OLCF Best Practices and Overview for New Users

General Information

- This presentation gives a brief introduction to using OLCF resources & covers systems, policies, and where to find help
    - This is by no means an all-inclusive presentation
    - Feel free to ask questions

- Much of this may be a reminder; it's largely an update to previous presentations

  https://vimeo.com/channels/olcftraining/254494153
  https://vimeo.com/channels/olcftraining/343636411
  https://vimeo.com/channels/olcftraining/405885960
  https://vimeo.com/channels/olcftraining/427792537
  https://vimeo.com/channels/olcftraining/519216250

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General Information

- Video/Slides will be uploaded to the event page (hopefully by the end of the week)

- All URLs are summarized at the end of the presentation

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Overview

1. Staying Informed
2. OLCF Policies
3. Authentication with RSA Tokens
4. Projects & User Accounts
5. Data Management
6. Finding and Building Software
7. Using Summit
8. Training Opportunities
9. Getting Help

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Staying Informed

Staying Informed

- We provides multiple layers of user notifications about system status and downtimes
  - Email lists
  - Status indicators on https://www.olcf.ornl.gov (at the bottom)
  - Twitter (@OLCFStatus)

- For more information, see the OLCF website: https://www.olcf.ornl.gov/for-users/user-assistance/

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Staying Informed – *Email Lists*

- *Announce* list
  - All users are required to be members
  - System-specific & center-wide announcements
  - olcf@olcf-communications.org
    (We use Mailchimp for this…It's an external address, but yes, it's us!)
  - Major announcements, weekly notice, etc.

- *Notice* lists
  - By default, "recent" users (active in last 2 weeks)
  - Permanent opt-in/opt-out possible (contact help@olcf.ornl.gov)
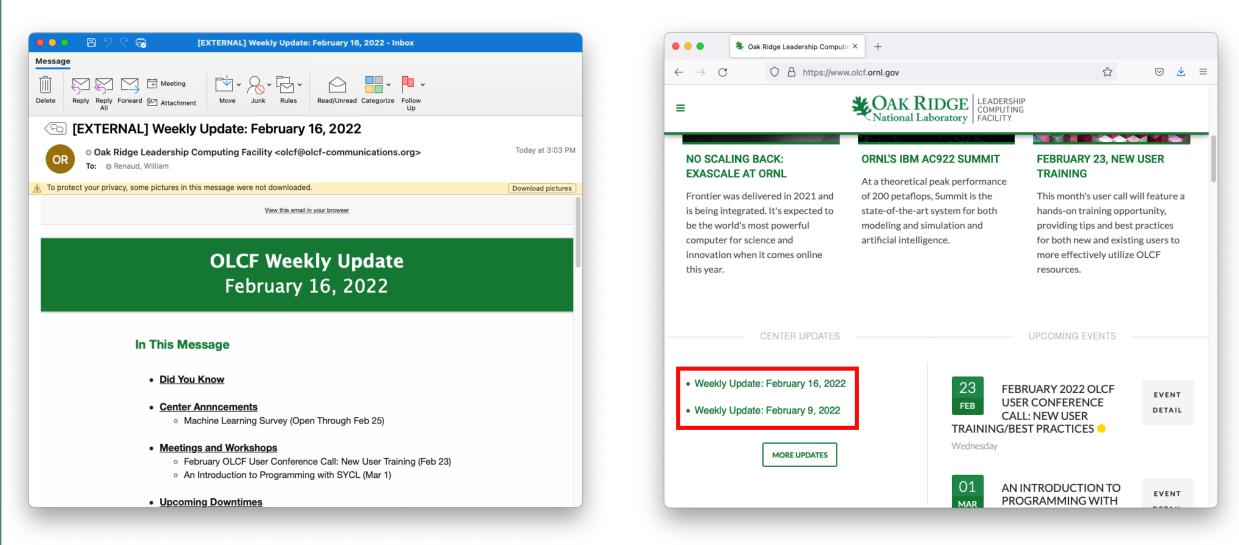 - Minor updates, system status, etc.

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Staying Informed – *Weekly Update*

- Sent before noon (Eastern) on Wednesday

- Announcements about outages, training, etc.

- ***ALL USERS* should receive this email**

- Also posted on OLCF home page

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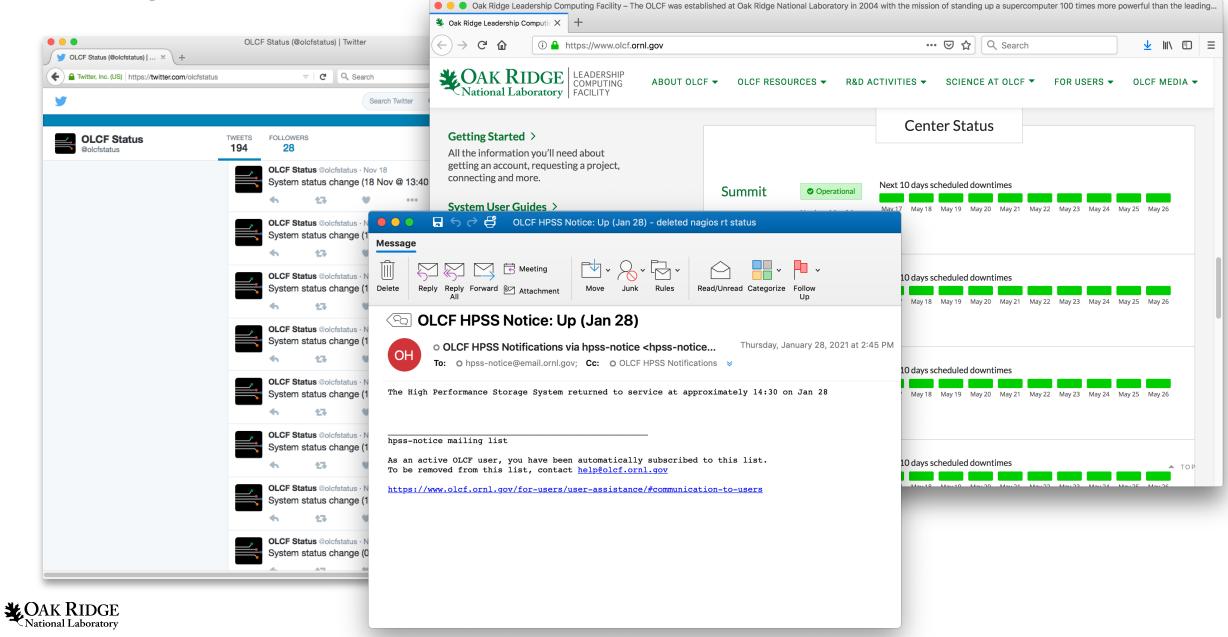
Staying Informed – *Weekly Update*

Staying Informed – *System Status*

- Logs from monitoring software are parsed to make educated guess on system status which is sent to multiple destinations
  - OLCF Website
  - Twitter (@OLCFStatus)
  - Appropriate *notice* list

- Fairly accurate, but still a fully automated process
  - Possibility of both false positives and false negatives
  - We do take some measures to mitigate this

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Staying Informed – *System Status*

OLCF Policies

OLCF Policies

- Various OLCF policies are available at
  https://docs.olcf.ornl.gov/accounts/olcf_policy_guide.html
  - Computing Policy
  - Security Policy
  - Data Management Policy
  - Various Project Policies
    (Reporting, Allocation Utilization, User Agreement)

- The site also includes the acknowledgement statement for publications related to work done on OLCF resources.

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Authentication with RSA Tokens

Authenticating to OLCF Systems

- Interactive login access is via Secure Shell (SSH)

- Systems use two-factor authentication via user-selected PINs and RSA SecurID tokens
  - Tokencodes can only be used once
  - Other methods (password, public key, etc.) are not permitted

- RSA terminology
  - *Tokencode*: The 6 digit number on your RSA token
  - *PIN*: An alphanumeric string of 4-8 characters known only to you
  - *PASSCODE*: Your PIN followed by the current tokencode

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Common Login Issues: Incorrect Username

- SSH (typically) doesn't prompt for a username
  - Nor does it tell you which one it's using
    - Unless you request verbose output (`-v[v[v]]`)
  - By default, it uses your username on the client system; you must tell it if your username differs
    - Command line: `ssh olcfusername@home.ccs.ornl.gov`
    - Via settings in `~/.ssh/config` file
    - Various ways to do this in graphical SSH clients

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Common Login Issues: Password Prompt

- SSH prompts for a password after PASSCODE fails
  - Typically happens after three PASSCODE failures…this is a fallback behavior of SSH (PASSCODE didn't work, so it's trying something else)
  - Your only option here is to kill the process (`ctrl-c`) & try again.
  - *Tip: If your PASSCODE has failed twice, let the tokencode change before you try again (to avoid token being locked out)*

```
Enter PASSCODE:
Enter PASSOCDE:
Enter PASSCODE:
user1@summit.olcf.ornl.gov's password:
```

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Common Login Issues: Token Synchronization

- RSA token gets out of sync with the server
  - Sometimes you may be prompted for the 'next tokencode'

  ```
  Enter PASSCODE:
  Wait for the tokencode to change, then enter the new tokencode :
  ```

  - If this happens, enter (only) the next tokencode your RSA token generates

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Projects & User Accounts

System & Group Access

- Projects
  - Are granted system access/assigned to Unix groups
- Users
  - Are assigned to projects
  - Inherit the project's groups & system accesses (they're not directly added to systems/groups)
- So…
  - For access to a group/system, you must join a corresponding project
  - If your project ends, your system access ends (unless you're on another project w/access to that system)
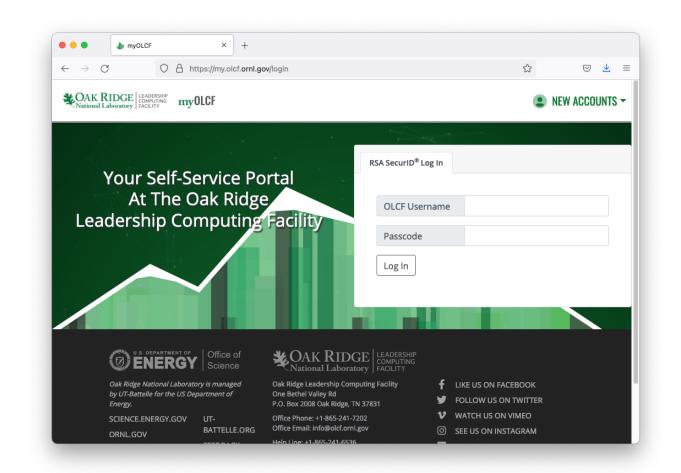
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Managing Your Allocation

- Projects are not disabled for going over allocation; they keep running, albeit at reduced priority
  - slight for 100-125% of allocation
  - larger for >125% of allocation (also incurs a limit of 1 running job)

- Since we don't disable projects, we don't give refunds (*per se*)
  - We can delay priority reduction if lots of jobs were affected by a particular system issue (same effect but easier to manage)
  - If you notice jobs being impacted by system issues, try to keep track of affected jobs

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myOLCF

- myOLCF allows you to
  - apply for projects (initial/renewal)
  - view your projects
  - get usage information
  - update your contact information
  - And more!

- https://my.olcf.ornl.gov

https://docs.olcf.ornl.gov/services_and_applications/myolcf/index.html

Project Closeout

- When your project ends:
  - You'll no longer be able to access OLCF resources associated with that project *unless* you have access via another project
  - You'll lose access to that project's Unix groups (and therefore the project's directories)
  - You'll have 1 extra month for data retrieval
    - But only on `home.ccs.ornl.gov` and `dtn.ccs.ornl.gov`
    - Don't wait to move data, though…

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Data Management

Storage Areas

By Scope	By Intended Use
• User	• Semi-Permanent/Home Directory
• Share among project members	• Scratch
• Shared with (possibly) all users	• Archive

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Data Storage Locations

Storage Area	Technology	Purpose of Area
User home	NFS	Frequently accessed user data
Project home	NFS	Frequently accessed project data
User work	Spectrum Scale/GPFS	User's scratch files
Project work	Spectrum Scale/GPFS	Project's scratch files
Global work	Spectrum Scale/GPFS	Sharing data among all users/projects on the system
User archive	HPSS[1]	Long-term storage for user data
Project archive	HPSS[1]	Long-term storage for project data
Global archive	HPSS[1]	Long-term storage for system-wide shared data

[1]HPSS is not mounted as a filesystem; access is discussed in upcoming slides

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Data Storage Locations

Storage Area	Location[1]	Default Permissions	Change Permissions?	Backed Up?
User home	`/ccs/home/$USER`	0750	Yes	Yes
Project home	`/ccs/proj/proj_id`	0770	No[3]	Yes
User work[2]	`/gpfs/alpine/proj_id/scratch/$USER`	0700	No[3]	**No**
Project work[2]	`/gpfs/alpine/proj_id/proj-shared`	2770	No[3]	**No**
Global work[2]	`/gpfs/alpine/proj_id/world-shared`	2775	No[3]	**No**
User archive	`/hpss/prod/proj_id/users/$USER`	0700	No[3]	**No**
Project archive	`/hpss/prod/proj_id/proj-shared`	2770	No[3]	**No**
Global archive	`/hpss/prod/proj_id/world-shared`	2775	No[3]	**No**

[1] *These are recommended ways to reference directories, not necessarily absolute path names.*

[2] *Or, $MEMBERWORK/proj_id, $PROJWORK/proj_id, $WORLDWORK/proj_id*

[3] *Top-level directory permissions "enforce" proper scope of user/project/global directories.*

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Data Backups - NFS

- NFS areas are backed up to a limited extent via the `.snapshot` subdirectory
  - Subdirectories are copies of the directory as of the snapshot time
  - Note that `.snapshot` won't show up in "`ls -al`"

```
$ ls –al /ccs/proj/abc123/important_data |grep .snapshot

$ ls /ccs/proj/abc123/important_data/.snapshot
daily.2022-02-10_0010    hourly.2022-02-15_1605    hourly.2022-02-16_0005    hourly.2022-02-16_0805
daily.2022-02-11_0010    hourly.2022-02-15_1705    hourly.2022-02-16_0105    hourly.2022-02-16_0905
daily.2022-02-12_0010    hourly.2022-02-15_1805    hourly.2022-02-16_0205    hourly.2022-02-16_1005
daily.2022-02-13_0010    hourly.2022-02-15_1905    hourly.2022-02-16_0305    hourly.2022-02-16_1105
daily.2022-02-14_0010    hourly.2022-02-15_2005    hourly.2022-02-16_0405    hourly.2022-02-16_1205
daily.2022-02-15_0010    hourly.2022-02-15_2105    hourly.2022-02-16_0505    hourly.2022-02-16_1305
daily.2022-02-16_0010    hourly.2022-02-15_2205    hourly.2022-02-16_0605    hourly.2022-02-16_1405
hourly.2022-02-15_1505   hourly.2022-02-15_2305    hourly.2022-02-16_0705    weekly.2022-02-13_0015
```

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Data Backups – GPFS and HPSS

- GPFS *is not* backed up (*AND* is purged)
  - GPFS directories are scratch areas (not intended for long-term storage)
  - To ensure available space, files not accessed/modified recently are purged (see Data Management Policy for the purge threshold)
  - *Archive data in GPFS to a more permanent location as soon as possible after creation!*

- HPSS *is not* backed up

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Monitoring Storage Usage

- For home directories, use the `quota` command

```
$ quota -Q
Disk quotas for user user1(uid 98765):
    Filesystem  blocks   quota   limit   grace    files   quota    limit    grace
nccs-svm1.lb.ccs.ornl.gov:/nccs/home1
               116432  52428800 52428800            1007  4294967295 4294967295
```

- No good tool for GPFS at present…ask help@olcf.ornl.gov if you need to know.

- For archive directories, use `showusage`

```
$ showusage -s hpss
HPSS Storage in GB:
                    Project Totals      user1
Project             Storage             Storage
_____|_____|_____
user1      |        550.65  |        550.65
abc123     |       2107.18  |        106.52
```

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Data Considerations

- OLCF systems generate lots of data very quickly; projects should develop a data strategy ***as soon as possible***. (It's easier to fix things with 100 files than with 100,000!)

- Some things to consider
  - How are files/directories shared among project members?
    - Where will project members store data?
    - What file attributes (permissions, group, etc.) are needed?
  - What happens when someone leaves the project?
  - What happens when the project ends?
    - Where does the data need to go?
    - How much data is there, who's moving it, and how long will it take?

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Whose Data Is It?

- Data in the User Home is considered the user's data
  - Normally, user must approve transfer to others
  - Anything that's part of the project needs to be elsewhere

- Data in other directories is considered project data
  - *Including User Scratch & User Archive areas*…yes, they're for things the user doesn't want to share, but they still are part of the project's data
  - PI approval is sufficient to change permissions/move this data

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Transferring Data

- https://docs.olcf.ornl.gov/data/transferring.html

- Data transfer nodes (`dtn.ccs.ornl.gov`) are the preferred place for internal & external data transfers

- Command-line transfer available with `hsi/htar` & `scp/sftp`

- Globus transfers available via two endpoints
  - OLCF DTN: for NFS and GPFS
  - OLCF HPSS: for HPSS

- Start early/transfer data as it's generated

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HPSS: The High Performance Storage System

- HPSS is the proper location for long-term storage
  - Not space-constrained like NFS "home" areas
  - Not subject to purge like GPFS

- Directories are project-centric with spaces for user, project, and globally-shared data

- Accessing HPSS:
  - From OLCF systems: via the `hsi` and `htar` commands
    - Preferably from `dtn.ccs.ornl.gov`; `hsi` from Summit/Andes logins should be OK
  - Externally: via Globus ("OLCF HPSS" endpoint)

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HPSS Directory Structure Changes - Overview

- Old structure had `/home/$USER` and `/proj/proj_id` storage areas

- New structure is project-based and mimics GPFS
  - `/hpss/prod/proj_id/[users|proj-shared|world-shared]` (old `/proj/proj_id` areas point to `/hpss/proj/proj_id/proj-shared`)
  - New users: Home directories are a link farm to proj areas
  - Existing users: Old home areas remain; users should migrate files to appropriate project areas & system will then convert to link farm)

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More HPSS Information

- Great presentation from Gregg Gawinski last month: https://www.olcf.ornl.gov/calendar/userconcall-jan2022/

- Data transfer information is available in OLCF User Guides on the website (links at the end of this presentation)

- For even more HPSS information, see the presentation by George Markomanolis
  - https://www.olcf.ornl.gov/wp-content/uploads/2018/12/storage_areas_summit_links.pdf
  - https://vimeo.com/306433952

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Finding & Building Software

Finding Software

- Basic commands are part of the default environment

- Other software via Lmod
  - Similar to Environment Modules (`module load`, etc.) but more powerful
  - https://lmod.readthedocs.io/

- Compilers, debugging/optimization tools, other libraries & some scientific apps available

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Finding Software

- Special case: python
  - We provide python+anaconda distributions
  - Recommend using those + conda/venv to build modules you need
  - You may need to build from source for Summit
  - Good presentation from OLCF's Matt Belhorn:
    - https://www.olcf.ornl.gov/wp-content/uploads/2020/06/20200603_summit_workshop_python.pdf
    - https://vimeo.com/427794043

- Other software
  - If you think something might be of general interest, you can request via email to help@olcf.ornl.gov

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Building Software

- Consider building/installing software in an NFS area
  - Avoids the scratch area purge
  - Also can be "friendlier" to the system, since compiling involves lots of metadata which can impact/be impacted by large parallel filesystems

- Might be possible to build in a ramdisk with an NFS directory as the installation prefix
  - Be sure to set appropriate permissions

- Review may be needed prior to adding software that wasn't listed on your project application; you must also comply with licensing/export control requirements

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Using Summit

Summit Considerations

- Running Jobs
  - Summit uses LSF for the batch queue system
  - Summit uses `jsrun` as its parallel launcher

- Processor Architecture
  - POWER9™
  - **Not compatible with x86_64 binaries!** You may have issues with prebuilt software (including python modules via conda as noted earlier)

- Filesystems
  - NFS areas are read-only on compute nodes
  - NVMe areas only available if you submit with
    `#BSUB -alloc_flags "nvme"`

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Job Step Viewer

- The `jsrun` command can be tricky…it's a different approach than other parallel launchers

- We provide a tool, Job Step Viewer, that runs a `jsrun` command & displays job placement on nodes via the web
  - https://jobstepviewer.olcf.ornl.gov/)
  - To use it, simply load the module (`module load job-step-viewer`) and run your command. It'll echo the URL that shows job/task placement
  - Must be run from within a batch job

- For more info, see slide presentation on https://www.olcf.ornl.gov/calendar/userconcall-mar2020/

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Summit Training Resources

- https://github.com/olcf-tutorials

- https://docs.olcf.ornl.gov/training/training_archive.html, in particular:
  - https://www.olcf.ornl.gov/calendar/introduction-to-nvidia-profilers-on-summit/
  - https://www.olcf.ornl.gov/calendar/summit-training-workshop/
  - https://www.olcf.ornl.gov/calendar/introduction-to-summit-webinar/
  - https://www.olcf.ornl.gov/calendar/jsrun-tutorial/

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Training Opportunities

Training Opportunities

- We support numerous training events: concalls, software-specific courses, hackathons (https://gpuhackathons.org)

- Recent training has been virtual; we anticipate hybrid training for future events

- What training is coming up?
  - Watch for announcements in the Weekly Update
  - https://www.olcf.ornl.gov/for-users/training/training-calendar/

- Past training:
  - https://vimeo.com/channels/olcftraining
  - https://docs.olcf.ornl.gov/training/training_archive.html

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Getting Help

Where do I find documentation?

- OLCF Website/User Documentation: https://docs.olcf.ornl.gov/
  - Summit/Andes User Guides
  - Slate/Jupyter documentation
  - Data storage/transfer
  - Training archive

- NVIDIA hosted documentation: http://docs.nvidia.com

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Working With User Support

- Email is often the best option to contact us
  - Especially for sending long/complicated error messages
  - Send as many error messages as possible
    (or place them in a file & direct us to the file)

- It's not necessary to send us codes/reproducers via email
  - More efficient to tell us where they are on the filesystem
  - If appropriate, set up a test directory or collect everything in a .tar file

- Report new issues in new tickets (not a reply to an old ticket)
  - Helps us in classifying/searching through old tickets
  - Gives it greater visibility

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Requesting Policy Exemptions

- The Resource Utilization Council accepts requests for temporary exemption from some policies (various job limits, purge exemptions, quota increases, etc.)

- Request exceptions via email to help@olcf.ornl.gov.
  - These are reviewed by the RUC, so make them well in advance
  - Let us know why the existing limits are an issue
  - If requesting a job priority boost…submit the job! It may more quickly than you expect.

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Finally

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

- Computer operations staff available 24x7 for limited troubleshooting via phone at (865) 241-6536

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Links

Links

- General
  - https://www.olcf.ornl.gov
  - https://www.olcf.ornl.gov/for-users/user-assistance/
  - https://docs.olcf.ornl.gov/accounts/olcf_policy_guide.html
  - https://my.olcf.ornl.gov
  - https://docs.olcf.ornl.gov/services_and_applications/myolcf/index.html

- Documentation
  - https://docs.olcf.ornl.gov/
  - http://docs.nvidia.com
  - https://lmod.readthedocs.io/

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Links

- Data Transfer
  - https://docs.olcf.ornl.gov/data/transferring.html
  - https://www.olcf.ornl.gov/calendar/userconcall-jan2022/
  - https://www.olcf.ornl.gov/wp-content/uploads/2018/12/storage_areas_summit_links.pdf
  - https://vimeo.com/306433952

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Links

- Summit Topics
  - https://jobstepviewer.olcf.ornl.gov/
  - https://www.olcf.ornl.gov/calendar/userconcall-mar2020/
  - https://www.olcf.ornl.gov/calendar/introduction-to-nvidia-profilers-on-summit/
  - https://www.olcf.ornl.gov/calendar/summit-training-workshop/
  - https://www.olcf.ornl.gov/calendar/introduction-to-summit-webinar/
  - https://www.olcf.ornl.gov/calendar/jsrun-tutorial/
  - https://www.olcf.ornl.gov/wp-content/uploads/2020/06/20200603_summit_workshop_python.pdf
  - https://vimeo.com/427794043

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Links

- Training
  - https://gpuhackathons.org
  - https://github.com/olcf-tutorials
  - https://www.olcf.ornl.gov/for-users/training/training-calendar/
  - https://vimeo.com/channels/olcftraining
  - https://docs.olcf.ornl.gov/training/training_archive.html
  - Previous Best Practices
    - https://vimeo.com/channels/olcftraining/254494153
    - https://vimeo.com/channels/olcftraining/343636411
    - https://vimeo.com/channels/olcftraining/405885960
    - https://vimeo.com/channels/olcftraining/427792537
    - https://vimeo.com/channels/olcftraining/519216250

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