Agenda

• NERSC Move Timeline Update
• Carver Retirement Reminder
• Hopper and Edison Status Updates
• HPSS Archival Storage System Enhancements
• Plans for Global Scratch
• NESAP Update
• New Batch Scheduler at NERSC: SLURM
• NIM (accounting interface) Enhancements
• Annual User Group Meeting: Your Opinion Wanted
• What is “Shifter”? (Think user-defined images; webinar Friday.)
• NERSC is Hiring!
NERSC Move to CRT

• NERSC will be moving systems and staff from downtown Oakland (OSF) to Berkley Lab main campus this year (CRT building)

• Timeline Highlights
  – Cori Phase 1 (Cray XC40/Haswell) user availability October 2015
  – Carver retires 9/30/2015
  – Global scratch retires 9/30/2015 (+14 days to retrieve files)
  – Hopper retirement after Cori Phase 1 stable and available to all users; expected December 2015
  – Edison moves from OSF to CRT beginning sometime in Nov.-Dec., unavailable for ~6 weeks
Carver Retirement Reminder

• Carver will be shut down on Sep. 30, 2015
• Running jobs will be terminated beginning at noon on Sep. 30
• Software stack frozen on July 1
• 14 days to retrieve files on scratch
  – $GSCRATCH on Edison
• Please move your work to Edison
• Contact NERSC consultants if you need help or advice
  – consult@nersc.gov
  – https://help.nersc.gov
  – https://my.nersc.gov
  – https://www.nersc.gov/users/computational-systems/carver/retirement-plans/
Edison Updates

Zhengji Zhao
NERSC User Services
Edison Updates

• Queue change to decrease wait for debug, medium and large jobs (end of March, 2015):
  – Debug, reg_xbig, reg_big, and reg_med queues priority increase
  – reg_small jobs can move to Hopper, which has shorter wait times

• Edison compute nodes can now access remote networks (RSIP configuration change, end of March 2015)
  – Provides remote (outside of NERSC) database access from compute nodes.
  – Web portals, ipython notebook server, etc., can run on Edison compute nodes (via remote secure tunneling).
  – Working to increase the number of ports per RSIP node

• TMPDIR=/tmp on Edison login nodes (May 8, 2015)
  – Compilations should be faster than before
Edison Updates - continued

• Increasing Minimal Bias (IMB) setting for Aries is in place now to address the performance variation on Edison (experimental, May 8, 2015)
  – env MPICH_GNI_ROUTING_MODE=ADAPTIVE_1. Slight non-minimal bias at injection point, but increasing bias toward the minimal path as the packet traverses the network. It does help with intermediate group interference.

• VTUNE is now available on Edison (Feb, 2015)
  – VTUNE provides a rich set of performance insight into hotspots, threading, locks & waits, bandwidth and more. Use powerful analysis to sort, filter and visualize results on the timeline and on your source. VTUNE is a preferred performance analysis tool for on-node code optimization for Cori and Edison.
Hopper Updates

Helen He
NERSC User Services
Recent Changes on Hopper

• Scratch file systems updated to Lustre 2.4.1
  – Required so we could keep OS up to date
  – Feb 3-4: /scratch2
  – Feb 18: /scratch

• Mar 11: OS upgraded to CLE52UP02
  – New default Cray programming environment software
  – NERSC Software and user applications rebuilt

• May 12: Batch queue changes for reg_long queue
  – Max global run limit increased from 50 to 100
  – Max user run limit increased from 16 to 32
Current Issues on Hopper

• A handful of users reported jobs got run time error of compute nodes OOM (out-of-memory) after the OS upgrade.
• Narrowed down to a bug in the Lustre client triggered by heavy IO.
• Available workarounds are:
  – Use a non-Lustre file system, such as /project or /global/scratch2
  – Use fewer cores per node
  – Use larger memory nodes
  – Use Edison
Future Plans for Hopper

• Keep system stable to maximize your productivity
  – No more major system upgrades
  – Plan to change RSIP configuration to allow outgoing network connection on the compute nodes as recently done on Edison

• Hopper retirement expected December 2015
  – Exact date TBA
  – After Cori Phase 1 is stable and available to all users
HPSS Enhancements and Global Scratch Plans

Lisa Gerhardt, Data & Analytics Services
In looking at how our archive (HPSS) is being used, we observe:
- High read-rate of files, about 40% of files read occur within 30 days of being archived
- Growing at a total of about 1.5 PB per month

Previously, the disk cache was optimized exclusively for writes
- 5 peak days of data ingest
- Total aggregate bandwidth was 12GB/sec

With the increase, we have sized the disk cache for both reads and writes
- Retains data for about 30 days
- Total aggregate bandwidth is 40GB/sec
• /global/scratch will retire with Carver system on 9/30/2015
  – Will remain read-only on other systems through 10/14/2015
  – Archive needed files to HPSS or move to Edison or Hopper scratch

• Purge policy reduced from 12 to 8 weeks (5/11/2015)
  – This will reduce usage and allow some hardware to aid in the relocation of the /project file system to CRT
  – Remainder of /global/scratch capacity will be added to project file system after relocation to CRT

• NERSC plans to provide a global scratch file system when Cori and Edison are co-located in CRT
The compute and storage systems 2015

Hopper: 1.3PF, 212 TB RAM
Cray XE6, 150K Cores

Edison: 2.5PF, 357 TB RAM
Cray XC30, 130K Cores

Sponsored Compute Systems
Carver, PDSF, JGI, KBASE, HEP
8 x FDR IB

Vis & Analytics, Data Transfer Nodes,
Adv. Arch., Science Gateways

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

3 PB
3 x SFA12KE

5 PB
DDN9900 & NexSAN

250 TB
NetApp E5460

70 PB stored, 240 PB capacity, 40 years of community data

HPSS

2 x 10 Gb
1 x 100 Gb

Science Data Network
• NERSC Exascale Science Application Program
• NERSC continues to actively engage with code teams and vendors (Intel, Cray) to prepare codes for Cori
• Trainings, teleconferences, visits, dungeon sessions
• http://www.nersc.gov/users/computational-systems/cori/nesap/
• Three postdocs have been selected (of ultimately 8)
  – Optimization of the BoxLib Adaptive Mesh Refinement Framework for Scientific Application Codes, PI: Ann Almgren (Lawrence Berkeley National Laboratory)
  – High-Resolution CFD and Transport in Complex Geometries Using Chombo-Crunch, David Trebotich (Lawrence Berkeley National Laboratory)
  – Materials Science using Quantum Espresso, Paul Kent (Oak Ridge National Laboratory)
SLURM @ NERSC

Computational Systems Group

NUG Meeting
May 14, 2015
The Cori Phase 1 system will be using SLURM as the Workload Manager (WLM).

SLURM will provide both Resource Manager (RM) functionality and Scheduler functionality.

WLMs have traditionally interfaced with ALPS on the Crays.
- ALPS is a lower-level application placement scheduler.

SLURM can be run in “native” mode – i.e. without the use of ALPS.
- More details later.
• SLURM provides all of the same functionality as Torque/Moab (a few differences).

• SLURM is fully open source

• In the Cori time frame, SLURM will be able to better support our mixed Data-HPC needs.

• SLURM is extensible (plugin architecture).

• SLURM provides a PBS translator
  – Allows scripts written for Torque to be submitted to SLURM
SLURM vs Torque/Moab

Torque/Moab (#PBS)
- qsub/qdel/qstat
- qstat –a
- -l nodes/mppwidth
- -l walltime
- -t [array]
- -Wdepend=

SLURM (#SBATCH)
- sbatch/scancel/squeue
- sinfo
- -N (nodes) / -n (PEs)
- -t (min)
- --array=[array]
- --depend=

Not exhaustive, See: http://slurm.schedmd.com/rosetta.pdf for details
High Level Plan – 2015-2016

- SLURM testbed on Alva, Babbage
- SLURM Deployed on CP1, Hopper/Edison/Carver run Torque
- SLURM run on CP1, testing for Edison, Hopper, Carver run Torque
- SLURM runs on Edison at CRT, Hopper continues to run Torque
- ...
- Cori comes in with SLURM
WLM/ALPS Interactions on the Cray

• Batch Script runs on a shared service node
  – Level of indirection to access compute nodes
  – “CCM” required to run applications unable to utilize hierarchical compute model
  – Resources directly managed by ALPS, indirect communication with WLM

• ALPS manages compute node resources, application placement, Aries High-speed Network (HSN) access
Native SLURM on the Cray

- Batch Script runs directly on a compute node
  - Simpler access to compute resources (especially for x86_64 and KNL environments)
  - No bottleneck in shared “MOM” node
  - Implicit “CCM” functionality for many applications; NERSC adding ssh-based access for others
  - Resources directly managed by SLURM on each compute node (memory, processes)

- Interaction with Native Cray networking libraries for full access to Aries HSN

- Reduced complexity by not interacting with separate resource manager (ALPS)
Testing Plans

• Continual use of Alva, Babbage
  – test development
  – test new SLURM releases

• Full Scale tests of SLURM on Hopper/Edison
  – production queue structure
  – slurm Unit Test suite developed at NERSC
    • reservations * serial jobs * preemption * job dependencies * job arrays * routing queues * MPI * PBS emulation
  – simulated workload reflecting the spectrum of job sizes on Edison and create a backlog of several thousand jobs

• Allows us to tune scheduler settings to maximize efficiency and fairness
User Resources for SLURM

• User Services Group will have
  – Documentation
  – SLURM usage examples
  – Sample Job Script Files

• NERSC Documentation
  – Using SLURM on Babbage and Cori Phase 1 pages are forthcoming

• References
What do We Need From You?

• Check to see how you use the WLM
  – Simple submission/query
  – Complicated workflows?
  – Workflow tools?
    • Fireworks
    • Qdo
    • Others?

• Simple use cases will translate to SLURM easily

• If you have complicated workflows, please contact us (consult@nersc.gov) to test out SLURM
Allocating Fixed Hours to Users Instead of Repo Percentage in NIM

Clayton Bagwell
NERSC Account & Allocations Support
NIM Development Team

Oakland Scientific Facility
May 14, 2015
The original model for allocating time to users within a repository has been to allow them access to a percentage of the repo’s total allocation.

- This meant that the number of hours a user could access would fluctuate with the changes to a repo’s allocation.

Many of our PIs have requested the ability to allocate a fixed number of hours to their users.

On April 15th, the NIM Development Team released modifications to NIM to accommodate Fixed Hour Allocations.
User Requests an Account

- New user submits an account request
- PIs and Proxies get email notification and reminder upon logging into NIM
Pending Users tab info

- Clicking on the reponame takes you to the Pending Users tab for the project

### Project Information

<table>
<thead>
<tr>
<th>Project</th>
<th>Project Repos</th>
<th>Project Unix Groups</th>
</tr>
</thead>
<tbody>
<tr>
<td>testmpp#15</td>
<td>testmpp testpdfsf</td>
<td>c_claveyrv c_pishou/dowthis c_testdir c_troutcrk includef pishouid richards_dir testint testint2 testmpp testpdfsf testpid</td>
</tr>
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</table>

**Test project/repositories**

### Pending Account Requests

<table>
<thead>
<tr>
<th>Name</th>
<th>Uname</th>
<th>Organization Label</th>
<th>Email</th>
<th>Workphone</th>
<th>Remarks</th>
<th>Submit Date</th>
<th>Reponame</th>
<th>Resource Type</th>
<th>% Allowed</th>
<th>Hours Allowed</th>
<th>Update Allocation</th>
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<tbody>
<tr>
<td>User, Test Fixed Hour</td>
<td>tthu</td>
<td>NERSC</td>
<td><a href="mailto:ncbovy@nersc.gov">ncbovy@nersc.gov</a></td>
<td>510-486-8612</td>
<td>Testing the Fixed Hour Allocation process.</td>
<td>13-MAY-2015</td>
<td>testmpp</td>
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<td></td>
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2 records found
Updating Allocation before Approval

- You can either adjust the % Allowed or enter a value for Hours Allowed

<table>
<thead>
<tr>
<th>Full Name</th>
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<tbody>
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<td>Project Name</td>
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</tr>
<tr>
<td>Repository Name</td>
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<td>Hours Allowed</td>
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update successful.
Return To Form
Return to List
Approve Account Request

- Clicking Return to List takes you back to the Pending Account Requests where you can now approve the account

<table>
<thead>
<tr>
<th>Project</th>
<th>Project Repos</th>
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</thead>
<tbody>
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<td>testmp testpdsf</td>
<td>c_claveyr c_pshouldowthis c_testpidir c_troutork includex pishould Richards_dir testint testint2 testmpp testpdsf testpid</td>
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<td><strong>Test project/repositories</strong></td>
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Pending Account Requests

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<tr>
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<th>Organization Label</th>
<th>Email</th>
<th>Workphone</th>
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<th>Reponame</th>
<th>Resource Type</th>
<th>% Allowed</th>
<th>Hours Allowed</th>
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<td>tfhu</td>
<td>NERSC</td>
<td><a href="mailto:nobody@nersc.gov">nobody@nersc.gov</a></td>
<td>610-486-6512</td>
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<td>testmp</td>
<td>REPO</td>
<td>500</td>
<td>Upcista Allocation</td>
<td>Approve</td>
</tr>
</tbody>
</table>
Manually Adding a User to Your Repo

• When you use Add/Revive User to add a user to your repo, you can allocate either by % Allowed or Hours Allowed

Add a new NERSC User

For NERSC Principal Investigators, Account Managers, and NERSC staff.

Please fill out a separate request for each new NERSC user that you want added to your repositories (repos), and then click the “Submit” button at the bottom of the form.

Your request will be reviewed by NERSC Account Support. After it has been received and processed, the user will need to submit a Computer Use Policy form and then the Ac an email regarding their account password information.

User First Name: ____________________________
Middle Initial: ____________________________
User Last Name: ____________________________
NERSC Username: ____________________________ (If user does not have a NERSC username, enter a preferred username.)
Citizenship: ____________________________
Email Address: ____________________________
Telephone: ____________________________
Organization: ____________________________
Mail Stop (optional): ____________________________

Repository Information

Choose the platforms on which you would like an account created, select the repository name and the percentage or amount of the total allocation you would like the user to be able to use (where applicable).

Add? | Host | Repository Name | % Allowed | Hours Allowed
--- | --- | --- | --- | ---
X | MPP: carver.edson,hopper.matscomp | testmpp | | |
| HPSS | | | | |
| pdsf | | | | |
Allocating to Existing Users

- You can set or adjust Fixed Hours for existing users through the MPP Usage & Quotas tab

<table>
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**Test project/repositories**

*Format: Read-only -> Edit user allocations*

**NOTE:** all hours displayed below are user hours, not repo hours.

**testmp MPP Users, AY 2015 --> Show users for prior AY**

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<th>Login</th>
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<th>User Hrs Used</th>
<th>User Charged</th>
<th>Avg CF</th>
<th>% Used</th>
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<th>User Balance</th>
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**Total:**

|   |   |   |   |   |   |   |   |   |   |

**15 records found**
Adjusting User Allocations

- Click on the Edit user allocations link, enter new % Allowed or Hours Allocated values, click on Save All Rows

Format: Read-only <-> Edit user allocations

NOTE: all hours displayed below are user hours, not repo hours.

testmpp MPP Users, AY 2015 <-> Show users for prior AY

<table>
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<th>Base Repo?</th>
<th>Diff New?</th>
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15 records found
Instructions in the NIM User’s Guide for PIs

• You can find detailed instructions in the NIM Guide for PIs and Project Managers

• http://www.nersc.gov/users/accounts/nim/nim-guide-for-pis/
Annual Users Group Meeting

• Floating a trial balloon:

• What do you think about an annual user group meeting for the three ASCR facilities (NERSC, ALCF, OLCF)
  – Hosts move on a rotating basis
  – Would you be more/less likely to attend in person?
  – Advantages?
  – Disadvantages?
  – Let us know what you think.
What is Shifter?
User Defined Images/Containers in HPC

- Data Intensive computing often require complex software stacks
- Efficiently supporting these in HPC environments offers many challenges
- shifter – Prototype containers in HPC
  - NERSC R&D effort, in collaboration with Cray, to support User-defined, user-provided Application images
  - “Docker-like” functionality on the Cray
  - Efficient job-start & Native application performance
Want to Know More?

Please come see our upcoming talk:

Contain This, Unleashing Docker for HPC
Douglas Jacobsen and Shane Canon

Friday, May 15, 2015, 12:00PM – 1:00PM
NERSC, Oakland Scientific Facility, Room 238

Remote Access Info:
https://nersc-training.webex.com
Password: shifter
NERSC is Hiring!

- Application readiness/HPC consultants
- High Energy Physics/Nuclear Physics consultant
- NESAP Postdocs
- Network Engineer
- Data Analytics
- Security Analyst
- Computer Systems Engineer

- NERSC Users Make Great NERSC Staff!
Section Title