

NERSC



SciDAC PI Meeting
Rockville, MD

Richard Gerber
HPC Department Head
Senior Science Advisor
14 Sept 2023

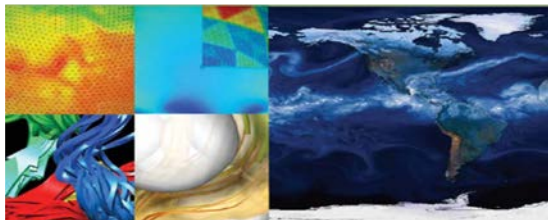
NERSC: Mission HPC for DOE Office of Science Research



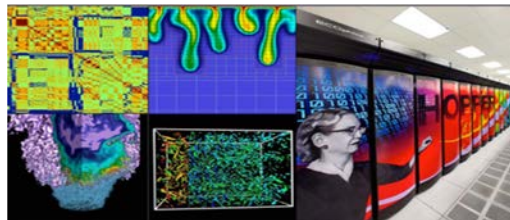
U.S. DEPARTMENT OF
ENERGY

Office of
Science

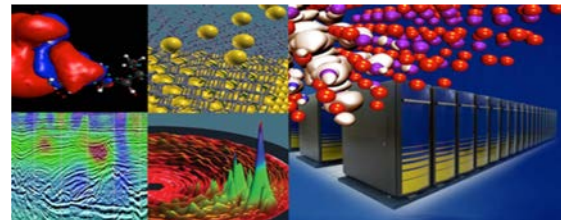
Largest funder of physical
science research in the U.S.



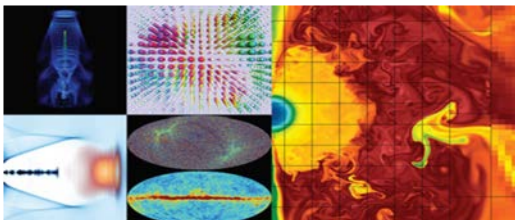
Biological & Environmental Research



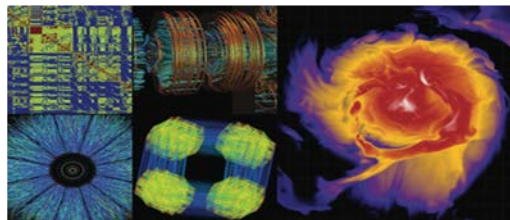
Computing



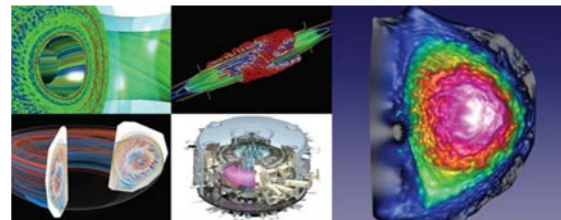
Basic Energy Sciences



High Energy Physics



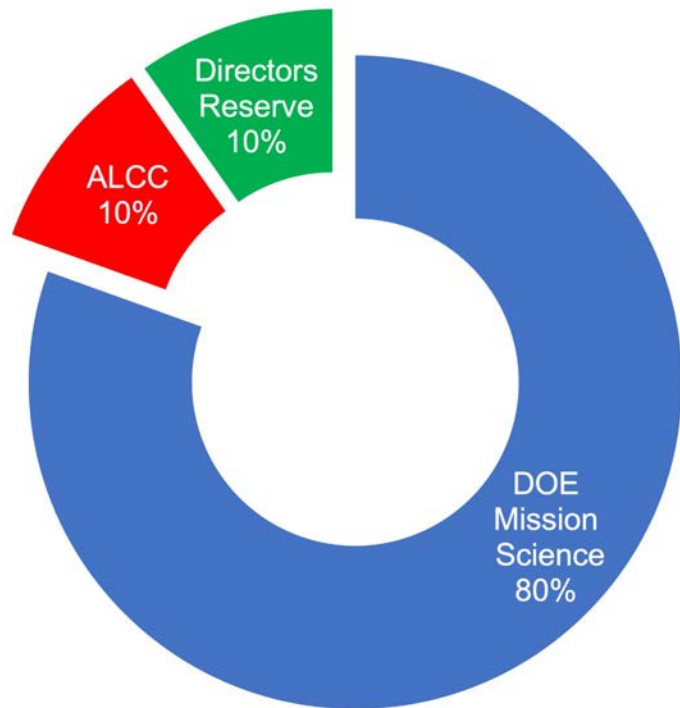
Nuclear Physics



Fusion Energy, Plasma Physics



Allocation Programs



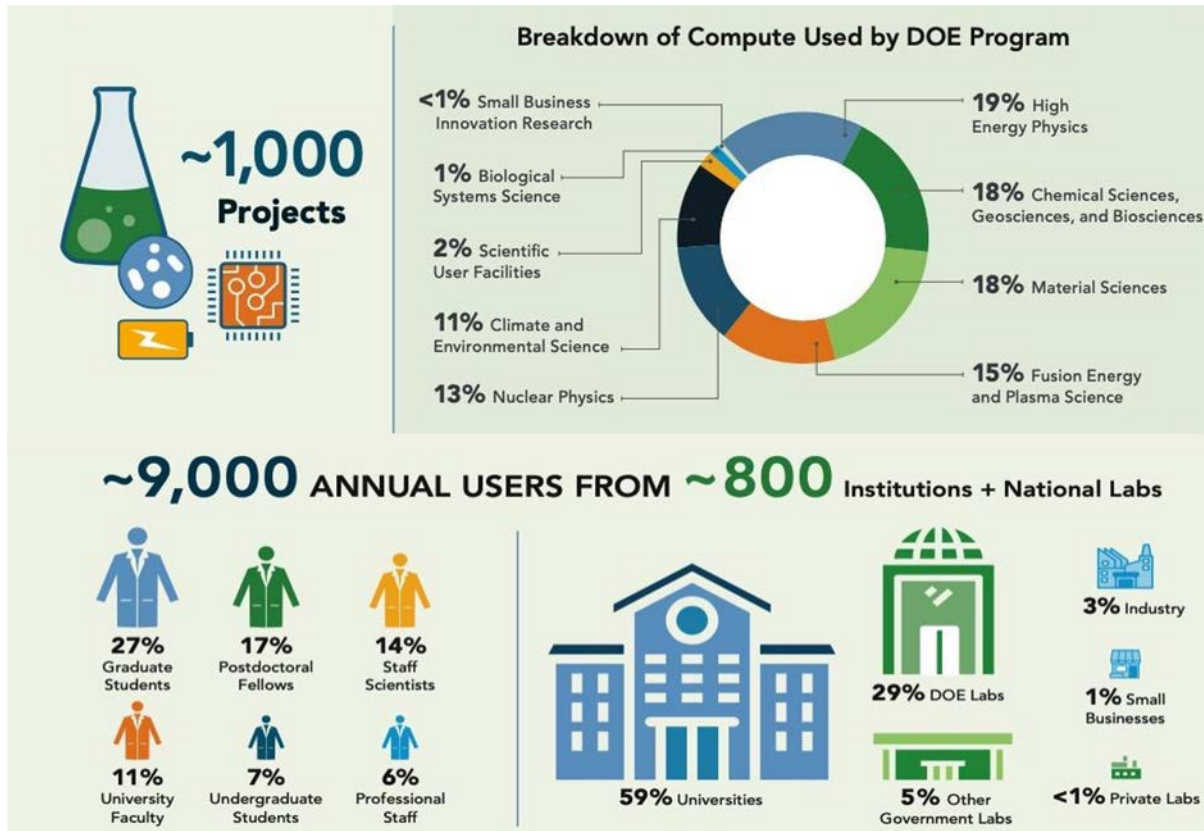
Distributed by DOE Office of Science program managers

Competitive awards run by DOE Advanced Scientific Computing Research Office

Strategic awards from NERSC

NERSC doesn't pick its users, so we have to meet them where they are and try to guide them towards increased productivity

A Diverse Scientific Community of Users



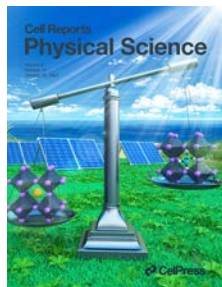
NERSC's Users Produce Groundbreaking Science



New Materials for More Efficient Solar Cells

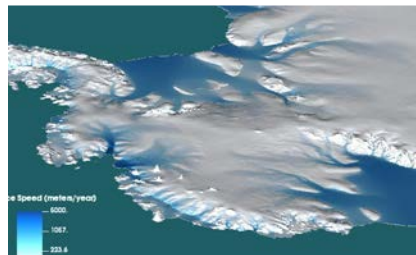
New study reveals the promise of using all-inorganic perovskite materials for solar energy conversion.

Cell Reports Physical Science



Climate & Extreme Weather

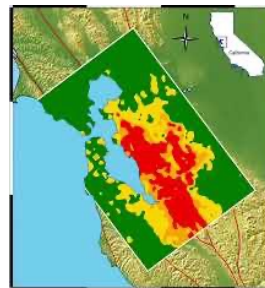
NERSC is a hub for climate and extreme weather research and the impacts on diverse communities.



Land Ice Contributions to 21st Century Sea Level Rise

Scientists quantify the effect of melting land ice on the global sea level.

Nature



World Most Advanced Coupled Earthquake-Building Simulations

Public planners can now access advanced models of different earthquake rupture scenarios will affect the public through an open-access database.

Machine Learning Technique Adds Depth, Breadth & Speed for Sky Survey Analysis

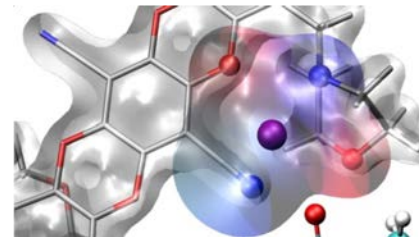
Self-supervised representation learning overcomes shortcomings of existing methods for enabling discovery.

Astrophysical Journal Letters



Breakthrough in Efficiency of Membranes for Batteries, Fuel Cells and Water Purification

Researchers have designed a membrane with “solvation cages” that can greatly speed up the flow of the desired molecules through an interface.

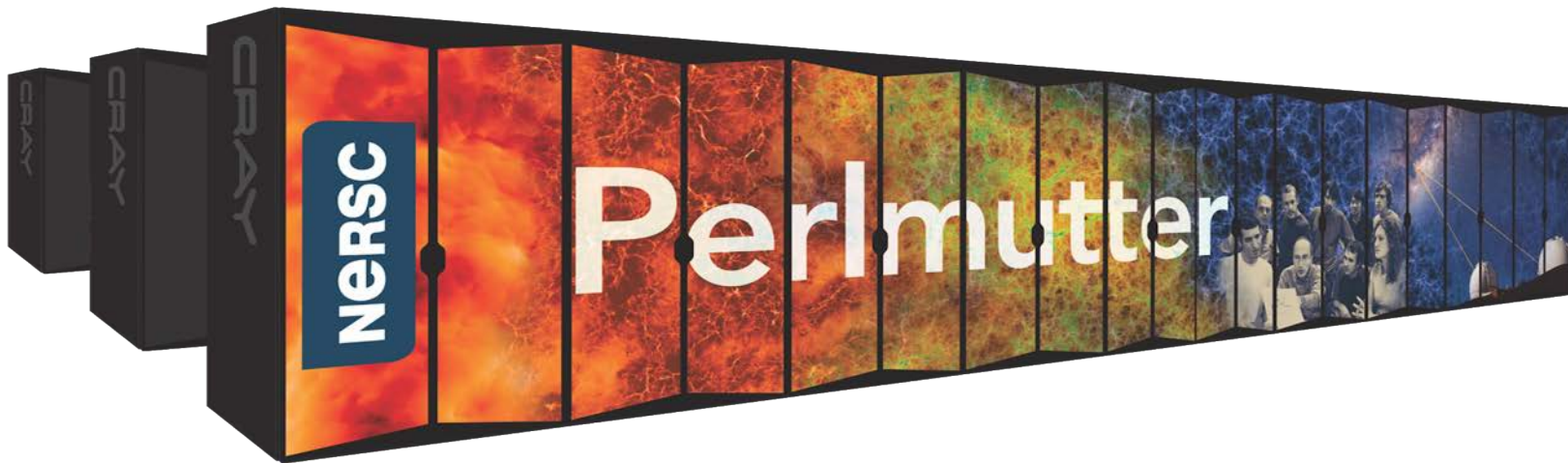


Nature



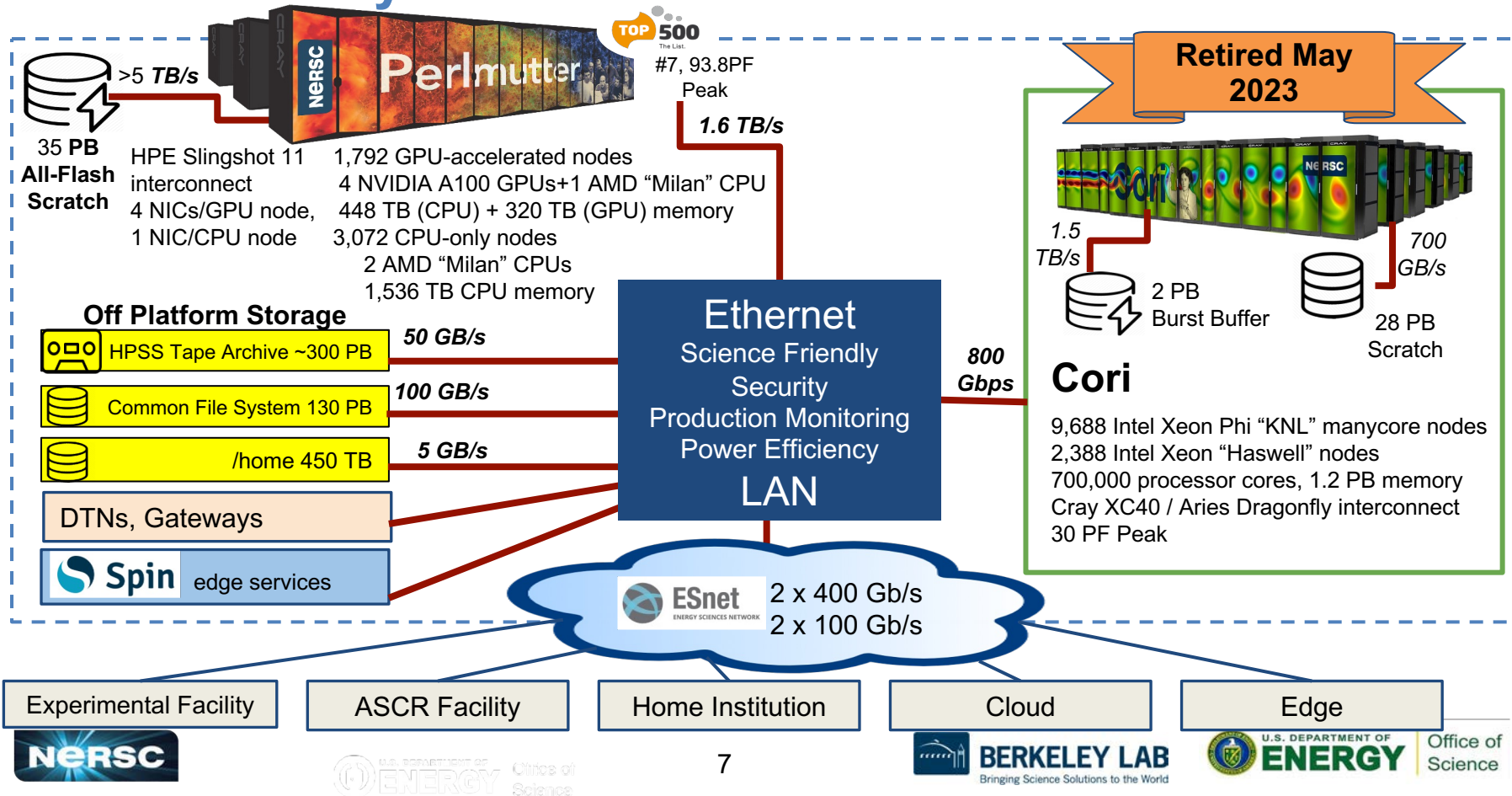
Perlmutter

The full Perlmutter System was formally accepted this summer

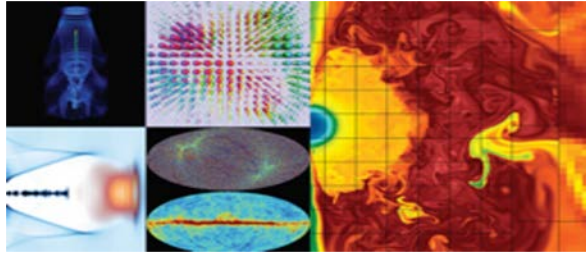


- 1,792 GPU Accelerated Nodes
 - 4 NVIDIA A100 per node
 - 7,168 GPUs
 - 1 AMD “Milan” per node
- 35 PB FLASH scratch filesystem
- 3,072 CPU only nodes
 - 2 AMD “Milan” per node
 - 512 GB memory per node
 - 393K cores
- HPE Cray “Slingshot 11” network

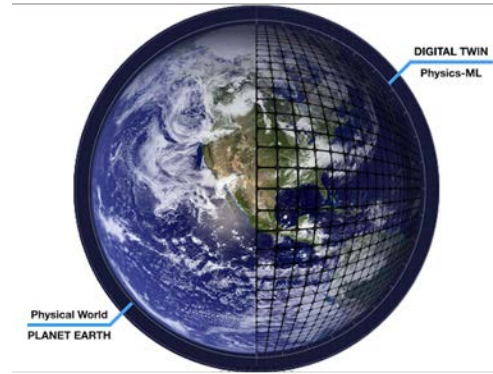
NERSC Ecosystem



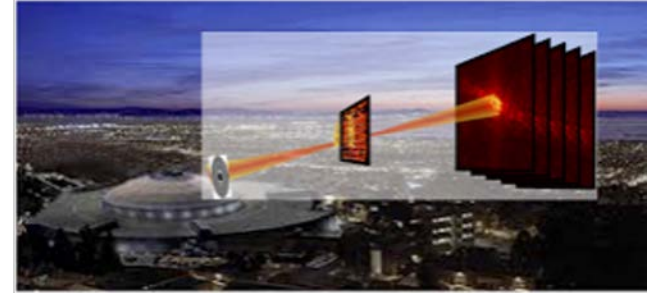
NERSC Has a Diverse Workload



Large-scale applications
for simulation, modeling
and data analysis



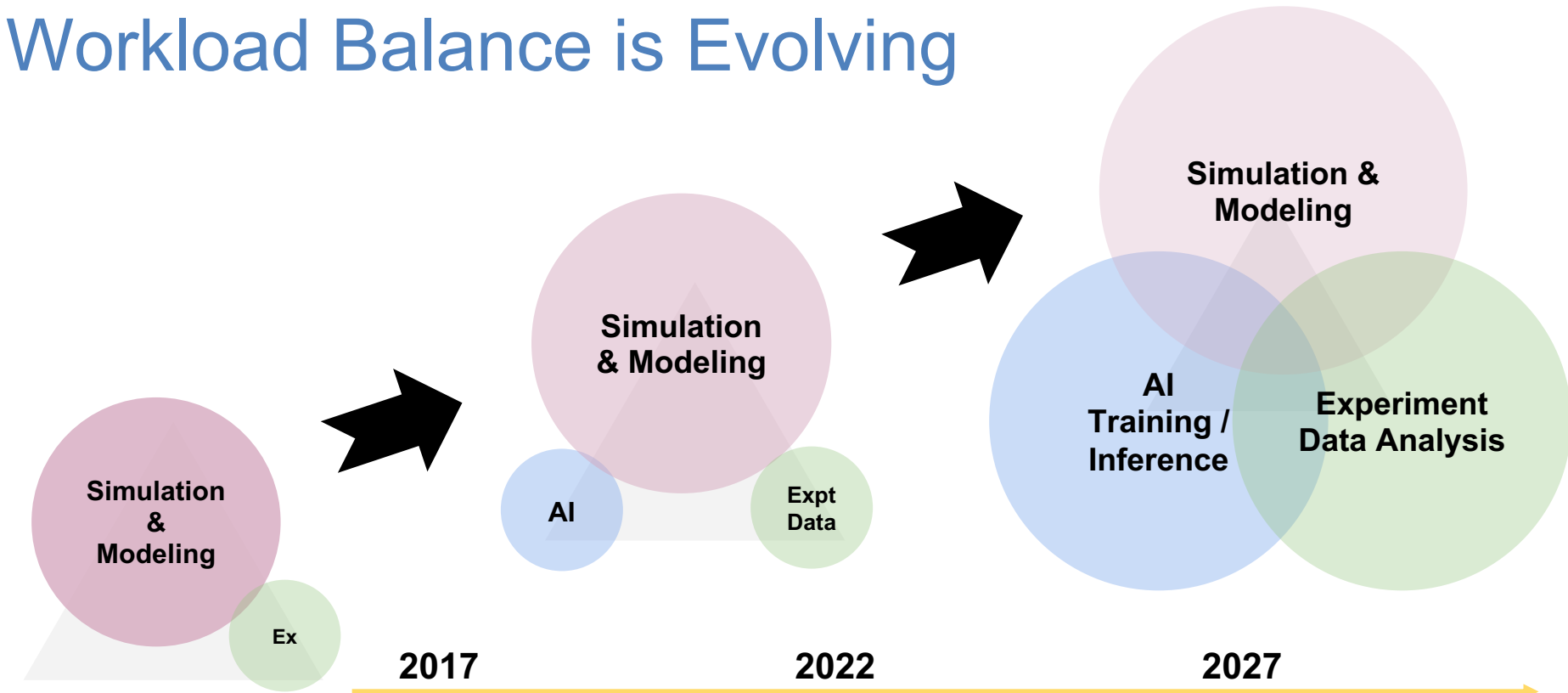
AI based discovery



Data-driven workflows
from experiments

The NERSC workload is diverse with growing emphasis on integrated research workflows

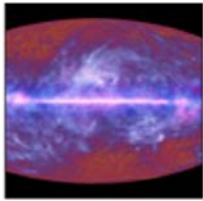
User Community - HPC Facility Workload Balance is Evolving



NERSC supports a large number of users and projects from DOE SC's experimental and observational facilities



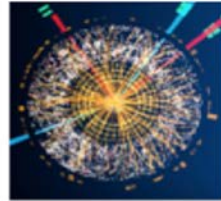
Palomar Transient
Factory
Supernova



Planck Satellite
Cosmic Microwave
Background
Radiation



Star
Particle Physics



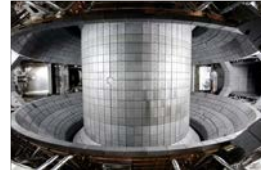
Atlas
Large Hadron Collider



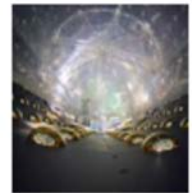
APS



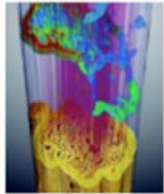
DUNE



KSTAR



Daya Bay
Neutrinos



ALS
Light Source



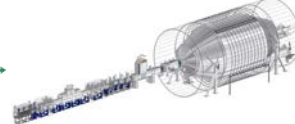
LCLS
Light Source



Joint Genome Institute
Bioinformatics



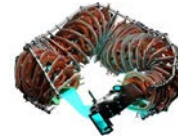
ARM



Katrin



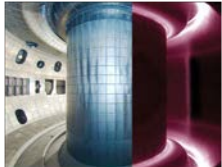
NSLS-II



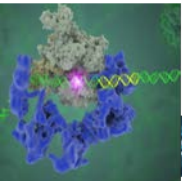
HSX



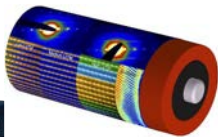
Majorana



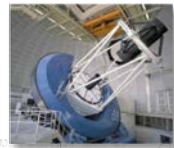
DIII-D



Cryo-EM



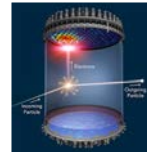
NCEM



DESI



LSST-DESC



LZ



IceCube

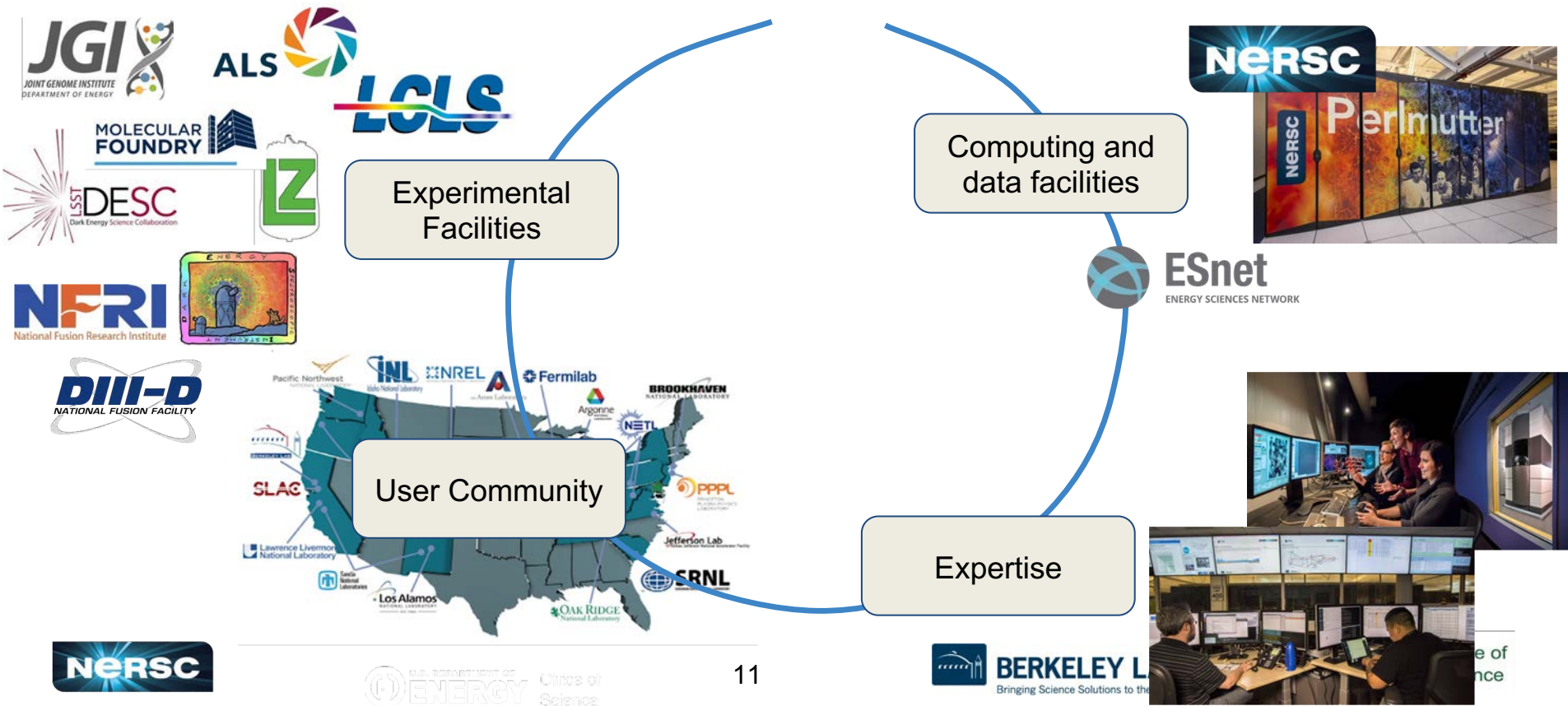


EXO



Joint BioEnergy Institute

The Superfacility concept: connecting experiment and compute facilities with the expertise and community they need for success



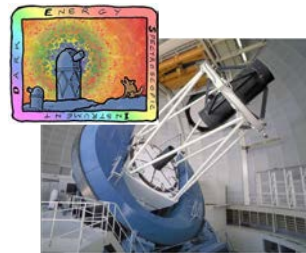
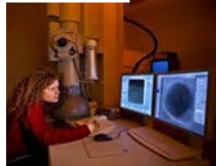
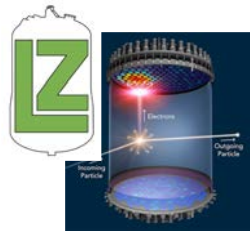
Multiple science teams are using NERSC for superfacility-enabled science, in production

The 3 year Superfacility project kick-started this work, building the base infrastructure and services. We now support multiple science teams using automated pipelines to analyze data from remote facilities at large scale, without routine human intervention, using:

- **Real-time** computing support
- Dynamic, high-performance **networking**
- Data management and movement tools, incl. **Globus**
- **API**-driven automation
- HPC-scale notebooks via **Jupyter**
- Authentication using **Federated Identity**
- Container-based edge services supported via **Spin**

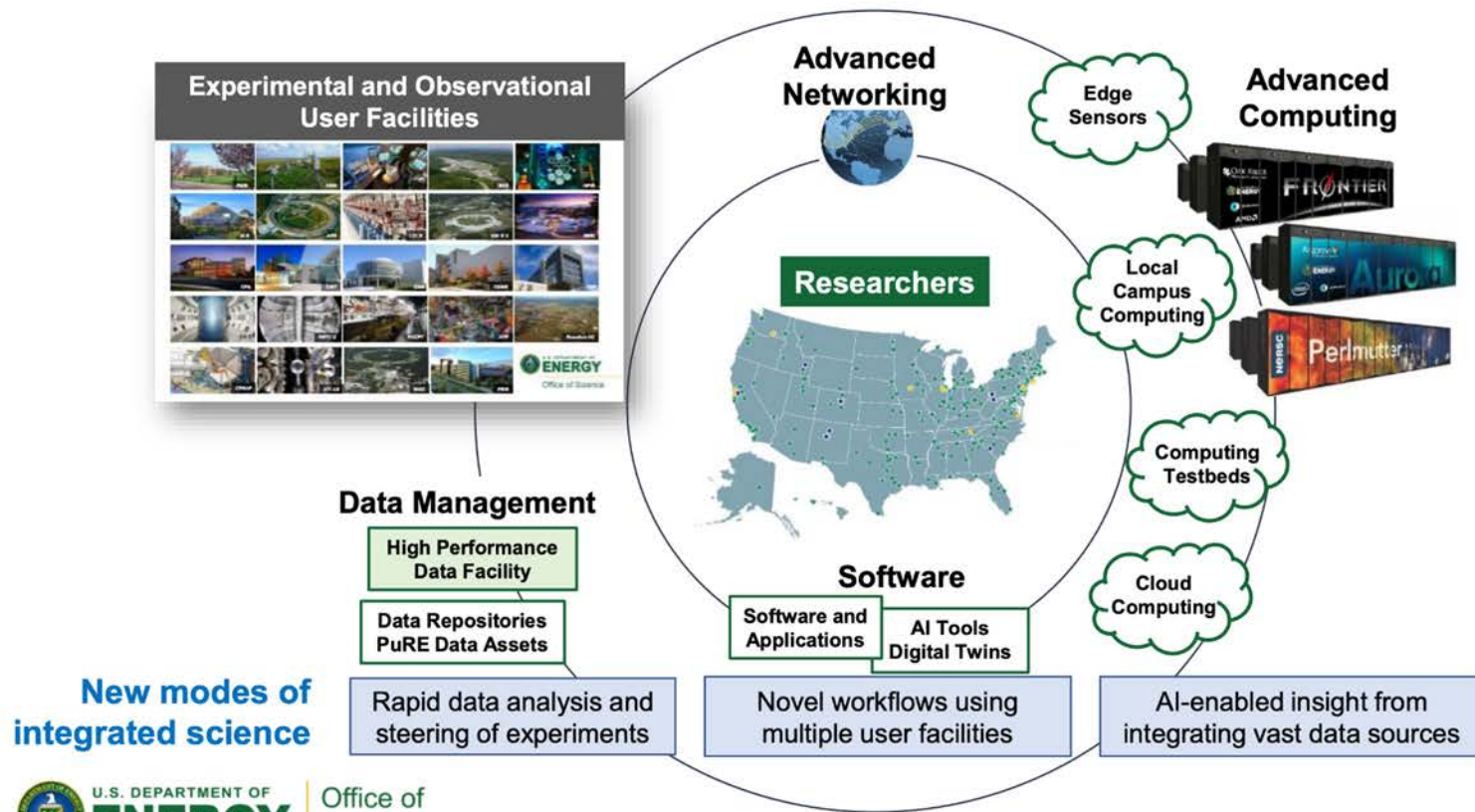


AMCR
SciData



DOE's Integrated Research Infrastructure (IRI) Vision:

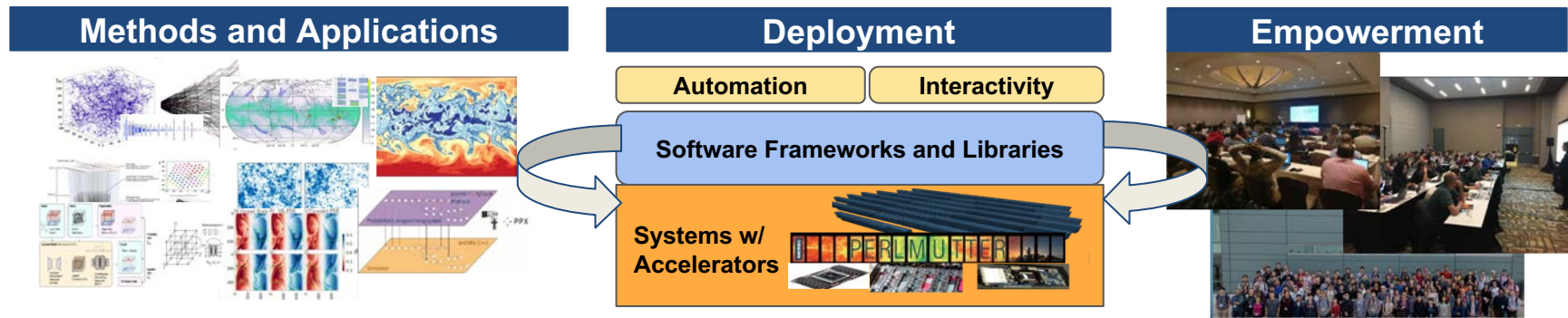
To empower researchers to meld DOE's world-class research tools, infrastructure, and user facilities seamlessly and securely in novel ways to radically accelerate discovery and innovation



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Office of
Science

NERSC AI Strategy



- **Deploy** optimized hardware and software systems
 - Currently Perlmutter >6000 A100 GPUs; Work with vendors for optimized AI software
 - >6x increase in number of users of DL frameworks since 2018
 - Improve performance, e.g through benchmarking (e.g. [MLPerf HPC](#)))
- **Apply ML** for science using cutting-edge methods
 - “NESAP for Learning” application readiness program with postdocs, early access etc.
 - Other targeted engagements that push model development, scale and performance
 - Leverage lessons learned for all users
- **Empower** through seminars, training and schools
 - E.g. Deep Learning at Scale tutorial at Supercomputing

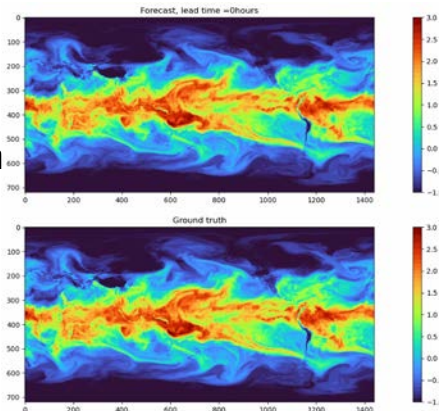
Transformative AI for new science - powered By Perlmutter

FourCastNet

Pathak et al. 2022 [arXiv:2202.11214](https://arxiv.org/abs/2202.11214)

Forecasts global weather at high resolution. Hybrid data/ model parallel @ 4000 GPUs

First deep-learning with skill of numerical weather prediction

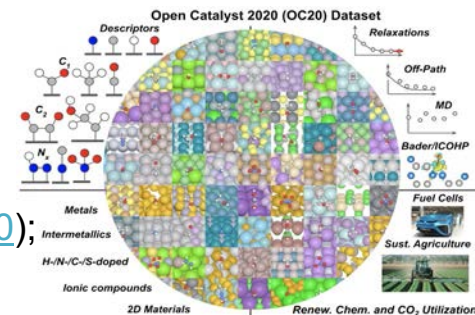


CatalysisDL

Chanussot et al. 2021

[arXiv:2010.09990](https://arxiv.org/abs/2010.09990)

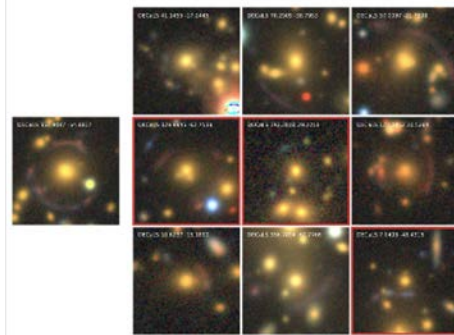
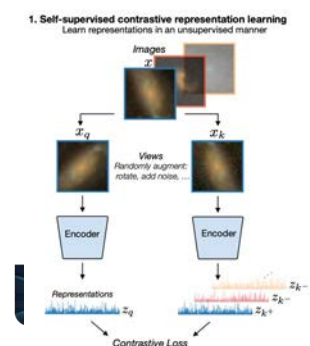
Co-developed largest catalysis dataset ([OC20](https://oc20.org/)); [Graph-parallel NN approaches](#) and [NeurIPS 2021 + 2022 Competitions](#)



Self-supervised sky surveys

Stein et. al. (2021) [arXiv:2110.00023](https://arxiv.org/abs/2110.00023)

Uncovered thousands of undiscovered strong-lenses

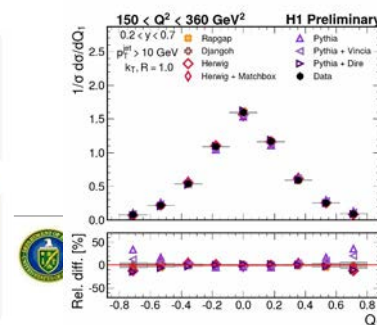
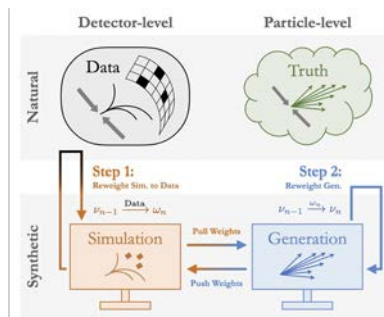


Unfolding for particle physics

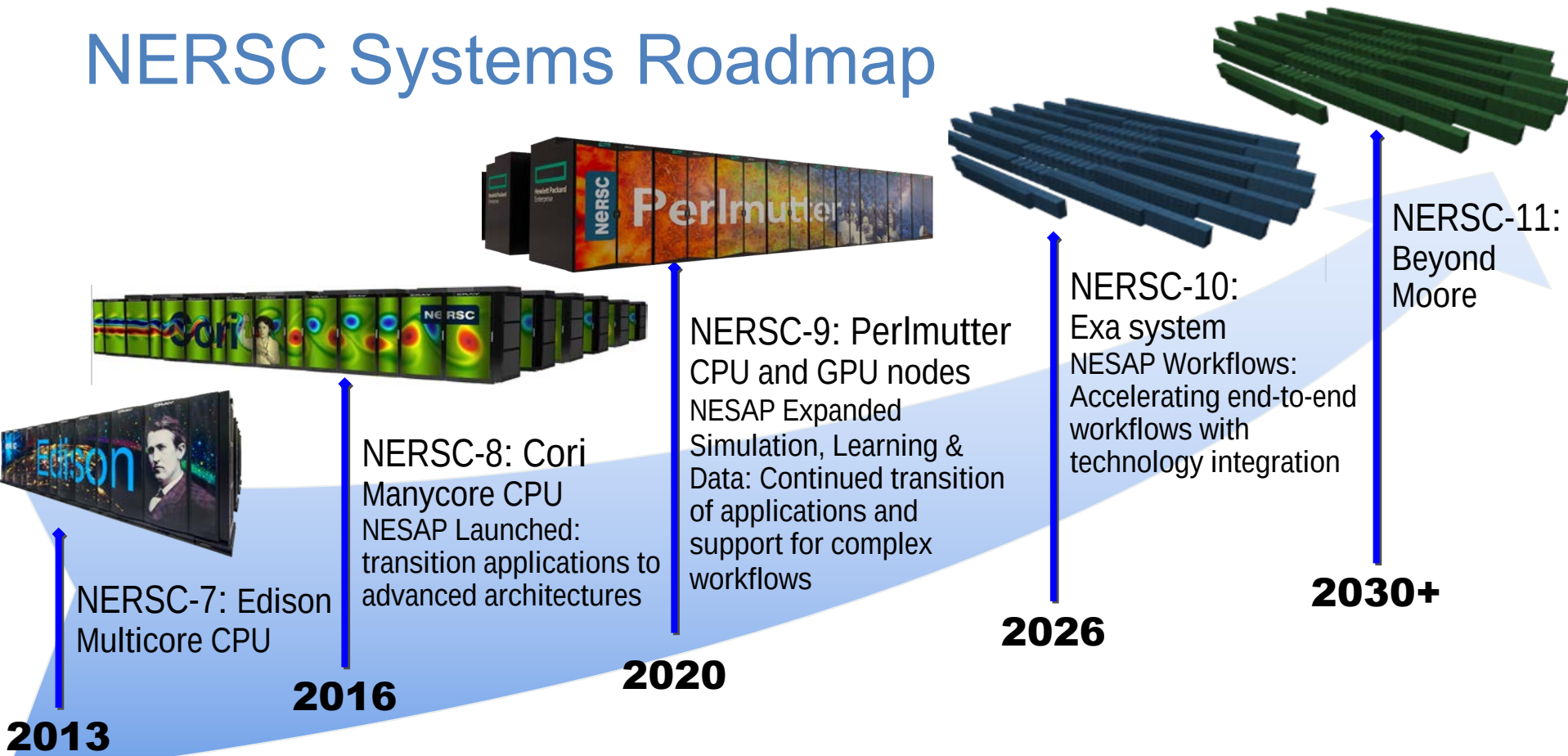
H1 Collaboration ([...] Mikuni et. al.) announced [at DIS2022](https://arxiv.org/abs/2110.00023)

New ML approach extracts new physics insights from old data.

Requires Perlmutter for multiple distributed training runs



NERSC Systems Roadmap



NERSC 10: Workflows and Integration

*Users require an **integrated ecosystem** that supports new paradigms for **data analysis** with **real-time interactive feedback** between experiments and simulations. Users need the ability to **search, analyze, reuse, and combine data** from **different sources** into **large scale simulations and AI models**.*

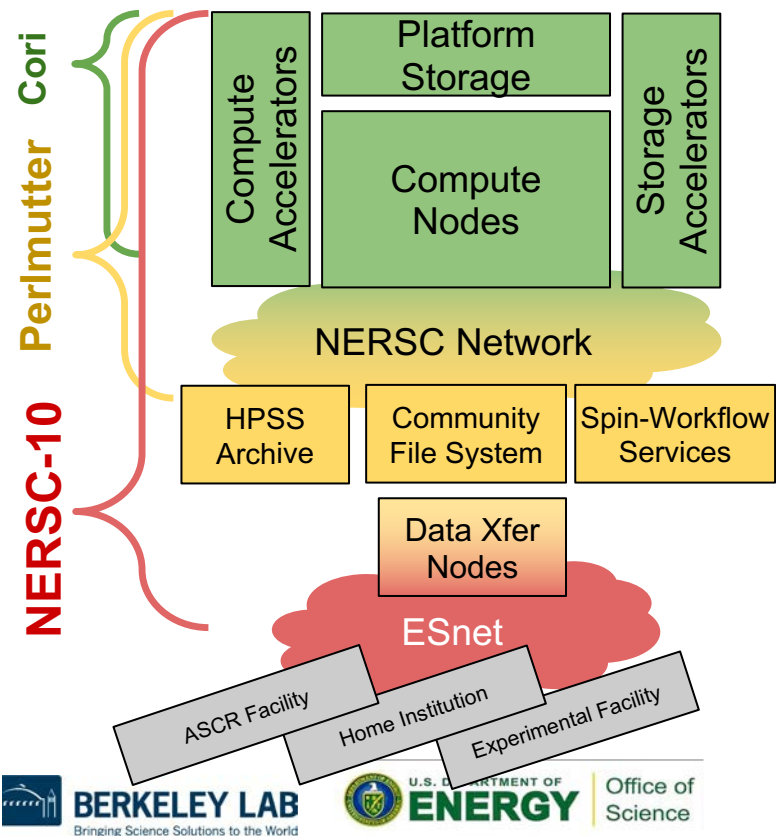
NERSC-10 Mission Need Statement: The NERSC-10 system will accelerate end-to-end DOE SC workflows and enable new modes of scientific discovery through the integration of experiment, data analysis, and simulation.

NERSC-10 CD-0 (Mission Need) has been approved



NERSC-10 Architecture: Designed to Support Complex Simulation and Data Analysis Workflows at High Performance

- **Quality of Service** – computation, storage and networking designed to emphasize response-time plus throughput/utilization.
- **Seamlessness** – tight integration of system components to enable high performance across workflow steps.
- **Portability** – Modular workflow execution across heterogeneous HPC, edge and cloud.
- **Programmability** – APIs to manage data, execute distributed code, and interact with system resources.
- **Orchestration** – coordinate resource management across different resource domains.
- **Security** – authentication, authorization and auditing (e.g., identity proofing, access/privacy control, records of transactions).



Innovation in software is key to enabling complex workflows

New capabilities:
FaaS/serverless,
specialized HW, AI
deployment, data
lifecycle, quantum...

Support usage of both
ssh and Jupyter

Meet federal security
requirements

User software/ workflows

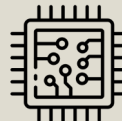


Workflow environment

System software



System hardware



RESTful user-facing
APIs support
automation

System-side APIs for
workflow observability,
administration and
reconfigurability

Containerize the user
environment

NESAP is NERSC's Vehicle for Preparing Users for Current and Future Systems

NESAP is a collaboration between NERSC, Strategic Science Teams, and Technology Vendors to prepare science workflows for systems at NERSC

NESAP is evolving from a focus on single application performance to consider the entire science workflow

- Science Workflow and Technology **CoDesign**
- **Early Access** to Advanced Hardware
- Deep-Dive Collaborative **Code Development, Analysis and Optimization**
- Mutual **Staff Embedding, Training, and Experience Sharing**
- Creation of Lessons Learned and Best Practices to be shared with HPC community

NESAP Call for Term Projects in Key Areas:

Workflow Performance /
Portability

Advanced capability areas
anticipated in **IRI** and **N10**

Workflows Yet to
Benefit from Perlmutter
GPUs

Frontier and
Aurora
Portability

AI in the
Loop

Smart
Networking /
Compression

QoS storage
system (QSS)

API
Driven
Workflows

IRI / Multi-site
workflows

QoS Network /
scheduling

Programming
Env.

Reduced Precision /
Tensor Instructions

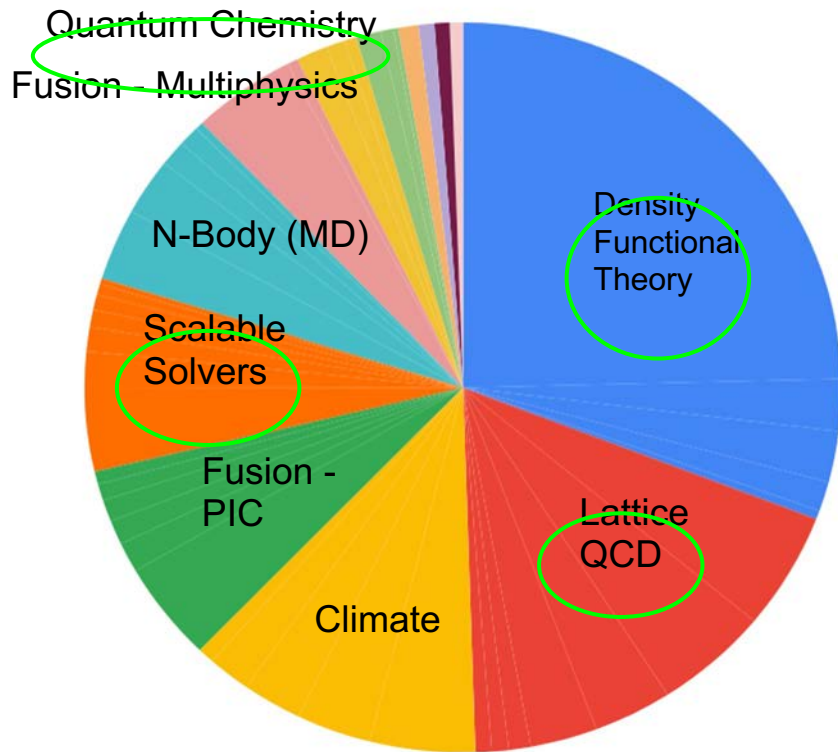
Containers /
Cloud Native

Workflow
Enablement
Nodes (WEN)

Pathfinding: Quantum Computing will be relevant to big parts of NERSC workload

	Logical Qubits	Note
Quantum Chemistry	$\propto$ active orbitals 10^1 - 10^2	Possible NISQ “killer app” - NAS
Density Functional Theory	$\propto$ bands 10^3 - 10^5	Algorithm published. Like ab initio, but larger systems.
Lattice QCD	$\propto$ lattice sites. 10^6 - 10^9	Algorithm published.
Machine Learning	???	Frameworks published. TensorFlow Quantum, TorchQuantum
Scalable Solvers	???	Kernels published. ($Ax=b$, FFT)

Top Algorithms among NERSC codes Allocation Year 2018



NERSC Quantum Computing Roadmap

2022	2022-2024	2024-2028	2028-203?
• Ramp up engagement with QIS community • Director's Discretionary Reserve Call for quantum information science (QIS) on Perlmutter	• Engage with quantum hardware companies • Enable user access to quantum hardware • Development of hybrid algorithms • Identify opportunities for quantum accelerated HPC codes • Benchmarking quantum hardware	• Integration of near-term (NISQ) quantum hardware becoming standard • Users requesting both classical and quantum resources	• High-performing quantum hardware becoming available • Full integration with traditional HPC • Users routinely solve problems using quantum hardware !

Optimal integration of classical and quantum processors is an open area of research



Thanks!