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

Initial Allocation of Hours by DOE Office of Science Program Office 2017

<table>
<thead>
<tr>
<th>Office of Science</th>
<th>Percentage</th>
</tr>
</thead>
<tbody>
<tr>
<td>ASCR</td>
<td>Advanced Scientific Computing Research</td>
</tr>
<tr>
<td>BER</td>
<td>Biological &amp; Environmental Research</td>
</tr>
<tr>
<td>BES</td>
<td>Basic Energy Sciences</td>
</tr>
<tr>
<td>FES</td>
<td>Fusion Energy Sciences</td>
</tr>
<tr>
<td>HEP</td>
<td>High Energy Physics</td>
</tr>
<tr>
<td>NP</td>
<td>Nuclear Physics</td>
</tr>
<tr>
<td>SBIR</td>
<td>Small Business Innovation Research</td>
</tr>
</tbody>
</table>
Over 600 Codes Run at NERSC

- Ten codes make up 50% of NERSC workload
- 25 codes make up 66% of NERSC workload
NERSC users produce publish more than any other center in the world*; ~2K/year

1,300 citations via Web of Science in 2017 (underestimate!)

* 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-accounts/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

NERSC-7: Edison
Multi-core CPU

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

2013
2016
2020
2024
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”
HPC Systems

Edison:
- Large, stable machine
- Shorter queues
- Lower charge factor
- Retiring March 31, 2019

Cori:
- 2 types of nodes: Haswell and KNL
- *Haswell nodes*: for throughput
  - Queues allow single-core jobs
  - Longer walltime limits for smaller jobs
- *KNL nodes*: for performance
  - Codes should exploit many-core architecture
  - Large jobs encouraged
Filesystms

- Global Filesystems:
  - Home
  - Project

- Local Filesystems:
  - Scratch
  - Burst Buffer

- Long-term Storage System:
  - HPSS
<table>
<thead>
<tr>
<th></th>
<th>Home</th>
<th>Project</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>● Permanent, relatively small storage</td>
<td>● Permanent, larger storage</td>
</tr>
<tr>
<td></td>
<td>● Mounted on all platforms</td>
<td>● Mounted on all platforms</td>
</tr>
<tr>
<td></td>
<td>● NOT tuned to perform well for parallel jobs</td>
<td>● Medium performance for parallel jobs</td>
</tr>
<tr>
<td></td>
<td>● Quota cannot be changed</td>
<td>● Quota can be changed</td>
</tr>
<tr>
<td></td>
<td>● Snapshot backups (7-day history)</td>
<td>● Snapshot backups (7-day history)</td>
</tr>
<tr>
<td></td>
<td>● <strong>Perfect for storing data such as source code, shell scripts</strong></td>
<td>● <strong>Perfect for sharing data within research group</strong></td>
</tr>
</tbody>
</table>
Local Filesystems

Scratch

- Large, temporary storage
- Local on Edison, Cori scratch also mounted on Edison
- 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)

- 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
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
https://www.flickr.com/photos/14730981@N08/13475333725/
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!)
Chemistry & Materials Applications

- More than 13.5 million lines of source code Compiled, Optimized, and Tested

Codes and Tools:
- VASP
- Quantum ESPRESSO
- SIESTA
- NAMD
- GAMESS
- CPMD
- LAMMPS
- WANNIER90
- NERSC
- BERKELEY LAB
- U.S. DEPARTMENT OF ENERGY

b-initio package simulation

U.S. DEPARTMENT OF ENERGY
Office of Science
Interacting with NERSC

- NERSC Consulting
- NERSC Operations
- NERSC User Group (NUG)
- The first people you interact with when submitting a ticket or calling
- In 2018, handled 7194 tickets from 2350 unique users
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 staff answer phone and forward to consultants during business hours if necessary
- 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

● 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!