Support for Astronomy & Astrophysics at NERSC

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Outline

• What is NERSC
• Who uses NERSC?
• How to get access to NERSC Resources
• NERSC Requirements Gathering
NERSC is the Production HPC & Data Facility for DOE Office of Science Research

Bio Energy, Environment

Computing

Materials, Chemistry, Geophysics

Particle Physics, Astrophysics

Nuclear Physics

Fusion Energy, Plasma Physics
Some Benefits of NERSC

- Large, state-of-the-art computing and data systems
- Consulting, system admin, 24x7 operations support
- Well maintained software environment, prebuilt optimized applications & libraries
- Designed for massive parallelism, but supports all scales
- Easily share data and codes
- Easy to use account management
- Large permanent archival data storage
- Ongoing technology refreshes
- Word-class cybersecurity
- Open science environment
- Web-based science /data gateways
Focus on Science
• A word-class resource to support world-class science.
• 1,500 refereed journal publications per year
• Supports Nobel-prize winning projects: Chemistry 2013, Physics 2011, Peace 2007

Large diverse user community
• 5,000 users, 700 projects
• From 48 states, 65% from universities
• Many large international collaborations

Science-driven systems and services
• Designed to support science
• Optimized for scientific productivity at cutting-edge scale
Demographics

642 users from outside the U.S.
NERSC Systems Today

**Edison: 2.57PF, 357 TB RAM**
- Cray XC30
- 5,576 nodes
- 134K Cores

**Hopper: 1.3PF, 212 TB RAM**
- Cray XE6
- 6,384 nodes
- 150K Cores

**Production Clusters**
- Carver, PDSF, JGI, KBASE, HEP
- 14x QDR

**Vis & Analytics**
- Data Transfer Nodes
- Adv. Arch. Testbeds
- Science Gateways

**Ethernet & IB Fabric**
- Science Friendly Security
- Production Monitoring
- Power Efficiency
- WAN

**WAN**
- 2 x 10 Gb
- 1 x 100 Gb

**Software Defined Networking**

**Global Scratch**
- 3.6 PB
- 5 x SFA12KE

**Home**
- 5 PB
- DDN9900 & NexSAN

**HPSS**
- 250 TB
- NetApp 5460

**Local Scratch**
- 50 PB stored, 240 PB capacity, 20 years of community data

**ESnet**
- Power Efficiency
- WAN
**Edison Quick Facts**

**First Petaflop system with Intel “Ivy Bridge” processors & Cray Aires High Speed Network**

<table>
<thead>
<tr>
<th>Nodes</th>
<th>5,576 dual-socket with 64 GB memory</th>
</tr>
</thead>
<tbody>
<tr>
<td>Processors</td>
<td>Intel “Ivy Bridge” 12-core, 2.4 GHz</td>
</tr>
<tr>
<td>Network</td>
<td>Cray “Aires” Dragonfly Topology</td>
</tr>
<tr>
<td>Scratch Disk</td>
<td>7.6PB with &gt;165 GB/sec bandwidth</td>
</tr>
<tr>
<td>Peak / Sustained</td>
<td>2.67 PF / 260 TF</td>
</tr>
<tr>
<td>Global Network Bandwidth</td>
<td>&gt; 11 TB/sec</td>
</tr>
<tr>
<td>Node Memory Bandwidth</td>
<td>90 GB/s</td>
</tr>
</tbody>
</table>

**High-Impact Results on Day One**

NERSC’s users started running production codes immediately on Edison.

Top projects: carbon sequestration, artificial photosynthesis, complex novel materials, cosmic background radiation analysis

*Edison is very similar to Hopper, but with 2-5 times the performance per core on most codes.*

NERSC 8 Benchmark Performance

- **GTCS**
- **MILC**
- **miniDFT**
- **MiniFE**
- **MiniGhost**
- **AMG**
- **UMT**
- **SNAP**
NERSC Supports Jobs of all Kinds and Sizes

High Throughput: Statistics, Systematics, Analysis, UQ

Larger Physical Systems, Higher Fidelity
NERSC-8 Mission Need

The Department of Energy Office of Science requires an HPC system to support the rapidly increasing computational demands of the entire spectrum of DOE SC computational research.

- Provide a significant increase in computational capabilities, at least 10 times the sustained performance of the Hopper system on a set of representative DOE benchmarks
- Delivery in the 2015/2016 time frame
- Provide high bandwidth access to existing data stored by continuing research projects.
- Platform needs to begin to transition users to more energy-efficient many-core architectures.
NERSC Data Resources

• Global shared filesystems (aka NGF)
  – Connected to all NERSC computational systems
  – Large, fast, permanent data storage
  – Intended for data sharing within and among projects
  – Many PBs
  – Default quotas ~ 5-10 TB, but often increased

• Hopper and Edison have dedicated “local” scratch systems
  – 2 PB & 7.6 PB, respectively

• Archival storage system
  – HPSS tape-backed storage
  – Permanent, many 10s of PB
  – No quotas per se, current 240 PB capacity

• Grid enabled for fast and easy transfers
• Dedicated data transfer nodes
• Science Data Gateways
Solving the Puzzle of the Neutrino

• HPC and ESnet vital in the measurement of the important “$\theta_{13}$” neutrino parameter.
  – Last and most elusive piece of a longstanding puzzle: why neutrinos appear to vanish as they travel
  – The result affords new understanding of fundamental physics; may eventually help solve the riddle of matter-antimatter asymmetry in the universe.

• HPC for simulation / analysis; HPSS and data transfer capabilities; NGF and Science Gateways for distributing results
  • All the raw, simulated, and derived data are analyzed and archived at a single site
  • => Investment in experimental physics requires investment in HPC.

• One of Science Magazine’s Top-Ten Breakthroughs of 2012

The Daya Bay experiment counts antineutrinos at three detectors (shown in yellow) near the nuclear reactors and calculates how many would reach the detectors if there were no oscillation. transformation.

PI: Kam-Biu Luk (LBNL)
The Planck Mission

• A European Space Agency (+NASA) satellite mission to measure the temperature and polarization of the Cosmic Microwave Background.
  – The echo of the Big Bang: primordial photons have seen it all.
  – Fluctuations encode all of fundamental physics & cosmology.
  – Planck results assumed by all Dark Energy experiments.

• Realizing the full scientific potential of Planck requires very significant computing resources
  – Tiny signal (µK - nK) requires huge data volume for sufficient S/N
  – 72 detectors sampling at 30-180Hz for 2.5 years => $10^{12}$ samples.
  – Analysis depends critically on Monte Carlo methods
    • Simulate and analyze $10^4$ realizations of the entire mission!

• One of Physics World’s Top 10 Breakthroughs of 2013
NERSC 2013 Usage by Scientific Discipline

- Materials: 22%
- Fusion: 18%
- Chemistry: 13%
- Climate: 11%
- QCD: 11%
- Geophysics: 5%
- Astrophysics: 4%
- Life Sciences: 4%
- Combustion: 3%
- Accelerator: 2%
- Other: 7%
NERSC (all) and HEP Computational Hours

2017 HEP Need: 42.8 Billion
2014 HEP Need: 2.4 Billion
2012 HEP Usage: 184 Million

NERSC 8 Target

All NERSC 2014 Allocation

HEP Need (Dashed)
Who Uses NERSC? – Archival Storage

Archival Data Stored at NERSC - March 2014

Tape-Backed Storage
NERSC Total: 38 PB
Astro: 6.5 PB

- Climate Research: 34%
- Astrophysics: 17%
- CMB Transient/SN searches: 11%
- Biosciences: 10%
- Applied Math: 6%
- Nuclear Physics: 4%
- Lattice QCD: 3%
- Fusion Energy: 3%
- Computer Science: 2%
- Other: 4%
- Combustion: 3%
- High Energy Physics: 3%
- Materials Science: 3%

NERSC Total: 38 PB
Astro: 6.5 PB
High Energy Physics (HEP) and All NERSC Archival Storage

- HEP Usage
- All NERSC
- All NERSC Trend
- HEP Trend
- HEP Need 2014
- All NERSC Need 2014
- HEP Need 2017

Data Stored (TB)

Year


HEP 2017 Need: 242 PB
HEP 2014 Need: 7.5 PB
HEP 2012 Usage: 4 PB
Who Uses NERSC? – Permanent Disk

Shared Permanent Disk Storage at NERSC - March 2014

- Nuclear Physics: 7%
- Materials Science: 8%
- Computer Science: 11%
- Climate Research: 12%
- Other: 6%
- High Energy Physics: 28%
- Astrophysics: 28%
- Planck: Cosmo Simulation Data

Permanenl Spinning Disk
(Shared)
NERSC Total: 3.25 PB
Astro: 0.9 PB
NERSC Resource Usage by Office 2013

- NGF Storage
- HPSS Storage
- MPP Compute

Percent of Total

ASCR | BER | BES | FES | HEP | NP
Astronomy & Astrophysics Projects at NERSC

• **55 Projects in 2014**
  – 250 Million hours of compute time allocated
  – 6.5 PB of archival data currently stored
  – 1 PB on permanent spinning disk shared among project members (/project)

• **Science Emphasis**
  – Planck data analysis and synthetic observations/maps
  – Supernova searches & transients
  – Cosmological simulations
  – Supernova simulations
  – Other: Neutrino astrophysics, radio astronomy data analysis, galaxy formation, X-ray bursts, MHD, ...
HPC Services at NERSC

User Services

HPC Consultants (1 open position)

Data & Analytics Services

JGI Consultants

PDSF Consultant

Postdoc Program Coming Soon

+ Many partial FTEs
Year to Year comparison: JGI overall satisfaction with NERSC

JGI Users

<table>
<thead>
<tr>
<th>Year</th>
<th>Satisfaction Level</th>
</tr>
</thead>
<tbody>
<tr>
<td>2011</td>
<td>5.32</td>
</tr>
<tr>
<td>2012</td>
<td>5.27</td>
</tr>
<tr>
<td>2013</td>
<td>6.25</td>
</tr>
</tbody>
</table>

MPP Users

<table>
<thead>
<tr>
<th>Year</th>
<th>Satisfaction Level</th>
</tr>
</thead>
<tbody>
<tr>
<td>2011</td>
<td>6.53</td>
</tr>
<tr>
<td>2012</td>
<td>6.48</td>
</tr>
<tr>
<td>2013</td>
<td>6.54</td>
</tr>
</tbody>
</table>
How to Get Access to NERSC Resources

• “ERCAP” allocations process
  – 80% of compute hours allocated by DOE program managers to projects doing research within the DOE mission
  – 10% allocated through ALCC (high-risk, high-payoff)
  – Archival storage (tape) also allocated
  – Project funding from DOE not required; at discretion of program managers

• NERSC Director’s Reserve for strategic projects
  – 10% of computer time (250 M hours)
  – NISE and Data Initiative exploratory programs

• Startup Projects
  – At NERSC’s discretion
  – Up to 50 K hours for 18 months
How to Get Access to NERSC II

• Buy-in model for hardware and support
  – PDSF cluster: Nuclear and High Energy Physics
  – Genepool cluster & file systems: Joint Genome Institute

• A La Carte resources run by NERSC
  – Planck bought a rack of a compute cluster
  – Fixed cost for 5 years of shared spinning disk (coming soon)
  – The Materials Project has dedicated nodes
  – Science Gateways
High Performance Computing is …

... the application of supercomputers, data systems, networking, and advanced algorithms & workflows to scientific problems that are either too large for standard computers or would take too long on them.

Understanding How Proteins Work

Designing Better Batteries

The Universe

Climate
HPC is a Tool for Discovery
Requirements Reviews

1½-day reviews with each Program Office

Computing and storage requirements for next 5 years

• Participants
  – DOE ADs & Program Managers
  – Leading NERSC users & key potential users
  – NERSC staff & CS Experts

Scientific Objectives

Computing, Storage, Software, Services Requirements
Reports From 8 Requirements Reviews Have Been Published

- Computing and storage requirements for 2014 & 2017
- Executive Summary of requirements
- Case studies
- Second round, for 2017 requirements, will be completed in April 2014 (NP)

http://www.nersc.gov/science/hpc-requirements-reviews/reports/
Impact

• Highly regarded within DOE
• Scientific justification for ASCR budget requests
  – Quantitative requirements
  – Documented science goals & needs from science teams
• Basis for NERSC 7 and NERSC 8 Mission Need documents
• Influence on NERSC services
  – e.g. application readiness, support for high-throughput computing, planning for NERSC data services
• Derivative publications and reports:
  – HEP community’s “Snowmass” Report
  – DOE ASCR white paper on data needs
HEP Executive Summary

• More computing and data resources needed
• Vastly improved I/O capabilities and better facilities for data-intensive science
• Need to support both large-scale and ensemble runs
• Assistance needed to transition to next-generation processors
• There are communities within DOE HEP that are not traditional users of large HPC centers, yet have a profound need for additional computing, storage, and analysis facilities. (LHC, sky surveys, ...)
### HEP Cosmic Frontier Requirements - MPP

<table>
<thead>
<tr>
<th>Project</th>
<th>Repos</th>
<th>2012 Usage</th>
<th>2017 Need</th>
<th>Factor Increase</th>
</tr>
</thead>
<tbody>
<tr>
<td>Experimental Cosmology</td>
<td>LSST, Boss, BigBoss, DES, DESSN, PTF, DESI, COSMO</td>
<td>2 M</td>
<td>82 M</td>
<td>41</td>
</tr>
<tr>
<td>Cosmological Simulations for Sky Surveys</td>
<td>Cosmosim, cusp, hacc</td>
<td>24 M</td>
<td>10,000 M</td>
<td>417</td>
</tr>
<tr>
<td>CMB Analysis</td>
<td>Planck, usplanck, mp107</td>
<td>13 M</td>
<td>500 M</td>
<td>38</td>
</tr>
<tr>
<td>Supernova Studies</td>
<td>m1400</td>
<td>13 M</td>
<td>200 M</td>
<td>15</td>
</tr>
</tbody>
</table>
## HEP Cosmic Frontier Requirements - HPSS

<table>
<thead>
<tr>
<th>Project</th>
<th>Repos</th>
<th>2012 Usage</th>
<th>2017 Need</th>
<th>Factor Increase</th>
</tr>
</thead>
<tbody>
<tr>
<td>Experimental Cosmology</td>
<td>LSST, Boss, BigBoss, DES, DESSN, PTF, DESI, COSMO</td>
<td>40 TB</td>
<td>1,000 TB</td>
<td>25</td>
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<tr>
<td>Cosmological Simulations for Sky Surveys</td>
<td>Cosmosim, cusp, hacc</td>
<td>70 TB</td>
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<td>143</td>
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<tr>
<td>CMB Analysis</td>
<td>Planck, usplanck, mp107</td>
<td>550 TB</td>
<td>50,000 TB</td>
<td>91</td>
</tr>
<tr>
<td>Supernova Studies</td>
<td>m1400</td>
<td>100 TB</td>
<td>2,000 TB</td>
<td>20</td>
</tr>
</tbody>
</table>

7.6 X is “Normal”
<table>
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<td>20TB</td>
<td>500 TB</td>
<td>25</td>
</tr>
<tr>
<td>Cosmological Simulations for Sky Surveys</td>
<td>Cosmosim, cusp, hacc</td>
<td>120 TB</td>
<td>10,000 TB</td>
<td>83</td>
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<tr>
<td>CMB Analysis</td>
<td>Planck, usplanck, mp107</td>
<td>200TB</td>
<td>5,000 TB</td>
<td>25</td>
</tr>
<tr>
<td>Supernova Studies</td>
<td>m1400</td>
<td>3 TB</td>
<td>200 TB</td>
<td>67</td>
</tr>
</tbody>
</table>
Extreme Data Strategy

- Develop and deploy new data resources and capabilities
- Partner with DOE experimental facilities and projects to identify requirements and create early success
- Provide expertise and services for extreme data
- Leverage ESnet and ASCR research to create end-to-end solutions
Thank you.