Data Management in the HPC

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What you will learn

What: understand how to transfer, organize, and use data on the HPC.

Why: Nice data makes things easier: collaboration, reproducibility => better research

Assume

• Basic understanding of how to use the Unix shell

How

• Overview of storage options on the HPC
• Methods of transferring data in and out
• Basic HPC data management /good enough practices
• Moving data around
Basic Pipeline

- Data input, processing, collaboration, sharing
Logging in
The diagram of the UA HPC cluster
Login node is like an elevator
Login node is like an elevator
Cluster Login

- Open ood.hpc.arizona.edu in your web browser and login with your NetID and password.

- From the “Clusters” drop-down menu choose “shell access”

or use ssh from command line

```bash
~/ $ ssh zwickl@hpc.arizona.edu
Last login: Tue Feb 22 15:50:18 2022 from on-campus-10-138-68-75.vpn.arizona.edu
This is a bastion host used to access the rest of the RT/HPC environment.
Type "shell" to access the job submission hosts for all environments

[zwiclk@gatekeeper ~]$ shell
```
Login node
Data Storage Options
HPC Storage

- Tiered storage
- HPC storage: Active data
- Google drive: Non-active data
- Cloud storage: Archived data
HPC Storage – Tier I

- Three storage options (all FREE):
  - User level
    - /home
      - 50 GB
      - aka home directory or ~/ 
  - Group (PI) level
    - /groups
      - 500 GB
  - /xdisk
    - temporary “scratch” storage
    - up to 20 TB for up to 150 days (plus another 150 day extension)
    - Requested and managed by PIs
  - No rented storage
HPC Storage – Tier I

NO BACKUP
NO MERCY
Monitoring storage

- portal.hpc.arizona.edu
Monitoring storage

- command line - uquota

[dshyshlov@login3 ~]$ uquota

<table>
<thead>
<tr>
<th>Directory</th>
<th>Used</th>
<th>Soft Limit</th>
<th>Hard Limit</th>
</tr>
</thead>
<tbody>
<tr>
<td>/groups/dshyshlov</td>
<td>209.6G</td>
<td>500.0G</td>
<td>500.0G</td>
</tr>
<tr>
<td>/home</td>
<td>13.9G</td>
<td>50.0G</td>
<td>50.0G</td>
</tr>
<tr>
<td>/xdisk/dshyshlov</td>
<td>3.9G</td>
<td>9.8T</td>
<td>9.8T</td>
</tr>
</tbody>
</table>
Monitoring storage – xdisk

- Xdisk is temporary storage
- Max duration – 150 days
- One extension – another 150 days
- PI’s can monitor and manage xdisk on the portal
Delegating xdisk permissions

- PI’s can delegate permissions to manage xdisk.
HPC Storage

- **Compute node disk**
  - `/tmp`
    - local disk on compute nodes
    - not connected to the main storage
    - the best performance for calculations
    - Ocelote – 800 GB is available on each node
    - Puma – 1.4 TB is available on each node
  
- data is removed once the job is finished, so need to script copying input/output data to the main storage
Transferring Files
File transfer between local computer and HPC

- GUI
  - WinSCP
  - FileZilla
  - Cyberduck
  - globus

- Command line
  - wget
  - scp
  - sftp
File transfer in web browser

- Open On Demand: ood.hpc.arizona.edu
Command line file transfer

• Command line transfer is easy with scp command

  - scp –rp what_to_copy where_to_copy

  remote cluster location
default target is home directory

  To download, use the remote location as the first argument

  ~/Desktop/ $ scp -rp data_dir zwickl@filexfer.hpc.arizona.edu:

  ~/Desktop/ $ scp -rp data_dir zwickl@filexfer.hpc.arizona.edu:/groups/chrisreidy/

  ~/Desktop/ $ scp -rp zwickl@filexfer.hpc.arizona.edu: data_dir .
Managing Files
Sharing data between HPC users

• You can share data with another HPC user without moving the data

• Open file permissions

• Create symbolic links
File permissions

- Check file permissions – `ls -l`

```
-rw-r--r-- 1 dshyshlov rc  639 Oct 10 15:58 script.pbs
```

Owner

Group

```
-rwx rwx rwx
```

Read, write, and execute permissions for all other users.

Read, write, and execute permissions for the group owner of the file.

Read, write, and execute permissions for the file owner.

File type:
- indicates regular file
- d indicates directory
File permissions

- View file permissions in OOD

Please NOTE: "windfall" jobs will be restarted or terminated without notice if pre-empted by a "standard" job in queue.

<table>
<thead>
<tr>
<th>Type</th>
<th>Name</th>
<th>Size</th>
<th>Modified at</th>
<th>Owner</th>
<th>Mode</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>bin</td>
<td>-</td>
<td>2/22/2022 2:18:45 PM</td>
<td>zwickl</td>
<td>755</td>
</tr>
<tr>
<td></td>
<td>containerTest</td>
<td>-</td>
<td>2/22/2022 9:55:45 AM</td>
<td>zwickl</td>
<td>755</td>
</tr>
<tr>
<td></td>
<td>DLcheckpointing</td>
<td>-</td>
<td>2/18/2022 4:50:14 PM</td>
<td>zwickl</td>
<td>755</td>
</tr>
</tbody>
</table>

Check this box

Permissions
## Numerical file permissions

<table>
<thead>
<tr>
<th>Octal Value</th>
<th>File Permissions Set</th>
<th>Permissions Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>--------</td>
<td>No permissions</td>
</tr>
<tr>
<td>1</td>
<td>------x</td>
<td>Execute permission only</td>
</tr>
<tr>
<td>2</td>
<td>-------w</td>
<td>Write permission only</td>
</tr>
<tr>
<td>3</td>
<td>----------wx</td>
<td>Write and execute permissions</td>
</tr>
<tr>
<td>4</td>
<td>r--------</td>
<td>Read permission only</td>
</tr>
<tr>
<td>5</td>
<td>r--x</td>
<td>Read and execute permissions</td>
</tr>
<tr>
<td>6</td>
<td>rwx</td>
<td>Read and write permissions</td>
</tr>
<tr>
<td>7</td>
<td>rwx</td>
<td>Read, write, and execute permissions</td>
</tr>
</tbody>
</table>
Numerical file permissions

- Permissions can be summarized with the digits 1-7
- One number appears for each of the user, group and all permission categories
- So, 777 = rwxrwxrwx
  755 = rwxr-xr-x
Change file permissions

• Command to change permissions – chmod

  • chmod $+$x filename - make file executable for everyone

  • chmod g+rwx filename - open all permissions for your group

  • chmod 777 filename - open all permissions for everyone

  • chmod $-R 777 filename - same as above but recursively (for all the subdirectories and files)
Symbolic links

• Create a soft link to a file or directory
  • `ln -s path/to/the/destination link_name`
  • perfect for situations when you need to share read only data
  • requires permissions to link directory of another user

• Examples:

  • Create a shortcut to your /groups in your /home
    • `ln -s /groups/PINetID ~/my_groups`

  • Share data on xdisk (permissions!)
    • `ln -s /xdisk/PINetID/project ~/project_data`
File & Space Management Tools

• Show disk usage command - du

$ du scripts/
24 scripts/slurm_testing
8 scripts/puma/test
380 scripts/puma
12 scripts/elgato
3304 scripts/ocelote
36 scripts/chaining
7264 scripts/

• Useful flags:
  • -h – human readable format
  • -s – display only the total
  • --max-depth=N – limit depth of subdirectories to N

$ du -sh scripts/
7.1M scripts/
File & Space Management Tools

- Checking your space & file limit: `uquota`

```bash
frios@login2 ~$ uquota
frios home & PBS
/extras/frios

used  soft limit  hard limit  files/limit
46.84M   14G      15G       1044
56.72G   200G     200G      2/120000
```

- Checking folder usage and count: `NCDU`

```
ncdu 1.14 ~ Use the arrow keys to navigate, press ? for help
--- /home/u17/frios -------
20.8 MiB [########]  4 /rcclone-v1.42-linux-amd64
12.2 MiB [#####]   619 /renameutils-0.12.0
9.7 MiB [#####]   13 /tmsu-x86_64-0.7.4
2.7 MiB [#]       149 /local
2.0 MiB [ ]      92 /ncdu-1.14
1.0 MiB [ ]      37 /hpc-test1
392.0 KiB [ ]    duc-1.4.3.zip
256.0 KiB [ ]    .duc.db
200.0 KiB [ ]    ./cache
144.0 KiB [ ]    ncd-1.14.tar.gz
16.0 KiB [ ]     /ondemand
16.0 KiB [ ]     .bash_history
8.0 KiB [ ]   143 ./cookiecutters
```
Operate on Data

- Things that can “break” the system:
  - heavy use of the login node
  - too many jobs
  - too many files
  - heavy I/O jobs
  - copying GB of data
Preview for Part 2

• File and folder tidiness
• Scriptable methods of transferring data into/out of the HPC
• Additional tools for managing files and projects
• Data archiving