Best Practices @OLCF (and more)

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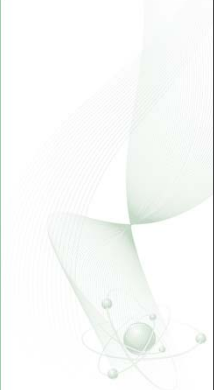
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General Information

- This presentation covers some helpful information for users of OLCF
  - Staying informed
  - Aspects of system usage that may differ from your past experience
  - Common error messages
  - Common questions
  - Quick tips & best practices
- This is by no means an all-inclusive presentation
- Feel free to ask questions

2 Best Practices @OLCF (& more)

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Staying Informed

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Staying Informed

- OLCF provides multiple layers of user notifications about system status and downtimes
  - OLCF Weekly Update
  - Status indicators on olcf.ornl.gov
  - Opt-in email lists (*subscription management currently unavailable*)
  - Twitter (@OLCFStatus)
  - StatusCast (*coming soon*)
- A summary of these items can also be found at http://www.olcf.ornl.gov/kb_articles/communications-to-users/

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Staying Informed-Weekly Update

- Sent weekly (Thu/Fri)
- Contains
  - Announcements about upcoming training
  - Announcements about system changes
  - Planned outages
- **All OLCF users should receive this email**
  - Let us know if you're not receiving it

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Staying Informed-System Status

- Logs from monitoring software parsed to make educated guess on system status
- Status is sent to multiple destinations
  - Websites
  - Twitter
  - Email lists
- Fairly accurate, but still a fully automated process
  - Possibility of both false positives and false negative
  - We do take some measures to mitigate this

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Staying Informed-System Status (via www.olcf.ornl.gov)
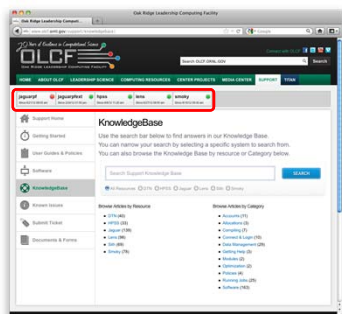
Staying Informed-System Status (via Twitter)

@OLCFStatus
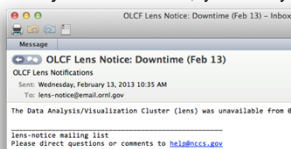

Staying Informed-System Status (via Opt-In Email Lists)

- We also send status up/down notices via email
  - These area available on an opt-in basis
  - Online sign up (*coming soon*) at http://www.olcf.ornl.gov/kb_articles/system-notification-lists/
  - Sign up now by emailing help@olcf.ornl.gov
- Lists aren't just for status; you may want to sign up

Staying Informed-System Status (via Opt-in Email Lists)
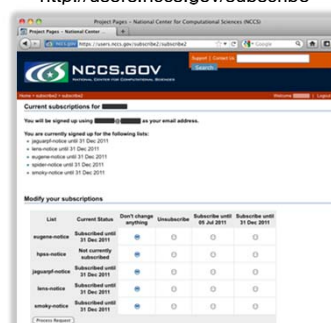
http://users.nccs.gov/subscribe

Staying Informed-System Status (via StatusCast)

- Users have told us via our survey that they'd like more status information online
- Work is ongoing on a new tool to provide that information
  - Current status
  - Outages (upcoming, current, and historical)
  - Announcements
- Stay tuned to the OLCF Weekly Update for more information

System Differences: Compiling & Finding Software

Finding Software

- Some is part of the default environment
  - Basic commands
  - Text editors
- Other software typically managed via 'modules'
  - Software is actually installed in `/sw`
  - "`module avail`", "`module load`", etc.
  - More information is available on the OLCF website
- Compilers, MPI and GPU libraries, etc. are also provided via modules (but are not in `/sw`)

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Software Updates

- Cray-provided software (compilers, MPI, CUDA, etc.) goes through testing before we receive it
  - Usually not available to us immediately after vendor releases it
- OLCF provided software is moving to a model of updates at certain intervals
  - Not all minor versions will be installed
  - We'll provide build "recipes" in case you want/need a minor version

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Software Installation

- You are free to install software in your directories
  - Subject to export control, license agreements, etc.
- If you think software would be of general interest, you might ask us to install it for general use
  - Via email to help@olcf.ornl.gov or the request form at http://www.olcf.ornl.gov/support/software/software-request/
  - Requests are reviewed by our software council

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Compiling for the XK7 and XC30

- May differ (greatly) from your previous experience
- Mix of `?-asyncpe` (`craype`) & `PrgEnv-?` modules
  - `PrgEnv` loads compiler, math, MPI, etc. modules
  - `craype`/`asyncpe` loads compiler wrapper scripts
- Regardless of actual compiler (PGI, Intel, etc), invoke with `cc`, `CC`, or `ftn`
- MPI, math, & scientific libraries automatically linked
  - No `-lmpi`, `-lblas`, etc.
  - Can be challenging for some build processes

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Compiling for the XK7 and XC30

- You are actually cross-compiling
  - Processors/instructions sets differ between login & compute nodes
  - It's very important to remember this…utilities like `configure` don't expect this
- Compiling for batch/login nodes is occasionally necessary
  - See §7.2 of the Titan User Guide for examples
    https://www.olcf.ornl.gov/support/system-user-guides/titan-user-guide/

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Running Jobs

- Batch job information is on the web site
- Note that XK7 queue policy favors large jobs
- Jobs are charged based on what you make unavailable to others, not what you use
- Requests for high priority/quick turnaround are considered

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Debugging/Optimization

- Several tools available: DDT, Vampir, ScoreP, CrayPAT

- Some documentation is available on the OLCF website; you can also contact User Assistance

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Common Runtime Error Messages

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Common Runtime Errors

- `Illegal Instruction`
  – A code compiled for compute nodes was executed on login/batch/service nodes
  – (Remember, you're cross-compiling)

- `request exceeds max nodes alloc`
  – The `aprun` request requires more nodes than the job requested
      -or-
  – Request was correct, but at launch time some nodes were discovered to be down (see potential fix later in this presentation)

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Common Runtime Errors (2)

- `relocation truncated to fit: R_X86_64_PC32`
  – Program is using too much static memory
  – Limit on Titan is 2GB
  – Solution: use dynamic memory allocation as much as possible

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Common Runtime Errors (3)

- `aprun: [NID 94]Exec a.out failed: chdir /autofs/na1_home/user1 No such file or directory`
  – Compute nodes only mount Lustre directories
  – When you launch aprun, you must be in a directory visible to compute nodes (in this example, it was launched from $HOME)
  – Any files used by the processes on compute nodes must also be in Lustre
  – The executable itself need not be in Lustre

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Common Questions

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Why isn't my job running?

- Can be a number of reasons
  - Insufficient nodes available
  - Pending downtime
  - Queue policy
  - Dependency on another job not met
- Use `checkjob <jobid>` to diagnose
  - Use `–v` for verbose mode
  - Reason for job not running is usually near the end
- Use `showres` to see upcoming reservations/outages
  - Also shows running jobs…look carefully

25 Best Practices @OLCF (& more)

Why isn't my job running? (2)

- Insufficient resources available
  ```
  NOTE:  job cannot run  (insufficient available procs:  3264 available)
  ```

- Unresolved dependency
  ```
  NOTE:  job cannot run  (dependency 1851375 jobcomplete not met)
  ```

- Queue policy issue
  ```
  NOTE:  job violates constraints for partition titan (job 1854474
  violates active HARD MAXJOB limit of 2 for qos smallmaxjobs user
  partition ALL (Req: 1  InUse: 2))

  BLOCK MSG: job 1854474 violates active HARD MAXJOB limit of 2 for qos
  smallmaxjobs user partition ALL (Req: 1  InUse: 2) (recorded at last
  scheduling iteration)
  ```

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Why isn't my job running? (3)

- Pending maintenance period/reservation
  - This is example output from `showres`
  - Look for alphanumeric `ReservationIDs` (those without letters are likely currently running jobs)
  - Note the full system reservation starting in 15 hours…am I asking for more than 15 hours in my job?

```
ReservationID Type S    Start      End  Duration    N/P     StartTime

DTNOutage.127 User -  15:05:13 1:03:05:13 12:00:00  11/176  Tue Jan 28 08:00:00
PM.128        User -  15:05:13 1:03:05:13 12:00:00 18688/299008 Tue Jan 28 08:00:00
PM_login.129  User -  15:05:13 1:03:05:13 12:00:00  16/2048 Tue Jan 28 08:00:00
```

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When will my job start?

- Can be difficult to tell since jobs submitted in the future can affect it
- `showstart <jobid>` is not always reliable
- `showq` output is sorted by priority (can be helpful)
- `mdiag –p` gives detailed priority info
  - Shows boosts based on job size
  - Shows overallocation penalties

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What is my project ID and what is the project allocation?

- Use `showproj` and `showusage` to list projects and usage, respectively
- Both commands have a help option (run with `–h`)

```
$ showproj

User1 is a member of the following project(s) on titan:
   stf007

$ showusage

titan usage for the project's current allocation period:
                          Project Totals           user1
  Project      Allocation    Usage    Remaining    Usage
                          |                     |
  stf007        7350000  |  11138    7338862  |     12
```

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What happens when my project overruns its allocation?

- Jobs will run with a lower priority to facilitate some degree of "fairshare" with projects that have allocation remaining
  - 30 day penalty for slightly over (usage 100-125% of allocation)
  - 365 day penalty for usage >125% of allocation
- Projects are *NOT* disabled for going over allocation

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My project lost *X* hours due to system issues…can I get a refund?

- Since we don't disable projects for going over allocation, we don't issue refunds (*per se*)
- If many jobs were affected, we can delay the priority reduction
  - This is the same thing as a refund but is much easier to manage

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Can I get a priority boost/higher walltime limit/purge exemption/etc?

- Perhaps
- Make request via https://www.olcf.ornl.gov/support/documents-forms/ (Forms to Request Changes to Computers, Jobs or Accounts)
- Reviewed by Resource Utilization Council
- Please make requests well in advance to allow for review
- If requesting job priority, make sure you submit the job…they often run more quickly than you expect

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Are my files backed up?

- NFS directories: Yes, to a limited extent

```
$ cd ~/SomeDir/SomeOtherDir
$ ls
file1 file2
$ rm file1
$ ls
file2
$ cp ~/.yesterday/SomeDir/SomeOtherDir/file1 .
$ ls
file1 file2
```

- Lustre: No
- HPSS: No
  (You might use it as a backup, but HPSS itself is not backed up. It's a good idea to have another level of backup at another site.)

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Where do I archive data? Is there a mass storage system available?

- Yes, HPSS
- Accessed via `hsi` and `htar`
- See the "Storage @ OLCF" presentation for details
  https://www.olcf.ornl.gov/wp-content/uploads/2013/02/Storage_at_OLCF_2-MG.pdf

34 Best Practices @ OLCF (& more)

How do I transfer my data? Can I access my data when Titan is down?

- System user guides discuss data transfer
- Data user guide:
  https://www.olcf.ornl.gov/computing-resources/data-management/data-management-user-guide/
- Data transfer nodes (`dtn.ccs.ornl.gov`) are the preferred place for internal and external data transfer
  - Often remain available during system outages
  - All users should have access

35 Best Practices @ OLCF (& more)

Where do I store data?

- Can be complicated
  - NFS, Lustre, HPSS
  - User directories, Project directories
- See the Data Management Policy
  https://www.olcf.ornl.gov/kb_articles/data-management-policy

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How do I check my disk usage?

- For home directories, use the quota command

```
$ quota
quota: error while getting quota from master:/cm/shared for user1 (id 98765):
Connection refused
quota: error while getting quota from master:/home for user1 (id 98765): Connection
refused
Disk quotas for user user1(uid 98765):
     Filesystem  blocks   quota   limit   grace   files   quota   limit   grace
nccsfiler3.ccs.ornl.gov:/vol/home1
                8  10485760 10485760              2 4294967295 4294967295
nccsfiler4.ccs.ornl.gov:/vol/home2
          8669108 15728640 15728640          51766 4294967295 4294967295
```

- For lustre directories, use lustredu

```
$ lustredu $MEMBERWORK/stf007
Last Collected Date        Size    File Count  Directory
2014-01-10 12:30:08      31.21 MB           9  /lustre/atlas1/stf007/scratch/user1
```

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Where do I find documentation?

- http://www.olcf.ornl.gov
  - User Guides available at https://www.olcf.ornl.gov/support/system-user-guides/
- http://docs.cray.com (CrayDocs)
- http://docs.nvidia.com (Nvidia hosted documentation)

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Quick Tips, Best Practices, and Other Useful Information

Quick Tip-Dealing With the Lustre Purge

- Problem: Needed files were deleted by the purge
- Several "fixes"
  - Pulling from HPSS every time: inefficient
  - Multiple scripts (data in/not in place): cumbersome
  - touch: not ideal
  - Conditional transfer: good

```
#!/bin/bash
...
if [[ ! -a $MEMBERWORK/stf007/some_important_file ]]; then
    hsi -q get /home/user1/data/some_important_file
fi

aprun -n 4096 ./a.out
...
```

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Quick Tip-Dealing With Failed Nodes

- Sometimes nodes fail when your job starts
  - Since node allocation has already happened, the batch system can't replace them
  - You can work around this by requesting "extra" nodes

```
#!/bin/bash
#PBS -lnodes=104
...
APRUN_RETURN_VALUE=1
while [[ $APRUN_RETURN_VALUE -ne 0 ]]; do
    aprun -n1600 ./a.out
    APRUN_RETURN_VALUE=$?
done
...
```

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Best Practices: Data Storage

- HPSS is the proper location for long-term sotrage
- Project areas offer a common area for files shared among project members, but is not long-term storage
  - Monitor disk usage
  - Should be backed up
  - May be purged

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Best Practices: Lustre Filesystem

- Codes may need revisions to prevent large metadata operations
- Compiling in Lustre can be slow
- There is a purge, but please delete files when no longer needed

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Best Practices: Using HPSS

- HPSS prefers a few large files rather than many small files (`htar` is your friend)
- Running many simultaneous transfers can be problematic
- Planned upgrades (larger disk cache) should make a notable difference in performance

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Best Practices: User Support

- Email is often useful if there are long/complicated error messages
- Send as many error messages as possible
  - Or place them in a file & direct us to it
- When sending codes, create a .tar file & direct us to it
  - Include all files necessary to run
  - More efficient than sending via email
- Send new issues in new tickets, not replies to old ones

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Finally…

- We're here to help you
- Questions/comments/etc. can be sent to the OLCF User Assistance Center
  - Staffed 9AM – 5PM US Eastern Time, exclusive of ORNL holidays
  - help@olcf.ornl.gov
  - (865) 241-6536

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