• National Energy Research Scientific Computing Center
  – Established 1974, first unclassified supercomputer center
  – Original mission: to enable computational science as a 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
• A national user facility
Today’s Talk

• A brief introduction to the Center and some simple rules for getting work done at NERSC.

Trajectory of an energetic ion in a Field Reverse Configuration (FRC) magnetic field. Magnetic separatrix denoted by green surface. Spheres are colored by azimuthal velocity. Image courtesy of Charlson Kim, U. of Washington; NERSC repos m487, mp21, m1552
You Are Not Alone!

A calculation of the self-generated plasma current in the W7-X reactor, performed using the SFINCS code on Edison. The colors represent the amount of electric current along the magnetic field, and the black lines show magnetic field lines. Image: Matt Landreman
**NERSC: Mission Science Computing for the DOE Office of Science**

- **Diverse workload:**
  - 4,500 users, 700+ projects
  - 700 codes; 100s of users daily

- **Allocations controlled primarily by DOE**
  - 80% DOE Annual Production awards (ERCAP):
    - From 10K hour to ~10M hour
    - Proposal-based; DOE chooses
  - 10% DOE ASCR Leadership Computing Challenge
  - 10% NERSC reserve
    - NISE, NESAP

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*Simulation of density-driven flow for CO₂ storage in saline aquifers. Shown is a snapshot of the CO₂ concentration after onset of convection overlayed on the AMR grid. Image courtesy of George Pau and John Bell (LBNL). Repo mp111*
NERSC 2013 Allocations
By DOE Office

<table>
<thead>
<tr>
<th>Office</th>
<th>Percentage</th>
</tr>
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<tbody>
<tr>
<td>ASCR</td>
<td>6%</td>
</tr>
<tr>
<td>BER</td>
<td>18%</td>
</tr>
<tr>
<td>BES</td>
<td>31%</td>
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<tr>
<td>FES</td>
<td>20%</td>
</tr>
<tr>
<td>HEP</td>
<td>13%</td>
</tr>
<tr>
<td>NP</td>
<td>12%</td>
</tr>
</tbody>
</table>

- **ASCR**: Advanced Scientific Computing Research
- **BER**: Biological & Environmental Research
- **BES**: Basic Energy Sciences
- **FES**: Fusion Energy Sciences
- **HEP**: High Energy Physics
- **NP**: Nuclear Physics
Science View of Workload

NERSC 2013 Allocations By Science Area
What Role Does NERSC Play?

Experimentation → Data Analysis → Simulation → Compute, Store, Analyze, Share

Theory

Compute, Store, Analyze, Share

NERSC Computing and Services
You Will Be Successful!

Collision between two shells of matter ejected in two supernova eruptions, showing a slice through a corner of the event. Colors represent gas density (red is highest, dark blue is lowest). Image courtesy of Ke-Jung Chen, School of Physics and Astronomy, Univ. Minnesota. Repo m1400
Make sure you acknowledge NERSC in publications; please use “official” acknowledgement

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

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.

Science highlights sent to DOE each quarter.
  – Send us links to your publications.

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

• Edison: fastest processors; fastest interconnect; best for scaling to large core counts; higher NERSC machine charging factor

• Hopper: previous generation processors; excellent scalability; lower charge factor

• Carver: compute nodes have more generic Linux; current serial queue
Simple Rules for Success

- Use our web site; use “Search…”
- Cray systems are not “typical” clusters, pay attention to differences
- Be kind to your neighbor users
- Back your stuff up
- Pick the right resource for your job and your data
- Use batch system effectively; pay attention to system-specific syntax and policies
- Use your allocation smartly
- Pay attention to security
Chemistry & Materials Applications

- NERSC compiles and supports many software packages for our users.

- More than 13.5 million lines of source code Compiled, Optimized, and Tested
NERSC User’s Group

• Get involved. Make NUG work for you.
• Provide advice, feedback – we listen.
• Monthly teleconferences with NERSC, usually the last Thursday of the month, 11:00 AM to noon Pacific Time.
• Executive Committee - three representatives from each office and three members-at-large.
• Community!
Rule # 4: Expect Consistency. And Change.

Molecular Dynamics simulation snapshot showing water molecules (red and white), and sodium, chloride ions (green and purple) encountering a sheet of graphene (pale blue, center) perforated by holes of the right size, with water passing through (left side), but sodium and chloride being blocked.
NERSC Roadmap

- Franklin (N5) + QC
  - 36 TF Sustained
  - 352 TF Peak

- Hopper (N6)
  - 1.25 PF Peak

- Edison (N7)
  - 2.4 PF Peak

- Cori (N8)
  - 10-30x Hopper

- CRT Facility
  - N10 ~1 EF Peak
  - N9 200-500 PF Peak

- Peak Teraflop/s
  - 10^7
  - 10^6
  - 10^5
  - 10^4
  - 10^3
  - 10^2
  - 10

- Year:
  - 2006
  - 2007
  - 2008
  - 2009
  - 2010
  - 2011
  - 2012
  - 2013
  - 2014
  - 2015
  - 2016
  - 2017
  - 2018
  - 2019
  - 2020
Change and Consistency

- NERSC will be physically moving to a new facility in 2015.
- Carver will retire September 30, 2015.
- Hopper will retire December, 2015.
- NERSC-8 (Cori)
  - Phase 1 Haswell late summer 2015
  - Phase 2 Knights Landing summer 2016
  - Disruptive change
    - Codes likely will run, but will need to be modified to achieve good performance
    - NERSC will help users make this transition.
- Edison will remain available for codes that cannot transition to NERSC-8
Thank you and welcome to NERSC!
Generic Multiprocessor Architecture