High Performance Computing (HPC) Club Training Session

Coco M. Mao June 1st 2018



Outline

- > Hyak and HPCC
- > Logging in to Hyak
- > Basic Linux Commands
- > Transferring Files Between Your PC and Hyak
- > Submitting Your Jobs



Hyak Overview

- > ~10000 nodes in total
- > STF has access to 1024 cores
- > ikt.hyak
 - 16 processors
 - 64GB memory
 - CentOS 6 Linux

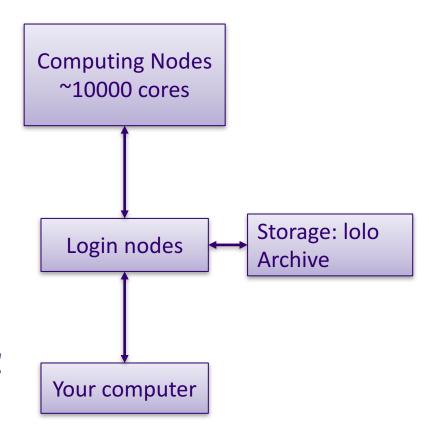
> mox.hyak

- 28 processors
- 128GB memory
- CentOS 7 Linux



Hyak Overview

- > Node type:
 - Computing nodes
 - > Production job
 - > ikt 'n012'
 - Login nodes
 - > Job submitting
 - > Files transferring
 - > 'ikt2'
- > Never run job on login nodes!
- > Hyak wiki:
 - http://wiki.cac.washington.edu/display/hyakusers/WIKI+for+Hyak+users



Logging in to Hyak

- > This is essentially remote-accessing a Linux System via SSH protocol
- > Linux & Mac
 - Mac: application->utilities->terminal
 - Ubuntu: Search for "terminal" in your applications

> Windows:

- SSH client alternatives
- Putty http://www.putty.org/
- cmder http://cmder.net/
- xshell

> More info here:

http://wiki.cac.washington.edu/display/hyakusers/Logging+In



HPC Club

- > High Performance Computing Club (HPCC):
 - http://students.washington.edu/hpcc/
- > As a club member, you can have access to thousands of CPU cores on UW Hyak supercomputer.
- > Become a member:
 - http://students.washington.edu/hpcc/getting-started-on-hyak/



Logging in to hyak

- > To connect to ikt.hyak
 - ssh -X yourUWnetid@ikt.hyak.uw.edu
- > To connect to mox.hyak
 - ssh -X yourUWnetid@mox.hyak.uw.edu
- > Enter your uwid password

```
D-10-18-220-168:~ maomoke$ ssh maomoke@ikt.hyak.uw.edu
Password:
Enter passcode or select one of the following options:

1. Duo Push to phone (XXX-XXX-4968)
2. Phone call to phone (XXX-XXX-4968)
Duo passcode or option [1-2]:
```

- > Confirm with Duo Mobile on your phone
 - https://itconnect.uw.edu/security/uw-netids/2fa/



Basic Linux Commands

- > Show current directory: pwd
 - + SHOME directory
- > Show contents in current directory: ls [options]
- > change current directory: cd + [path]
 - cd absolute path
 - cd relative_path
- > Create a new folder: mkdir folder_name
- > Remove a file/folder: rm [options]



Transfer files

- > Linux & Mac: SCP
 - Usage: scp [options] <source directory> <target directory>
- > Windows: WinSCP
 - Download: https://winscp.net/eng/download.php
- > Upload files to Hyak:
 - \$ scp filenameuser@ikt.hyak.uw.edu:path/to/destination/directory
- > Download files from Hyak:
 - scp user@hyak.washington.edu:path/to/file ./
- > Note that these all these commands should be executed on the remote host (your laptop).
- > More info: http://wiki.cac.washington.edu/display/hyakusers/Managing+your+Files#Managi



STF Workspace

> ikt

- gscratch:/gscratch/stf
- suppscr: /suppscr/stf
- lolo :/lolo/archive/hyak/stf/

> MOX

- /gscratch/stf
- > File scrubber:
 - http://students.washington.edu/hpcc/using-hyak/scrubber-dont-lose-your-files/



Interactive node usage

- > To get an interactive node in your own group for 2 hours:
 - qsub -I -1 walltime=2:00:00
- > To get 2 nodes for interactive use for 2 hours:
 - qsub -I -l nodes=2:ppn=16,feature=16core,walltime=2:00:00
- > When the above command runs, then you will have been allocated 2 nodes and you will be on one of the two nodes.
- > Interactive nodes are computing nodes. Can not transfer file between ikt/mox/lolo on interactive nodes. Can not submit jobs.



Submitting Batch Jobs

> qsub:

- qsub [options] command-for-running-your-job
- e.g. qsub -l walltime=2:00:00 -I -V matlab compute norm.m

> Use PBS (Portable Batch System) Jobscripts, which:

- Include instructions for the scheduler
- set up the work environment
- execute your program

> More info:

 http://wiki.cac.washington.edu/display/hyakusers/Hyak+Job+Schedule r#Hy%20akJobScheduler-ImportantInformation



Manage Jobs

- > Check the status of your job checkjob <job_id>
 - qstat -f <job_id>
- > Queue Status
 - showq -w qos=<your_group>
 - showq -w user=<your_netid>
 - e.g. showq -w qos=stf
- > To cancel a job:
 - mjobetl -c <job id>
 - qdel <job_id>
- > More info:
 - http://wiki.cac.washington.edu/display/hyakusers/Hyak+Job+Scheduler#HyakJo bScheduler-ManagingJobsinYourQueues

MOX

- > To connect to mox.hyak
 - ssh -X yourUWnetid@mox.hyak.uw.edu
- > **Show queue:** squeue
- > To get an interactive node in your own group for 2 hours:
- > srun -p xyz -A xyz --time=2:00:00 --mem=100G --pty /bin/bash
- > To get 2 nodes for interactive use:
- > srun -N 2 -p xyz -A xyz --time=2:00:00 --mem=100G --pty /bin/bash
- > **Submit:** sbatch -p <my short group> -A <my short group> test.sh
- > Use your group's nodes: squeue -p xyz
- > **Show Job Info:** scontrol show job <jobid>
- > Cancel Jobs: scancel <jobid>; scancel -u <username>
- > More info:
 - http://wiki.cac.washington.edu/display/hyakusers/Hyak+mox+Overview



Transfer between ikt and mox

> From ikt to mox

- ikt1\$ hyakbbcp myfile mox1.hyak.uw.edu:/gscratch/MYGROUP/
- ikt1\$ hyakbbcp -r mydirectory mox1.hyak.uw.edu:/gscratch/MYGROUP/

> From mox to ikt

- mox1\$ hyakbbcp myfile ikt1.hyak.uw.edu:/gscratch/MYGROUP/
- mox1\$ hyakbbcp -r mydirectory ikt1.hyak.uw.edu:/gscratch/MYGROUP/

> File scrubber

There's a scrubbed temporary filesystem available at /gscratch/scrubbed. Files can be removed at any time, but they will be removed on a periodic basis based on creation date (files created 30 days ago or more).

