OLCF Best Practices (and More)



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Overview

- This presentation covers some helpful information for users of OLCF
 - Staying informed
 - Some aspects of system usage that may differ from your past experience
 - Some common error messages
 - Common questions/Other tips on using the systems
- This is by no means an all-inclusive presentation
- Feel free to ask questions

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Staying Informed

- OLCF provides multiple layers of user notifications about system status and downtimes
 - OLCF Weekly Update
 - OLCF Status Page (https://users.nccs.gov/statuspages/summary)
 - Status indicators on olcf.ornl.gov
 - Opt-in email lists
 - Smartphone Apps
 - Twitter (@OLCFStatus)
- A summary of these items can also be found at http://www.olcf.ornl.gov/kb_articles/communications-to-users/



Staying Informed-Weekly Update

- Sent weekly (Thursday/Friday)
- Contains several items
 - Announcements about upcoming training
 - Announcements about upcoming system changes
 - Planned outages for the next week
- All OLCF users should receive this email
 - Let us know (help@olcf.ornl.gov) if you're not receiving it!



Staying Informed-System Status

- Automated scripts parse logs from our monitoring software and make an educated guess as to system state
- This status is then sent to multiple destinations: websites, Twitter, smartphone apps, and email lists
- While this is fairly accurate, it is a fully automated process
 - Thus, there is a possibility of both false positives and false negatives
 - We do take some measures to mitigate this



System Status: www.olcf.ornl.gov



OLCF Computing Resources:

System Status: users.nccs.gov

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https://users.nccs.gov/statuspages/summary





System Status: Twitter

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@OLCFStatus





System Status: Opt-In Email Lists

- We also send status up/down notices via email
 - These are available on an opt-in basis

- See http://www.olcf.ornl.gov/kb_articles/system-notification-lists/
- Subscribe only to lists of systems of interest to you
- Other notices are sent to these lists, so you may want to sign up





System Status: Opt-In Email Lists

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http://users.nccs.gov/subscribe





System Status: Smartphone Apps

- System status apps have been developed
 - Android: "OLCF StatusApp"
 - iPhone: "OLCF System Status"
- Choose systems to monitor
- Automated notifications of system changes
- Usage instructions on olcf.ornl.gov
- Currently unavailable due to app maintenance



Using the Systems at OLCF

- Software
- Compiling
- Common Error Messages
- Common Questions
- Other Tips/Best Practices





Finding Software

- Some software is part of the default environment
 - Basic commands
 - Text editing utilities
- Software is typically managed via the 'modules' utility
 - Software is actually installed in $/ \, {\tt sw}$
 - To list available software, use "module avail"
 - To use a package, use "module load"
 - More information is available on the OLCF website
- "Important" items, such as compilers, are also available via modules



Software Installation/Updating

- We are moving to a model of updates to software packages at certain intervals (or in the case of major revisions)
 - This means not all minor versions will be installed

- We'll move towards adding build instructions on the website so that you can build minor revisions/slightly different versions
- Look for information on the OLCF website and via Weekly Update emails



Software Installation

- You are free to install software in your directories (including your project directory)
 - Subject to terms of license agreements, export control laws, etc.
- If you think a piece of software would be of general interest, you might ask us to install it for general use
 - Preferred method: http://www.olcf.ornl.gov/support/software/software-request/, but email to help@olcf.ornl.gov works, too.
 - This will be reviewed by our software council



Compiling for the XK7

- The compilers on the XT/XE/XK line of systems may differ (significantly) from your previous experience
- Combination of ?-asyncpe and PrgEnv-? modules
 - ?-asyncpe provides compiler wrapper scripts
 - PrgEnv-? loads modules for compilers, math libraries, MPI, etc.
- Regardless of actual compiler being used (PGI, Intel, GNU), invoke with cc, cc, Or ftn
- MPI, math, and scientific libraries included automatically
 - NO -lmpi, -lscalapack, etc.
 - This can be challenging when dealing with some build processes



Compiling for the XK7

- You are actually cross-compiling...processors (& instruction sets) differ between login and compute nodes
 - It is very important to realize this ... utilities like "configure" often depend on being run on the target architecture, so they can be challenging to use on the XK7
- Compiling for login/batch nodes is occasionally necessary
- There are three ways to do this
 - module swap xtpe-interlagos xtpe-target-native
 - Add —target=native to cc/CC/ftn
 - Call the compilers directly (e.g. pgcc, pgf90, ifort, gcc)



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Common Runtime Errors

- Illegal Instruction
 - A code was compiled for the compute nodes but executed on login nodes
- request exceeds max nodes alloc
 - The number of cores required to satisfy the aprun command exceeds the number requested
 - Node allocation should be more intuitive now that we're using #PBS -1 nodes=n to request resources (as compared to #PBS -1 size=n)
 - Also happens when your request is correct, but at launch time a node is discovered to be down
 - Quick fix: request "extra" nodes & include logic to restart in your batch script



Common Runtime Errors

- relocation truncated to fit: R_X86_64_PC32
 - The static memory used by your code exceeds what's allowed by the memory model you're using
 - Only the "small" memory model is available (static size >= 2GB)
 - Solution: use dynamic memory allocation to the greatest extent possible



Common Runtime Errors

- aprun: [NID 94]Exec /tmp/work/userid/a.out failed: chdir /autofs/na1_home/userid No such file or directory
 - When you run 'aprun', you must do so from a directory visible to compute nodes (/tmp/work or /tmp/proj)
 - As a general rule, lustre directories are visible and others are not
 - When the job starts, it will attempt to 'cd' into the working directory from which you submitted aprun
 - In the example above, 'aprun' was executed from the user's home directory
 - Any files used by the processes running on compute nodes (input, output, .so, etc) must be in directories visible to the compute node.
 - This is not the case for executables...they can be in your home directory



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• Is my data backed up?

 NFS directories: Yes, to an extent. Take a look at /ccs/home/.snapshot/

\$ ls /ccs/home/.snapshot hourly.0 hourly.1 hourly.2 hourly.3 hourly.4 hourly.5 nccsfiler3(0151729160)_home.1 nightly.0 nightly.1

Lustre directories: No

- HPSS: No.

While you might use it as a backup of your directories, HPSS itself is not backed up. It's a good idea to have another level of backup at some other site if possible.



- What project am I on, and what's its allocation?
 - Use showproj to list your projects

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- Use showusage to display utilization
- Both commands have a "help" option...run them with _h for usage info

\$ showproj				
brenaud is a stf007	member of the	following pro	ject(s) on jagua	arpf:
\$ showusage				
jaguar usage in CPU hours:				
		Project Totals		brenaud
Project	Allocation	Usage	Remaining	Usage
stf007	600001	562227.60	37773.40	12968.42
stf007de1	500000	0.00	500000.00	0.00



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- What happens when my project overruns its allocation?
 - Most importantly, we do **not** disable the project...jobs simply run at lower priority
 - Jobs submitted to projects slightly over allocation (100-125%) receive a 30day priority reduction
 - Jobs submitted to projects well over allocation (>125%) receive a 365-day priority reduction
 - This allows a degree of "fairshare" while still allowing people to run when the system is quiescent



- My project has lost X hours due to system issues...can I get that time reimbursed?
 - Since we don't disable projects for going over allocation, we also don't deal with refunds *per se*
 - If many jobs are affected, the priority reduction can be delayed.
 This is basically a refund but is much easier to manage.



- I changed permissions on /tmp/work/\$USER, but they changed back...why?
 - Permissions in the lustre filesystem are controlled by settings in our accounts database
 - These settings only affect the top-level permission
 - Permissions are automatically (re-)set regularly
 - Most users can request they be changed
 - Send email to help@olcf.ornl.gov
 - Note that you need to email us to change them "back"
 - Of course, you can always just chmod everything under the top-level directory
 - We can't change permissions on directories associated with sensitive data



- Can I get a priority boost? ...a higher walltime limit? ... purge exemption? ...larger home directory quota ...etc?
 - Perhaps...

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- See https://www.olcf.ornl.gov/support/documents-forms/ (Forms to Request Changes to Computers, Jobs or Accounts)
- Once submitted, forms are sent to the Resource Utilization Council for approval
- Make request well in advance...it can be difficult to make last-minute changes
- If requesting job priority, be sure the job is submitted (the queue may move more quickly than expected, eliminating the need for the request)



- Where do I archive my data? Is there a mass storage system available?
 - HPSS
 - Accessed via hsi & htar
 - See the "Storage @ OLCF" presentation for full details



- How do I transfer my data? If the main system is down, can I access my data?
 - The Data Transfer Nodes are the preferred place for data movement (both internal and external)
 - dtn01.ccs.ornl.gov and dtn02.ccs.ornl.gov
 - Almost always available, even during outages of major resources
 - All users should have access

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Data Storage Practices

- HPSS is the proper location for long-term storage
- Project areas (NFS and lustre) offer a common area for shared data files, executables, but should not be considered long-term storage
 - Need to keep an eye on disk usage
 - Should still be backed up
- User scratch areas are intended for use during computations
 - Regularly purged
 - Store files to HPSS as soon as practicable
 - File cleanup is important



Lustre/Scratch Filesystem

- Remember that the current version of lustre has a single metadata server
- Codes may need revisions to prevent opening large numbers of files simultaneously
- Compiling in lustre can be slow
 - When possible, compile in NFS
- There is a purge, but if you delete files when not needed it will help



Dealing With the Scratch Purge-Conditional Transfers

- Many codes use files from previous iterations of the code, and those files may get deleted by the scratch purge
- This can present challenges
 - Pulling from HPSS every time is inefficient
 - Multiple scripts ("data in place", "data not in place") are cumbersome
 - touch isn't always ideal
- Conditional transfers help with this

```
#!/bin/bash
...
if [[ ! -a /tmp/work/brenaud/some_important_file ]]; then
    hsi -q get /home/brenaud/data/some_important_file
fi
aprun -n 4096 ./a.out
...
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```



Interacting with HPSS

- HPSS is a somewhat complex system
- HPSS prefers a small number of large files and not a large number of small files-htar is your friend in this regard
 - htar is (much) faster than a tar followed by hsi put
 - Limited disk space is no problem...data is streamed directly to HPSS so there is no "intermediate" local storage
- Running many transfers at a time can be problematic
 - Multiple transfers may not give you parallelism
 - Limiting the number of per-user transfers helps the system operate more efficiently (& therefore can be more efficient for you)
- Usage examples are on the OLCF web site



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Running Jobs at OLCF

- Batch job information is available on the OLCF Web Site
- Since we are designated as a "leadership-class" facility, queuing policy heavily favors large jobs
- Remember that jobs are charged based on what's made unavailable to others and not what you use
 - The system cannot allocate a single node to multiple aprun instances (much less multiple users)
- Requests for high priority/quick turnaround are considered
 - Submit your job ASAP...it may start more quickly than expected
 - Allow plenty of lead time when making a request...discussion may be necessary prior to a decision on approval



Running Jobs at OLCF

- From a user perspective, Titan has three major parts
 - The system proper
 - External login nodes
 - MOAB server

- Often, only the system proper is affected by outages
 - External login nodes and the MOAB server node remain up
 - This means you can compile/submit jobs/etc while titan is down
 - Jobs will be queued and will run when the system returns



Debugging/Optimization at OLCF

- Several software tools are provided for debugging and optimizing your applications
 - DDT
 - Vampir
 - CrayPAT
- Information on these tools is available on the web; you can also contact the OLCF User Assistance Center if you have questions





Support Best Practices

- Send as many error messages as possible
 - Or, place them all in a file and direct us to it
- When sending code, create a .tar file & direct us to it
 - Include all files necessary to build/run the code
 - More efficient than sending through email
- When possible, reduce error to a small reproducer code
 - We can assist with this
 - If the error has to go to the vendor, they'll want this
- Send new issues in new tickets, not replies to old ones



Finally...

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

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