# NERSC Overview



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#### Agenda



- Introduction to NERSC
- Hardware
- Software
- Interacting with NERSC
- User Responsibilities & Expectations





#### About NERSC



- National Energy Research Scientific Computing Center
  - Established 1974, first unclassified supercomputer center
  - Original mission: to enable computational science as complement to magnetically controlled plasma experiment
- Today's mission: Accelerate scientific discovery at the DOE Office of Science through High-Performance Computing and Extreme Data Analysis
- NERSC is a national user facility





#### About NERSC



- Diverse workload:
  - 7000 users, 800 projects
  - 600 codes, 100s of users daily
- Allocations primarily controlled by DOE
  - 80% DOE Annual production awards (ERCAP)
    - O(10K)-O(10M) hour awards
    - Proposal-based, chosen by DOE program managers
  - 10% DOE ASCR Leadership Computing Challenge
  - 10% NERSC reserve



#### Turbulence in Solar Wind





### DOE View of NERSC Workload





ASCR	Advanced Scientific Computing Research
BER	Biological & Environmental Research
BES	Basic Energy Sciences
FES	Fusion Energy Sciences
HEP	High Energy Physics
NP	Nuclear Physics
SBIR	Small Business Innovation Research





#### Over 600 Codes Run at NERSC





- Ten codes make up 50% of NERSC workload
- 25 codes make up 66% of NERSC workload





#### Focus on Science

NERSC users produce publish more than any other center in the world\*; ~2,500 / year



14 in Nature

NERSC







6 Nobel-prize winning users



\* as far as we can tell



### Help NERSC Help You!



- Be sure to acknowledge NERSC in publications!
  - This research used resources of the National Energy Research Scientific Computing Center, which is supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.
  - Available at:

https://www.nersc.gov/users/accounts/user-acco unts/acknowledge-nersc/

- Science highlights sent to DOE each quarter
  - Please send us links to your publications!



Magnetic field lines from HiFi simulations of two spheromaks. NERSC repo m1255 Image courtesy of Vyacheslav Lukin (NRL)





# **NERSC Systems Roadmap**

2016

NERSC-7: Edison Multi-core CPU

2013

NERSC-8: Cori Manycore CPU NESAP Launched: transition applications to advanced architectures NERSC-9: Perlmutter CPU and GPU nodes Continued transition of applications and support for complex workflows NERSC-10

2024



2020

#### **NERSC-9: A System Optimized for Science**



- Cray Shasta System providing 3-4x 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
  - Cray Slingshot high-performance network will support Terabit rate connections to system
  - Optimized data software stack enabling analytics and ML at scale
  - All-Flash filesystem for I/O acceleration
- Robust readiness program for simulation, data and learning applications and complex workflows
- Delivery in late 2020







# NERSC-9 will be named after Saul Perlmutter

- Winner of 2011 Nobel Prize in Physics for discovery of the accelerating expansion of the universe.
- Supernova Cosmology Project, lead by Perlmutter, was a pioneer in using supercomputers combine large scale simulations with experimental data analysis
- Login "saul.nersc.gov"





#### NERSC Systems Map 2019









#### HPC Systems: Cori



#### Haswell Nodes:

- For throughput
- Queues allow single-core jobs
- Longer walltime limits for smaller jobs
- Long queues

#### KNL Nodes:

- For performance
- Codes should exploit many-core architecture
- Large jobs encouraged
  - Large-job discount for jobs using ≥1024 nodes
- 4x larger than Haswell partition
- Shorter queues
- Flex queue increases throughput





#### Filesystems

NERSC

- Global Filesystems:
  - Home
  - Project
- Local Filesystems:
  - Scratch
  - Burst Buffer
- Long-term Storage System:
  HPSS







#### **Global Filesystems**



#### Home

- Permanent, relatively small storage
- Mounted on all platforms
- NOT tuned to perform well for parallel jobs
- Quota cannot be changed
- Snapshot backups (7-day history)
- Perfect for storing data such as source code, shell scripts

#### Project

- Permanent, larger storage
- Mounted on all platforms
- Medium performance for parallel jobs
- Quota can be changed
- Snapshot backups (7-day history)
- Perfect for sharing data within research group





#### Local Filesystems



#### Scratch

- Large, temporary storage
- Optimized for read/write operations, NOT storage
- Not backed up
- Purge policy (12 weeks)
- Perfect for staging data and performing computations

#### **Burst Buffer**

- Temporary per-job storage
- High-performance SSD file system
- Available on Cori only
- Perfect for getting good performance in I/O-constrained codes





### Long-Term Storage System



#### HPSS

- High-Performance Storage System
- Archival storage of infrequently accessed data
- Hierarchical storage:
  - Data first ingested onto high-performance disk arrays
  - Migrated to large enterprise tape subsystem for long-term retention
- (For more info please see later presentations)





### Using NERSC Filesystems (1)



- Analogy:
  - Computing = baking
  - Input = baking ingredients
  - Output = cake
- NERSC is gigantic shared kitchen space with all the latest kitchen gadgets
  - Computers = ovens
  - Home, project = pantry, fridge
  - HPSS = freezer
  - Scratch = kitchen counter







## Using NERSC Filesystems (2)

NERSC

- When baking, stage ingredients from pantry and fridge (plus maybe rarely used ingredients from freezer) onto kitchen counter
  - Likewise, stage data and executable onto scratch filesystem



New Mexico. Mrs. Fidel Romero proudly exhibits her canned food, 1946 US National Archives NWDNS-33-S-12785





## Using NERSC Filesystems (3)



- After baking, clean up after yourself!
- It's okay to let cake cool on kitchen counter, but need to leave space clean for next user
  - After a while, we will clean up if you don't, but not like you would want
  - We will throw all your materials in the trash (even your cake!)



Queen cakes cooling on a wire rack by James Petts <a href="https://www.flickr.com/photos/14730981@N08/13475333725/">https://www.flickr.com/photos/14730981@N08/13475333725/</a>





#### Software



- Cray supercomputers OS is a version of Linux
- Compilers are provided on machines
- Libraries: many libraries are provided by vendor, still others provided by NERSC
- Applications: NERSC compiles and supports many software packages for our users
- (For more details, please see later presentations!)











## Interacting with NERSC



- NERSC Consulting
- NERSC Operations
- NERSC User Group (NUG)





#### NERSC Consulting & Account Support





































### NERSC Consulting

The first people you interact with when

submitting a ticket or calling

 In 2018, handled 7194 tickets from 2350 unique users



Account Support = 1,598 (22.21%) Running Jobs = 1,317 (18.31%) Software = 1,248 (17.35%) Data/IO = 589 (8.19%) Other = 543 (7.55%) ERCAP = 402 (5.59%) Allocations = 385 (5.35%) Clogin Node = 320 (4.45%) Pogramming = 318 (4.42%) Performance = 120 (1.67%) Data/IO = 103 (1.43%) Network = 22 (1.14%) Other (more ...) = 159 (2.35%)





Nerso

#### NERSC Consulting: Expectations



- We will reply to you within four business-hours
- We will help you resolve your problem, and keep you apprised of progress
- We will attempt to accommodate user needs that don't fit within our operating structure
- We welcome user feedback and constructive criticism





### NERSC Consulting: Tips & Tricks

- Help us help you!
- Provide specifics:
  - What is the problem?
  - What machine?
  - When did it happen?
  - What modules were loaded?
  - How did you try to fix or work around it?





#### **NERSC** Operations



- Operations staff are on site 24/7/365 to supervise operation of the machine room
- Operations know the health of the machines and can help users with some tasks (password reset, killing jobs, changes to running reservation, etc.)





## NERSC User Group (NUG)



- Community of NERSC users
- Source of advice and feedback for NERSC (we listen!)
- Executive Committee: 3 representatives from each office + 3 members-at-large
- Monthly teleconferences hosted by NERSC (usually 3rd Thursday of the month, 11 am to noon)





### User Responsibilities & Expectations

NERSC

- Be kind to your neighbor users
  - Don't abuse the shared resources!
- Use your allocation smartly
- Pick the right resource for your job and your data
  - Small jobs are great on Cori Haswell, not so good on Cori KNL
- Back your stuff up
  - Especially from scratch, which has a purge policy
- Acknowledge NERSC in your papers
  - Acknowledge us so we can stay in business!
- Pay attention to security
  - Don't share your account with others!





Thank You and Welcome to NERSC!

