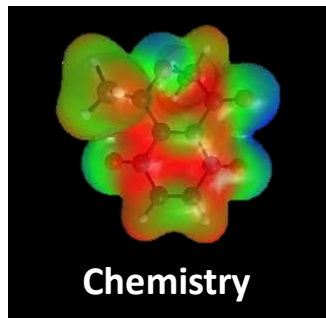
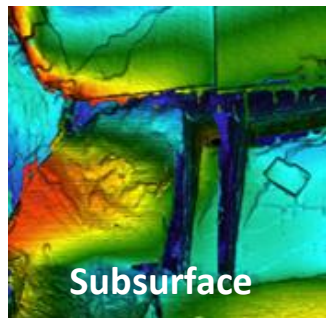
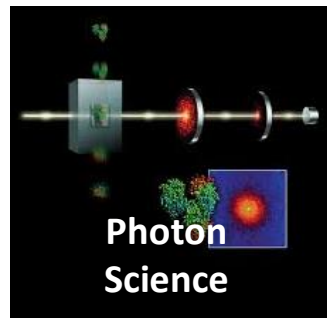
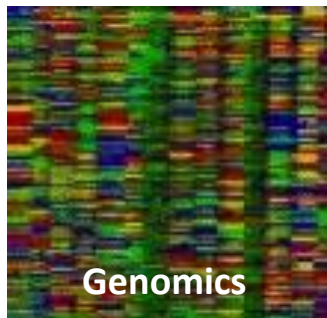
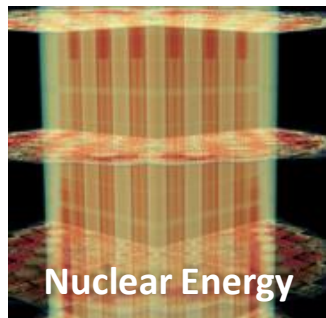
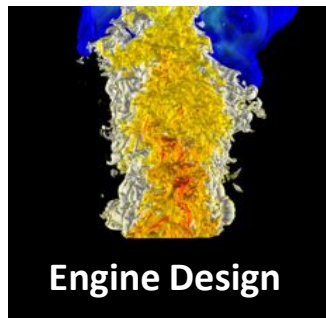
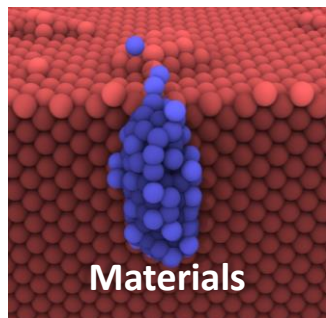
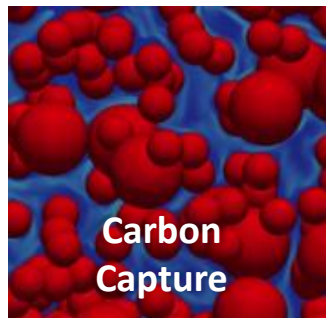
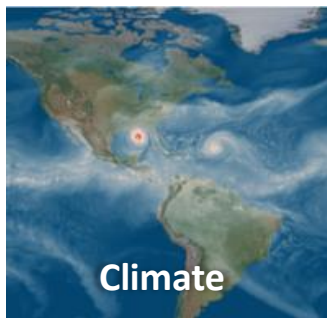
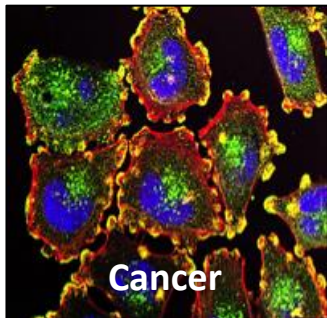
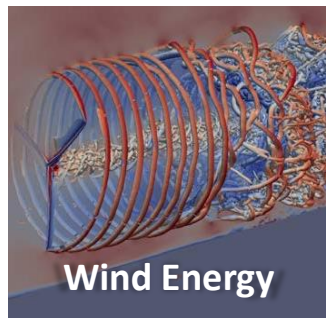


# ASCR investments significantly de-risked broader adoption of GPU technologies across agencies and industry



Opening the door to 100X improvements in capabilities and enabling faster adoption of AI technologies

# The breadth of exascale-ready applications is indicative of a sea change in computing abilities for DOE and the Nation



# Exascale Today Enables the AI of Tomorrow

Long-term investments in applied mathematics and computer science enabled exascale.



TOP500 # 1	GREEN500 # 2	HPL-MxP # 1
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Frontier, #1 on the Top500, **leads the world in computational capability**, and is also **#2 in the world in energy efficiency**, and is **#1 in the world for AI capability**.

The exascale and AI-enabled science era will lead to dramatic capabilities to predict extreme events and their impacts on the electric grid across weather and climate time scales...

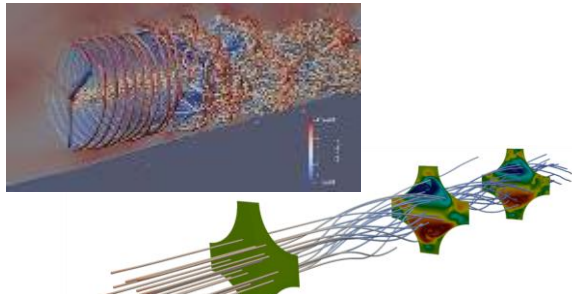


and will accelerate the design and deployment of clean-energy technologies to create a better future.



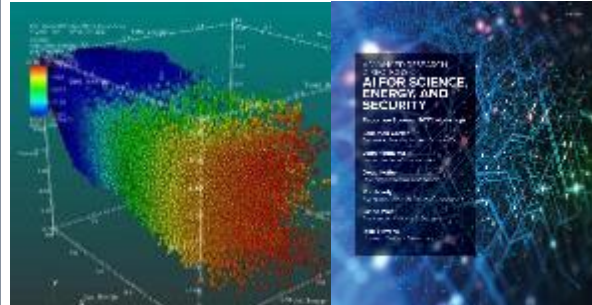
# ASCR Research Responds to Critical Technology Trends

## Advanced Modeling, Simulation, and Visualization



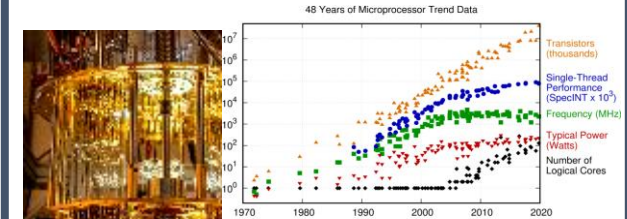
Empowering Science Through Fundamental Research

## Frontier AI & Data



Creating Trustworthy and Energy Efficient Frontier AI

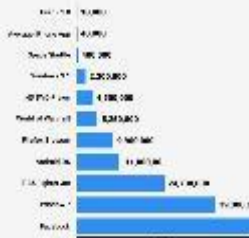
## Heterogeneous, Distributed, Co-Designed, Energy-Efficient Computing and Algorithms



Transforming Fundamentals of Computing

## Software Complexity for Increased Versatility

HOW MANY LINES OF CODE MAKE UP THESE POPULAR TECHNOLOGIES



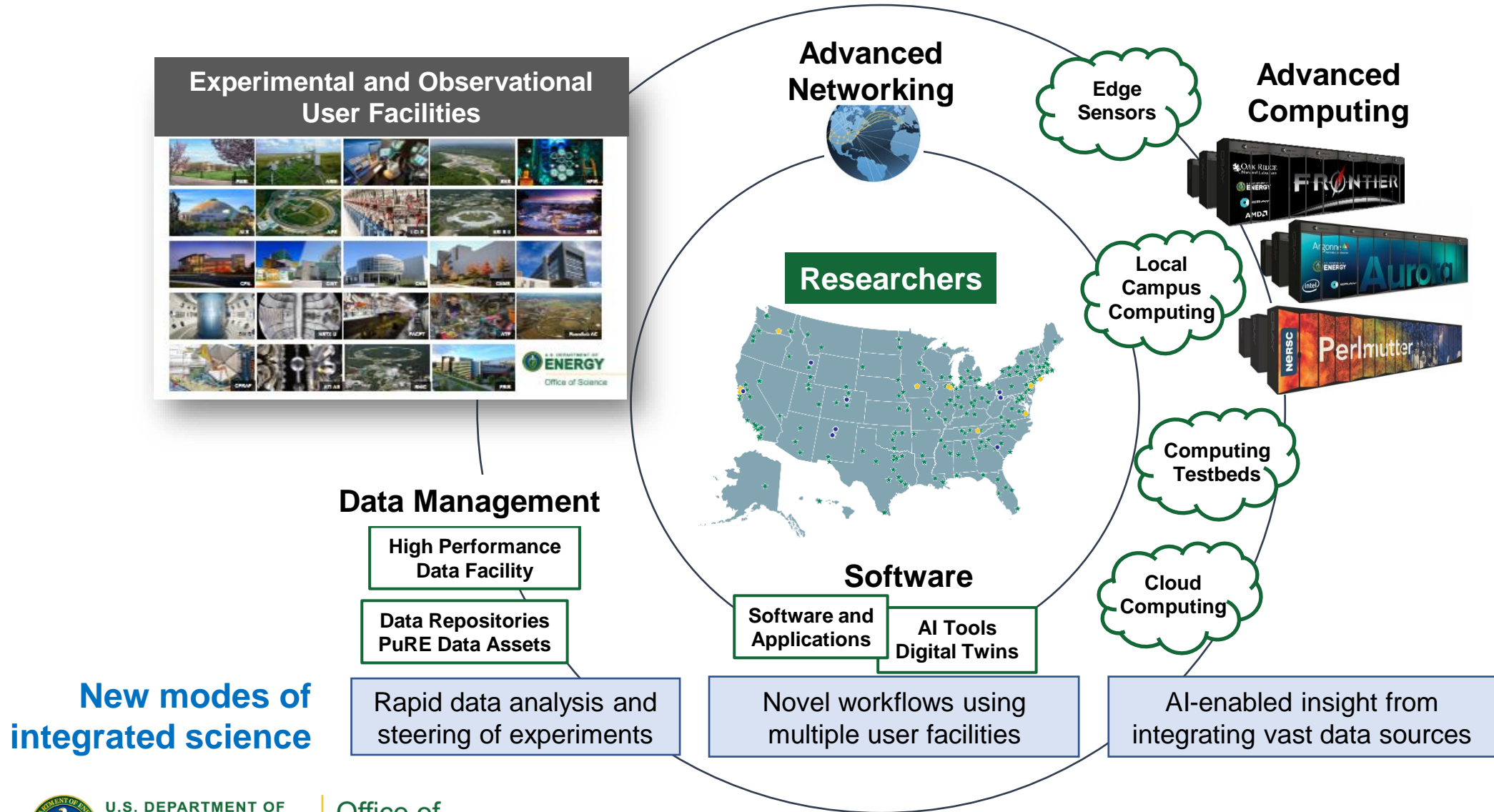
Enhancing Scientific Programming

## High-Performance Computing and Networking across Experiments, Exascale and the Edge



Accelerating Science from Exascale to the Edge

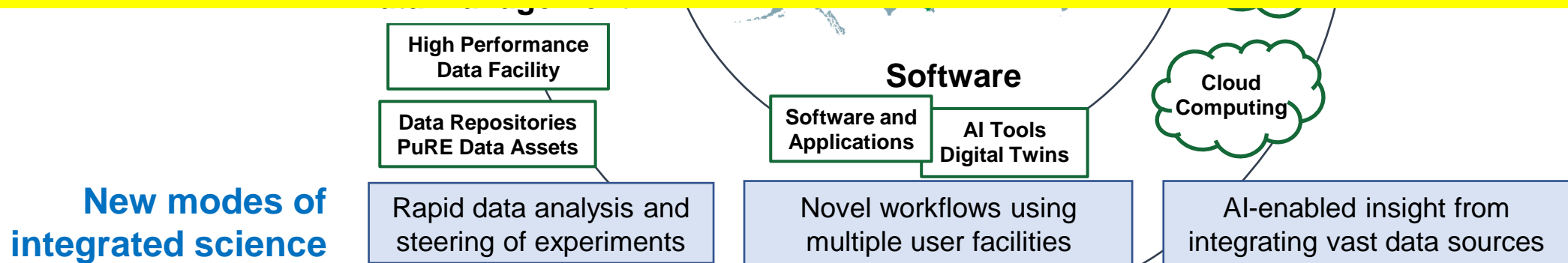
# DOE's Integrated Research Infrastructure (IRI) is a new effort to provide researchers with seamless interoperability of DOE's unique data, user facilities, & computing resources.



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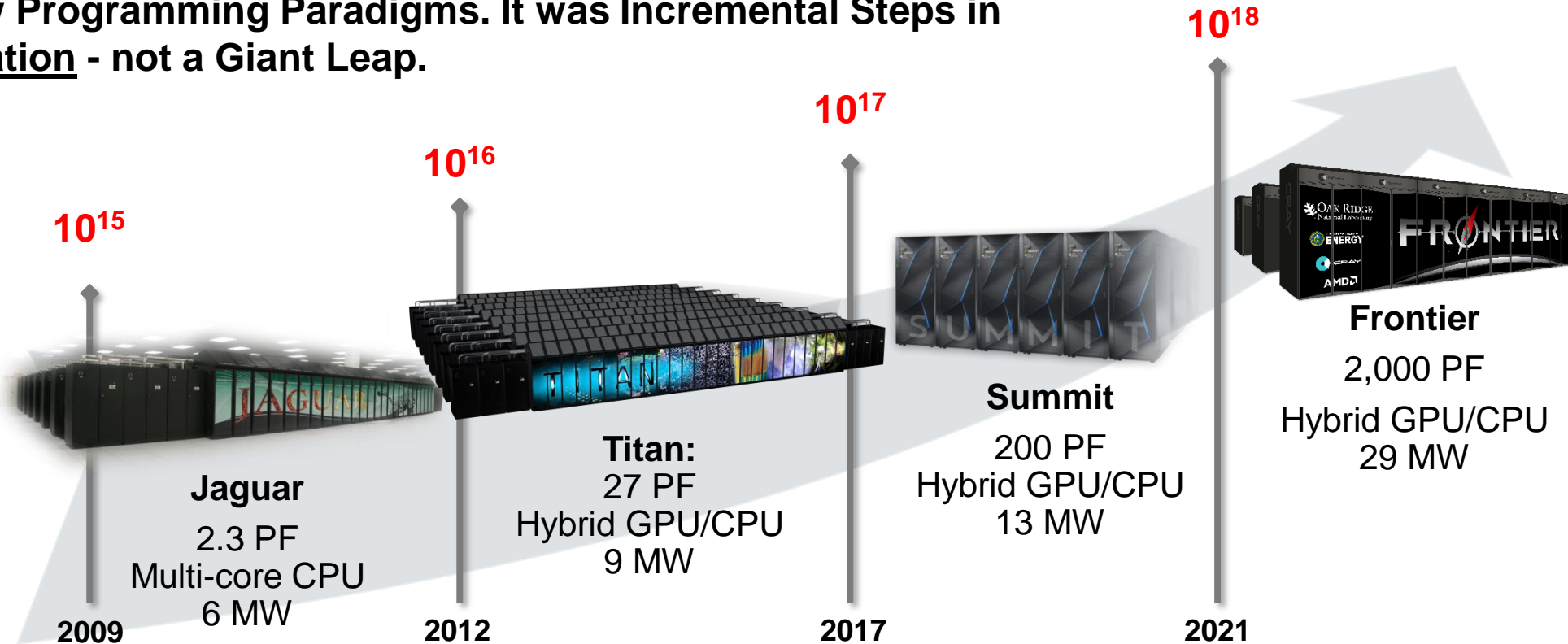


**HPDF Hub, a partnership between LBNL and TJNAF, was awarded in October 2023.**



# From 2009 to 2021 Exascale System

In the end, Exascale did not Require Exotic Technology, Architecture, or new Programming Paradigms. It was Incremental Steps in Innovation - not a Giant Leap.



**DOE must and will continue pushing Innovation in HPC.**