High Performance Computing (HPC) Club
Training Session
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Outline

• The Hyak Supercomputer
• Log in to Hyak
• Transfer files between your PC and Hyak
• Submitting your first job
• Practice
The Hyak Supercomputer

- A typical node has 16 processor cores and 128GB of memory
- All the nodes run CentOS 6 Linux
- ~10000 cores in total
- Club members have access to 1028 cores
- Node types
  - Computing nodes
  - Login nodes
    - Submitting jobs
    - Transferring files
Log in to Hyak

Remotely Accessing a Linux System via SSH protocol

• Use a SSH client program
  • Linux & Mac: just open a terminal
    • Mac: application->utilities->terminal
    • Ubuntu: Search for “terminal” in your applications

usage: ssh [options] user@IP-address

  e.g

  ssh xsqin@hyak.washington.edu
  ssh xsqin@americano.amath.washington.edu
  ssh shawn@128.95.220.141

  Then enter your password and PRN from your token

• Windows: putty
  • http://www.putty.org/
Log in to Hyak

- putty
- More info here: http://wiki.cac.washington.edu/display/hyakusers/Logging+In
Linux command basis

- Show current directory: `pwd`
- `$HOME` 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]`
- Rename a file/folder: `mv old_name new_name`
Managing your files

• Transfer files from your local desktop to the server
  • Linux & Mac: SCP
    • `scp [options] <source directory> <target directory>`
  • Windows: WinSCP
    • [https://winscp.net/eng/download.php](https://winscp.net/eng/download.php)

• Where should I put my job outputs?
  • Gscratch space: fast, temporary
    • `/gscratch/<your group>/<your netid>`
    • e.g. `/gscratch/stf/xsqin`
  • Lolo: slow, long-term storage
    • `/lolo/archive/hyak/<your group>/<netid>`
    • `/lolo/archive/hyak/stf/xsqin`
Submitting your first job

- Node types:
  - logging node: used to submit jobs. Don’t execute heavy tasks on it
  - computing node: where your jobs are running

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

- PBS (Portable Batch System) Jobscripts
  - instructions for the scheduler
  - setting up the work environment
  - executing your production program

- http://wiki.cac.washington.edu/display/hyakusers/Hyak+Job+Scheduler
  #HyakJobScheduler-ImportantInformation
Submitting your first job

```bash
#!/bin/bash

## name of the job
#PBS -N case17

## specify resources requested
#PBS -l walltime=1:00:00:00,nodes=3:ppn=16,mem=180gb,feature=16core

#PBS -d /civil/shared/motley/xsqin/tsunami_inundation/modified-3D/case17_force
#PBS -o /civil/shared/motley/xsqin/tsunami_inundation/modified-3D/case17_force

## Send an email to your UW email when the job begins, finishes or fails.
#PBS -m abe

## working environment
module load icc_14.0-1mpi_4.1.1

## executing your production program
source /gscratch/motley/shared/OpenFOAM231/OpenFOAM-2.3.1/etc/bashrc

#decomposePar -force
mpirun -np 64 interFoam -parallel

echo $MPI_ROOT
mpirun -np 64 interFoam -parallel >> run.log 2>&1
```
Submitting your first job

Practice:

Create a directory on Hyak for your code, e.g. $HOME/hello_world
go to:

https://github.com/xinshengqin/HPCC_training_session.git
copy and paste
• the code in ./hello_world/test.c
• the code in ./hello_world/run.sh
into two different text files on your laptop.

Edit run.sh:

change working directory and output directory (e.g. $HOME/hello_world)
Submitting your first job

Practice:
Upload the two text files to Hyak:
  e.g. $HOME/hello_world
Compile the c code:
  gcc test.c -o test
Test your code:
  ./test
For windows user:
  convert run.sh to UNIX
  format with command:
  dos2unix run.sh
Submit the job: qsub run.sh
Managing Jobs in Your Queues

• 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
  mjobctl -c <job_id>
  qdel <job_id>
Two types of jobs

• Background job
  • what we just submitted:
    • qsub some_script.sh

• Interactive jobs
  • qsub -l -V -W group_list=hyak-stf -l walltime=2:00:00