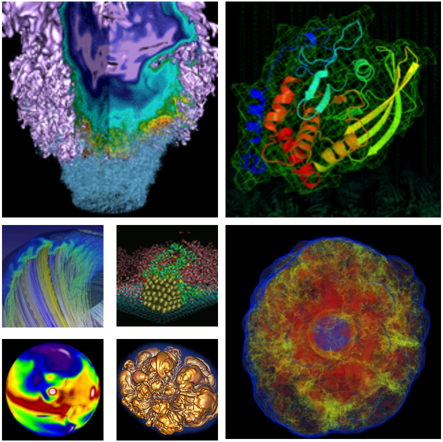
Mendel at NERSC:

Multiple Workloads on a Single Linux Cluster



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Snapshot of NERSC

- Located at LBNL, NERSC is the production computing facility for the US DOE Office of Science
  - NERSC serves a large population of ~5000 users, ~400 projects, and ~500 codes
- Focus is on “unique” resources:
  - Expert computing and other services
  - 24x7 monitoring
  - High-end computing and storage systems
- NERSC is known for:
  - Excellent services and user support
  - Diverse workload

NERSC Systems

- **Hopper**: Cray XE6, 1.28 PFLOPS
- **Edison**: Cray XC30, > 2 PFLOPS once installation is complete
- Three x86_64 midrange computational systems:
  - **Carver**: ~1000 node iDataPlex; mixed parallel and serial workload; Scientific Linux (SL) 5.5; TORQUE+Moab
  - **Genepool**: ~400 node commodity cluster providing computational resources to the DOE JGI (Joint Genome Institute). Mixed parallel and serial workload; Debian 6; Univa Grid Engine (UGE)
  - **PDSF**: ~200 node commodity cluster for High Energy Physics and Nuclear Physics; exclusively serial workload; SL 6.2 and 5.3 environments; UGE

Midrange Expansion

- Each midrange system needed expanded computational capacity
- Instead of expanding each system individually, NERSC elected to deploy a single new hardware platform (“Mendel”) to handle:
  - Jobs from the “parent systems” (PDSF, Genepool, and Carver)
  - Support services (NX and MongoDB)
- Groups of Mendel nodes are assigned to a parent system
  - These nodes run a batch execution daemon that integrates with the parent batch system
  - Expansion experience must be seamless to users:
    - No *required* recompilation of code (recompilation can be recommended)

Approaches

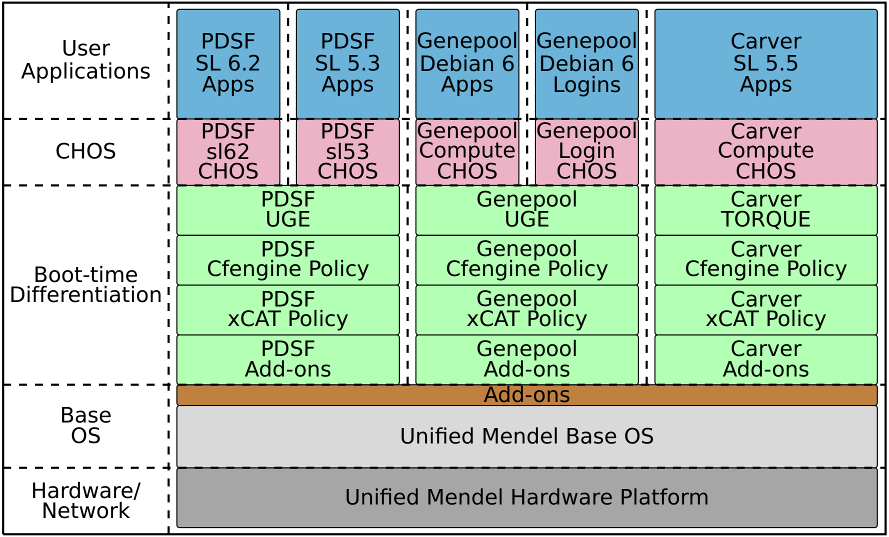
Multi-image Approach

- One option: Boot Mendel nodes into modified parent system images.
- Advantage: simple boot process
- Disadvantage: Many images would be required:
  - Multiple images for each parent compute system (compute and login), plus images for NX, MongoDB, and Mendel service nodes
  - Must keep every image in sync with system policy (e.g., GPFS/OFED/kernel versions) and site policy (e.g., security updates):
    - Every change must be applied to every image
    - Every image is different (e.g., SL5 vs SL6 vs Debian)
    - All system scripts, practices, and operational procedures must support every image
- This approach does not scale sufficiently from a maintainability standpoint

NERSC Approach

- A layered model requiring only **one** unified boot image on top of a scalable and modular hardware platform
- Parent system policy is applied at boot time
- xCAT (eXtreme Cloud Management Toolkit) handles node provisioning and management
- Cfengine3 handles configuration management
- The key component is CHOS, a utility developed at NERSC in 2004 to support multiple Linux environments on a single Linux system
  - Rich computing environments for users separated from the base OS
  - PAM and batch system integration provide a seamless user experience

The Layered Model



Implementation

Hardware

- Vendor: Cray Cluster Solutions (formerly Appro)
  - Scalable Unit expansion model
- FDR InfiniBand interconnect with Mellanox SX6518 and SX6036 switches
- Compute nodes are half-width Intel servers
  - S2600JF or S2600WP boards with on-board FDR IB
  - Dual 8-core Sandy Bridge Xeon E5-2670
  - Multiple 3.5” SAS disk bays
- Power and airflow: ~26kW and ~450 CFM per compute rack
- Dedicated 1GbE management network
  - Provisioning and administration
  - Sideband IPMI (on separate tagged VLAN)

Base OS

- Need a Linux platform that will support IBM GPFS and Mellanox OFED
  - This necessitates a “full-featured” glibc-based distribution
  - Scientific Linux 6 was chosen for its quality, ubiquity, flexibility, and long support lifecycle
- Boot image is managed with NERSC’s `image_mgr`, which integrates existing open-source tools to provide a disciplined image building interface
  - Wraps xCAT `genimage` and `packimage` utilities
  - `add-on` framework for adding software at boot-time
  - Automated versioning with FSVS
    - Like SVN, but handles special files (e.g., device nodes)
    - Easy to revert changes and determine what changed between any two revisions
    - http://fsvs.tigris.org/

Node Differentiation

- Cfengine rules are preferred
  - They apply and *maintain* policy (promises)
  - Easier than shell scripts for multiple sysadmins to understand and maintain
- xCAT postscripts
  - Mounting local and remote filesystems
  - Changing IP configuration
  - Checking that BIOS/firmware settings and disk partitioning match parent system policy
- `image_mgr` `add-ons` add software packages at boot time
  - Essentially, each `add-on` is a `cpio.gz` file, {pre-,post-}install scripts, and a MANIFEST file

CHOS

- CHOS provides the simplicity of a “chroot” environment, but adds important features.
  - Users can manually change environments
  - PAM and Batch system integration
    - PAM integration CHOSes a user into the right environment upon login
    - Batch system integration: SGE/UGE (`starter_method`) and TORQUE+Moab/Maui (`preexec` or `job_starter`)
  - All user logins and jobs are chroot’ed into `/chos/`, a special directory managed by sysadmins
  - Enabling feature is a `/proc/chos/link` contextual symlink managed by the CHOS kernel module
- Proven piece of software: in production use on PDSF (exclusively serial workload) since 2004.

/chos/

/chos/ when CHOS is not set:

```
/chos/bin    → /proc/chos/link/bin → /bin/
/chos/etc    → /proc/chos/link/etc → /etc/
/chos/lib    → /proc/chos/link/lib → /lib/
/chos/usr    → /proc/chos/link/usr → /usr/
/chos/proc   → /local/proc/
/chos/tmp    → /local/tmp/
/chos/var    → /local/var/
/chos/dev/     # Common device nodes
/chos/gpfs/    # Mountpoint for a shared filesystem
/chos/local/   # Mountpoint for the real root tree
```

/chos/

/chos/ when CHOS is sl5:

```
/chos/bin    → /proc/chos/link/bin → /os/sl5/bin/
/chos/etc    → /proc/chos/link/etc → /os/sl5/etc/
/chos/lib    → /proc/chos/link/lib → /os/sl5/lib/
/chos/usr    → /proc/chos/link/usr → /os/sl5/usr/
/chos/proc   → /local/proc/
/chos/tmp    → /local/tmp/
/chos/var    → /local/var/
/chos/dev/     # Common device nodes
/chos/gpfs/    # Mountpoint for a shared filesystem
/chos/local/   # Mountpoint for the real root tree
```

/chos/

/chos/ when CHOS is deb6:

```
/chos/bin    → /proc/chos/link/bin → /os/deb6/bin/
/chos/etc    → /proc/chos/link/etc → /os/deb6/etc/
/chos/lib    → /proc/chos/link/lib → /os/deb6/lib/
/chos/usr    → /proc/chos/link/usr → /os/deb6/usr/
/chos/proc   → /local/proc/
/chos/tmp    → /local/tmp/
/chos/var    → /local/var/
/chos/dev/     # Common device nodes
/chos/gpfs/    # Mountpoint for a shared filesystem
/chos/local/   # Mountpoint for the real root tree
```

CHOS Challenges

- CHOS `starter_method` for UGE enhanced to handle complex `qsub` invocations with extensive command-line arguments (e.g., shell redirection characters)
- UGE `qlogin` does not use the `starter_method`. Reimplemented `qlogin` in terms of `qrsh`
- TORQUE `job_starter` was only used for the launch of the first process of a job, not for subsequent processes through Task Manager (TM)
  - All processes need to run inside the CHOS environment
  - NERSC developed a patch to pbs_mom to use the `job_starter` for processes spawned through TM
  - Patch accepted upstream and is in 4.1-dev branch

Base OS Image Management

Image Management

- We needed an alternative to “traditional” image management:
  1. genimage (xCAT image generation)
  2. chroot…vi…yum
  3. packimage (xCAT boot preparation)
  4. Repeat steps 2 and 3 as needed
- The traditional approach leaves sysadmins without a good understanding of how the image has changed over time.
  - Burden is on sysadmin to log all changes
  - No way to exhaustively track or roll back changes
  - No programmatic way to reproduce image from scratch

image_mgr

- New approach: rebuild the image from scratch every time it is changed
  - `image_mgr` makes this feasible
  - We modify the `image_mgr` script, not the image
- Standardized interface for image creation, manipulation, analysis, and rollback.
- Automates image rebuilds from original RPMs
- Images are versioned in a FSVS repository
- “release tag” model for switching the production image

FSVS layout

```
/........................................The root directory of the repository
└── netboot/
    └── SL6.3/ ...................................... OS version
        └── x86_64/ ..................................Architecture
            └── mendel-core.prod/........................Image name
                ├── tags/
                │   ├── 2013-03-01-14-13-45-RELEASE-by-user/
                │   │   ├── rootimg/
                │   │   ├── add-ons/
                │   │   │   └── kvm/
                │   │   └── build-info/
                │   │       ├── image_mgr.sh ...........The build script
                │   │       └── stats .....................Build statistics
                │   └── 2013-02-27-11-10-02-RELEASE-by-user2/
                └── trunk/
```

image_mgr

`image_mgr` supports several subcommands: **create**, **tag**, **list-tags**, and **pack**

- **create**: Build a new image and commit it to `trunk/` (uses xCAT `genimage` and FSVS):

```
# image_mgr create -p mendel-core.prod -o SL6.3 -a
    x86_64 -m "Test build" -u user1
```

- **tag**: Create a new SVN tag of `trunk/` at the current revision, marking it as a potential production release

```
# image_mgr tag -p mendel-core.prod -o SL6.3 -a
    x86_64 -u user1
```

image_mgr

- **list-tags**: List all tags

```
# image_mgr list-tags -p mendel-core.prod -o SL6.3 -a
     x86_64
2013-03-01-14-13-45-RELEASE-by-user1
2013-02-27-11-10-02-RELEASE-by-user2
...
```

- **pack**: Pack a tag as the production image (uses xCAT packimage)

```
# image_mgr pack -p mendel-core.prod -o SL6.3 -a
    x86_64 -t 2013-03-01-14-13-45-RELEASE-by-user1
```

Feedback for CCS

CCS Feedback

Several areas for improvement. CCS is actively working with NERSC to improve.

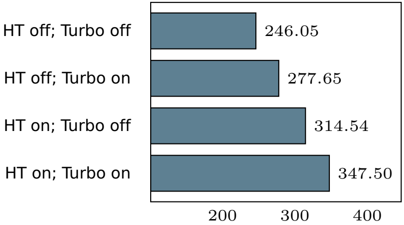
- Hardware supply chain issues
  - Delays getting parts from upstream vendor
- Proper cabling is **essential** when hundreds of cables are involved. We need to be able to service all equipment.
- 24x7 really means 24x7
  - NERSC users work around the clock, weekends, and holidays
  - The system is never “down for the weekend”
  - **Any** outage, planned or unplanned, is severely disruptive to our users
    - We need detailed timelines for all work requiring downtimes

Conclusion

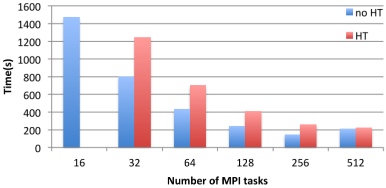
Acknowledgements

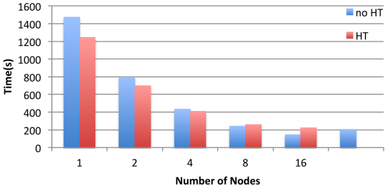
- **Doug Jacobsen**
  - Extensive Genepool `starter_method` and `qlogin` changes
- **Nick Cardo and Iwona Sakrejda**
  - Constructive feedback on the `image_mgr` utility
- **Shane Canon**
  - Original CHOS developer. Provided significant guidance for the Mendel CHOS deployment
- **Zhengji Zhao**
  - Early software tests on the Mendel platform.
- **Brent Draney, Damian Hazen, Jason Lee**
  - Integration of Mendel into the NERSC network
- This work was supported by the Director, Office of Science, Office of Advanced Scientific Computing Research of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.

Performance Data



Per-node HEPSPEC06 scores **on SL6** on dual Xeon E5-2670 servers with 64 GB RAM.





NAMD STMV benchmark (1,066,628 atoms, periodic, PME) on dual Xeon E5-2670, 128 GB RAM.

Data provided by Zhengji Zhao, NERSC User Services Group

Additional Resources

- FSVS: http://fsvs.sf.net/
- xCAT: http://xcat.sf.net/
- Original CHOS paper:
  - http://indico.cern.ch/getFile.py/access?contribId=476&sessionId=10&resId=1&materialId=paper&confId=0
- 2012 HEPiX presentation about CHOS on PDSF: http://www.nersc.gov/assets/pubs_presos/chos.pdf
- CHOS GitHub repository: https://github.com/scanon/chos/
- PDSF CHOS User documentation:
  - http://www.nersc.gov/users/computational-systems/pdsf/software-and-tools/chos/

Conclusion

- The layered Mendel combined cluster model integrates a scalable hardware platform, xCAT, Cfengine, CHOS, and `image_mgr` to seamlessly support diverse workloads from multiple “parent” computational systems and support servers
- Nodes can be easily reassigned to different parent systems
- Separation between the user and sysadmin environments, which can each be architected exclusively for their intended uses
- While this approach introduces additional complexity, it results in an incredibly flexible and maintainable system

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