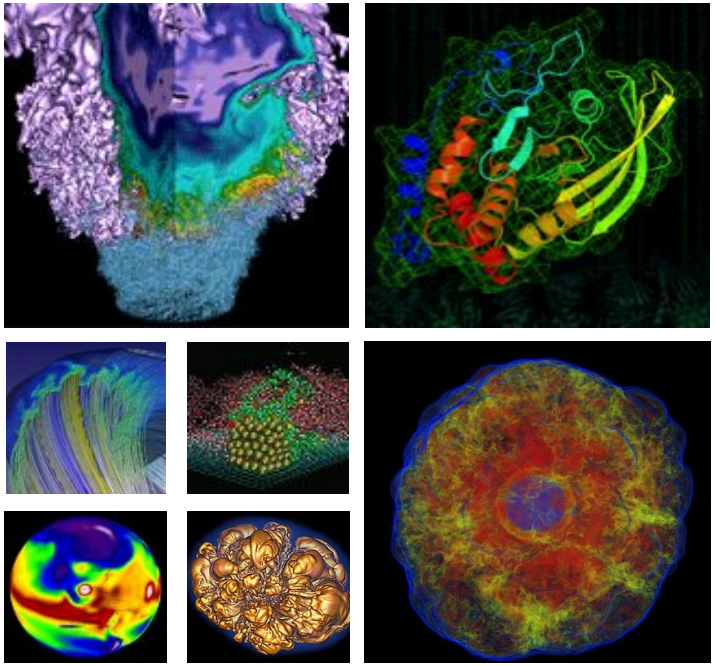
Future Advanced Computing Ecosystem



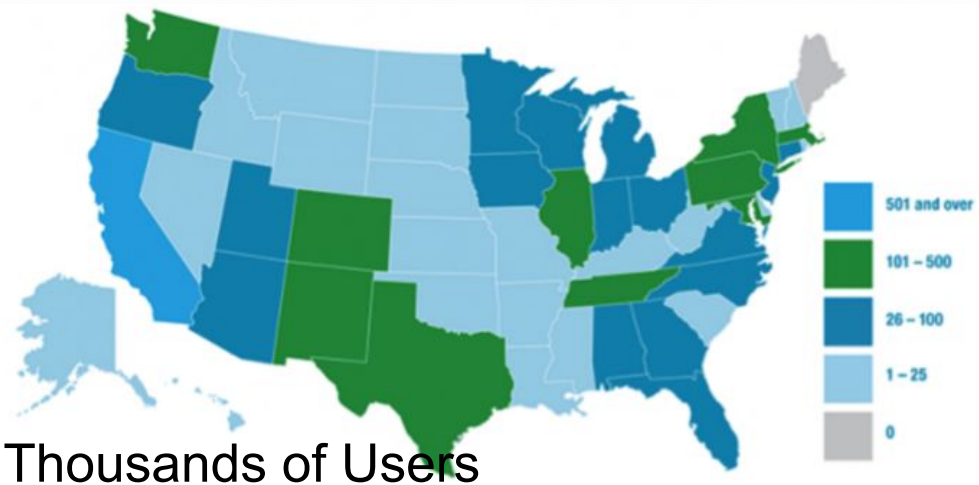
NERSC

Katie Antypas
NERSC Division Deputy
August 17, 2020

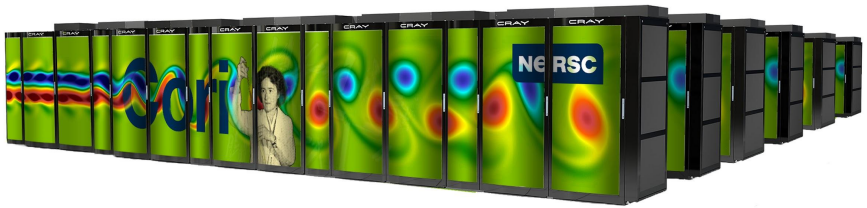
U.S. DEPARTMENT OF ENERGY | Office of Science

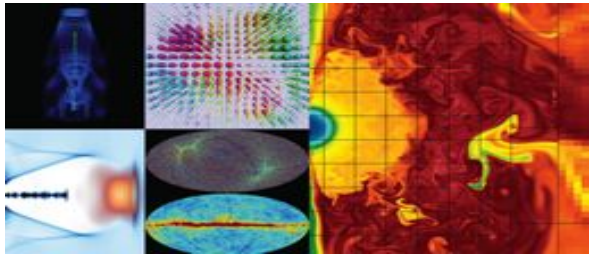
BERKELEY LAB

NERSC is the mission High Performance Computing facility for the DOE Office of Science

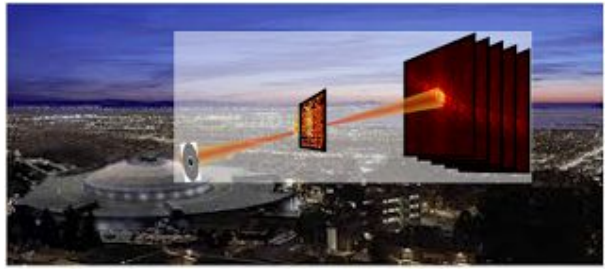


Thousands of Users
800 Projects
700 Codes
2000 NERSC citations per year





Simulations at scale



Data analysis support for DOE's experimental and observational facilities
Photo Credit: CAMERA

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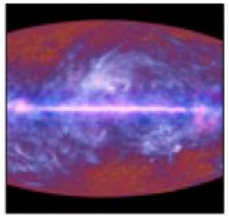
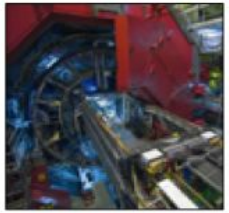
NERSC already supports a large number of users and projects from DOE SC's experimental and observational facilities

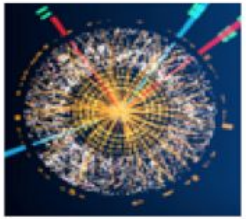
Palomar Transient Factory Supernova



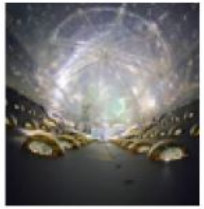
Planck Satellite Cosmic Microwave Background Radiation



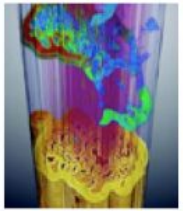
Alice Large Hadron Collider



Atlas Large Hadron Collider



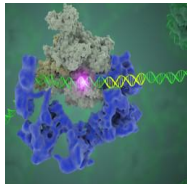
Dayabay Neutrinos



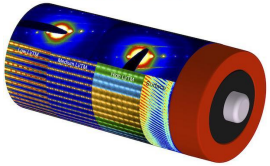
ALS Light Source

LCLS Light Source

Joint Genome Institute Bioinformatics



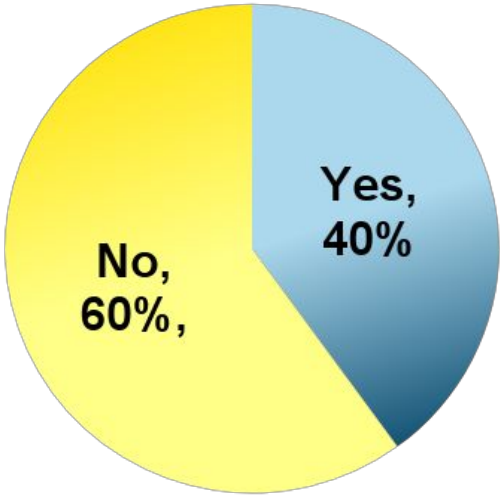
Cryo-EM



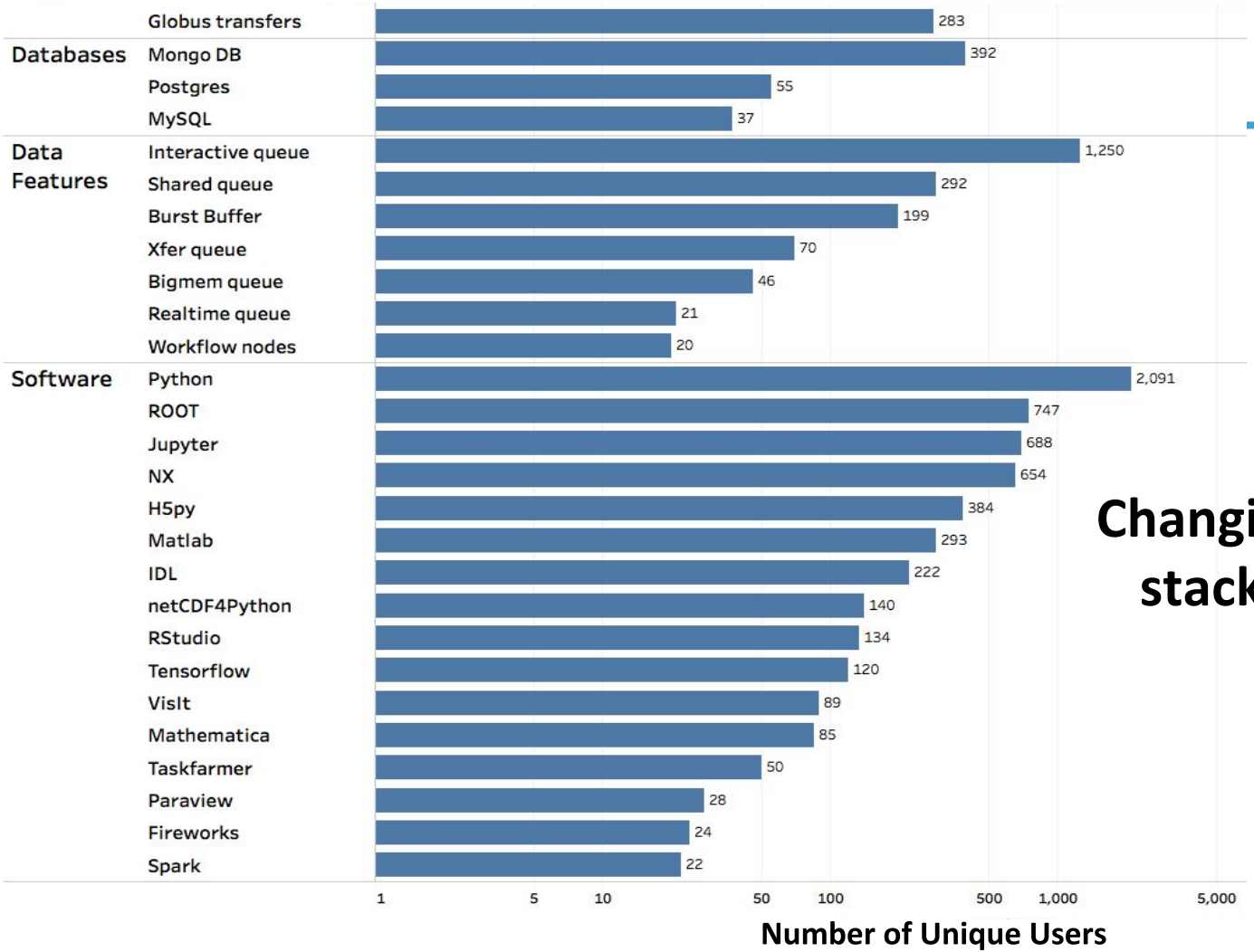
NCEM

DESI

2018 Call for Proposals Question

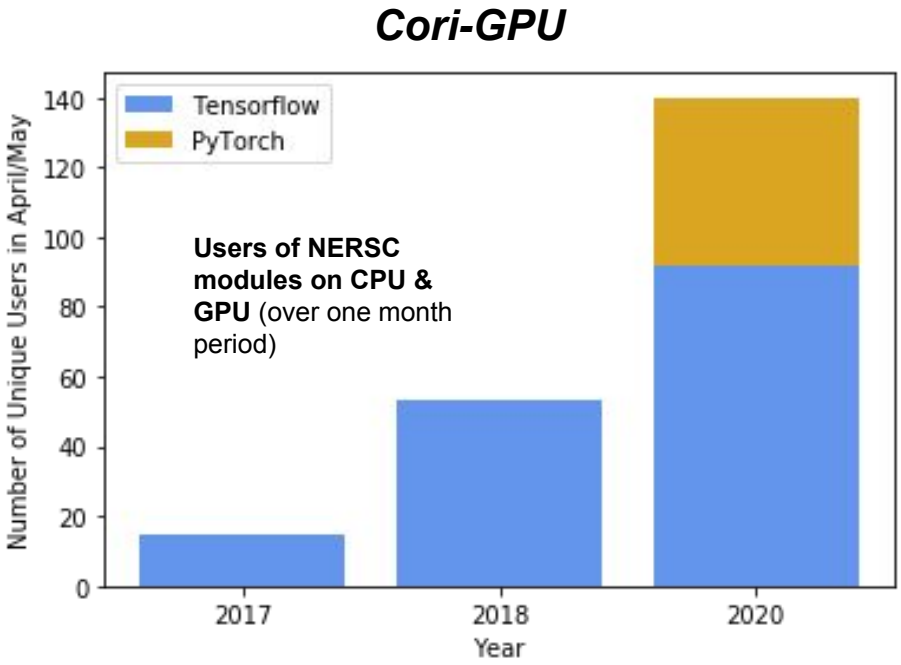


Is the primary role of this project to analyze data from experimental facilities; Or combined models and simulations with experimental data?



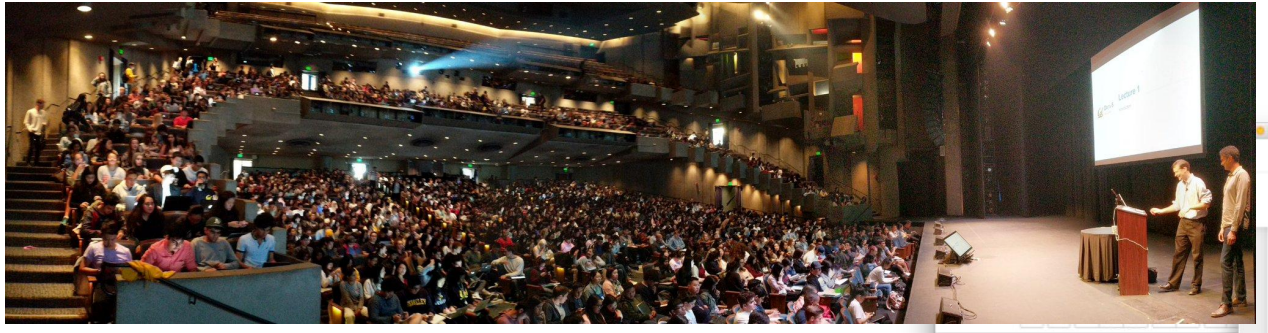
Changing software stack at NERSC

Growing AI and DL workload

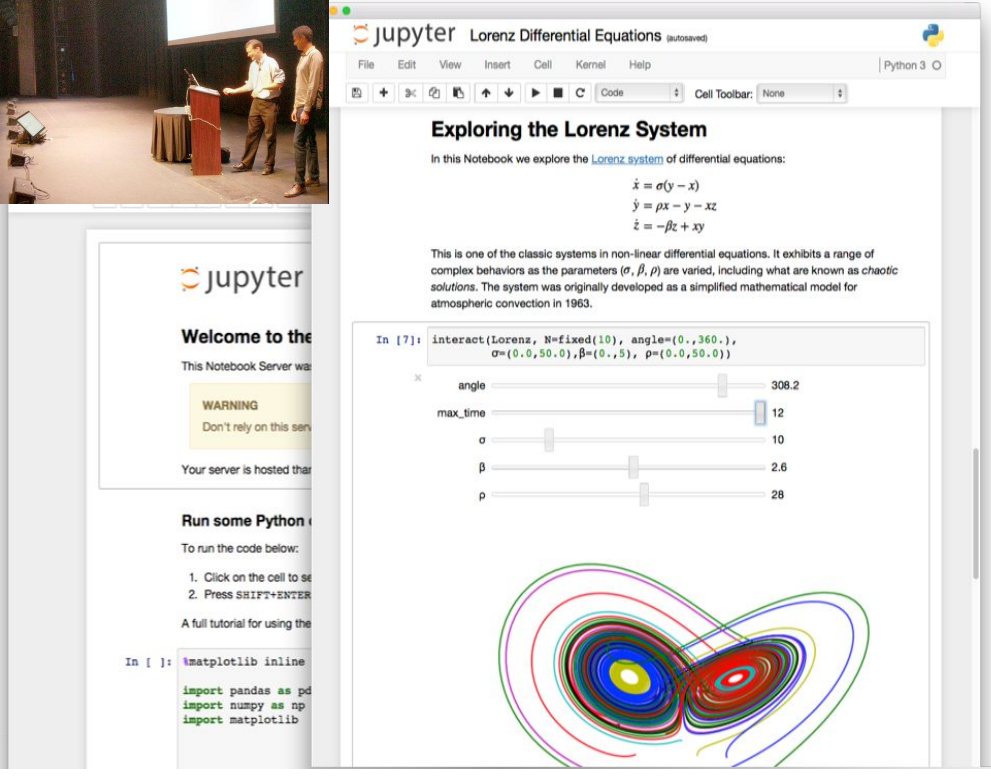


- **Deep learning (DL) users/workload growing**
- **Cori-GPU development system useful indicator for Perlmutter**
- **More than 75% of the compute hours are DL users**
- **Users routinely run distributed across multiple GPUs**

Jupyter: reproducible, sharable computing, now at scale



Data 8: Foundations of Data Science, Fall 2018, Zellerbach Hall



jupyter

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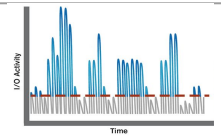
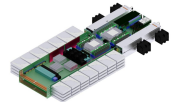
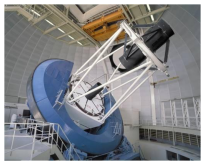
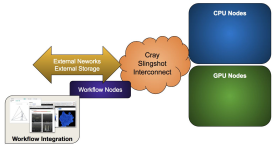
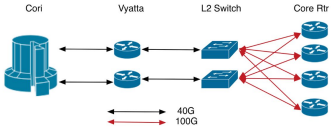
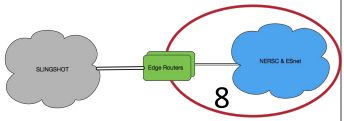
NERSC-9: A System Optimized for Science

- **Cray Shasta System providing >4x capability of Cori system**
- **First NERSC system designed to meet needs of both large scale simulation and data analysis from experimental facilities**
  - Includes both NVIDIA GPU-accelerated and AMD CPU-only nodes
  - All-Flash filesystem for I/O acceleration
  - Cray Slingshot high-performance network will support Terabit rate connections to system
  - Optimized data software stack enabling analytics and ML at scale
  - Dedicated workflow and data management nodes
  - Real-time and co-scheduling capabilities
- **Robust readiness program**
- **Delivery in 2 phases, GPU cabinets in late 2020**

Data Features	Cori System	NERSC Perlmutter
I/O and Storage	Burst Buffer 	All-flash file system: performance with ease of data management 
Analytics - **Production stacks** - **Analytics libraries** - **Machine learning**	User defined images with Shifter NESAP for data New analytics and ML libraries	 Complex workflow support Optimised analytics libraries and deep learning frameworks supported at scale
Workflow integration	Real-time queues	 SLURM co-scheduling Workflow nodes integrated
Data transfer and streaming	SDN 	Slingshot ethernet-based converged fabric 

In Summary:

- HPC Workloads are ***changing***: workflows are becoming more ***complex***, and ***need*** to be accommodated on HPC systems.
- Scientists need support for ***data management, data analysis, sharing and curation*** to enable their science: ***Machine learning*** is transforming science
- Much of this new robust ecosystem, now being deployed on HPC systems, originated ***outside*** the HPC community
- HPC Community has both an ***opportunity*** and a ***need*** to partner with existing communities and develop new capabilities to advance the software ecosystem for science.

"Any opinions, findings, conclusions or recommendations expressed in this material are those of the author(s) and do not necessarily reflect the views of the Networking and Information Technology Research and Development Program."

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