

This lecture:

- HPC introduction
- Python on HPC
- Hands-on
- Exercise

HPC - Introduction

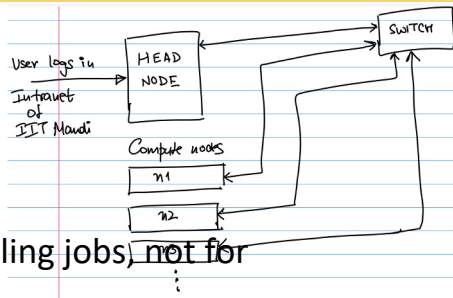
HPC topology

Head node:

Suited to login and scheduling jobs, not for computation

Compute nodes:

Suited for heavy computation, typically has 2 processors per node (machine), each processor has up to 12 cores, 64+GB RAM, 2TB local storage



HPC IIT Mandi (website tour)

• <https://sites.google.com/iitmandi.ac.in/hpc-iit-mandi/>

• CPUHPC (10.8.1.19): CPU-based parallelism

• GPUHPC (10.8.1.20): GPU-based parallelism

• 10G connectivity between nodes

• Filesystems

– Home: 10GB

– Working dir (wd): 2TB

• Software: basic software + *Singularity*

• Example PBS scripts

• Queue details

• Resources

Engineering

- Fluid flow and heat transfer (Open FOAM, Fluidity, ANSYS Fluent)
- Solid mechanics (ANSYS)
- Deep learning (Python modules)

Physics

- Molecular dynamics (in-house codes)

Chemistry

- Computational chemistry (Gromacs)

Biology

- Gene sequencing

IIT Mandi HPC cluster: 2884 processing cores; 300+ users • 169 nodes; 2884 cores

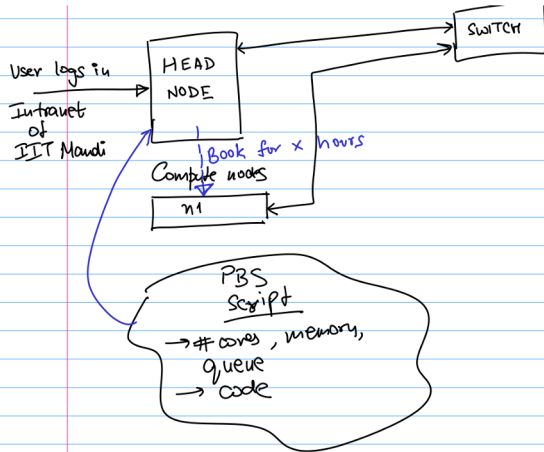
- Intel Xeon processors
- 11.5 TB memory
- 986 TB storage
- 33 Nvidia graphical processing units (GPUs) • 10Gb/s ethernet connectivity
- Cooling system

PBS: portable batch system

Queuing system for job submission which takes care of the number of jobs and excessive usage

Clusters

Filesystems



- Session screenshot to be recorded
- Logging in to the cluster(s) and directory structure
- Prepare virtualenv and install packages using pip
- PBS script for running a Python code
- Launching the PBS script using qsub
- Output and error files

Commands

```
scl --list - list all scl (Red Hat) packages available  
scl enable rh-python36 bash (exit to exit from the scl)  
pip3 install --user --upgrade --proxy=http://10.8.0.1:8080 pip  
pip3 install --user --upgrade --proxy=http://10.8.0.1:8080 virtualenv  
virtualenv ~/virtualenvs/testenv  
source ./virtualenvs/testenv/bin/activate  
pip3 install --upgrade --proxy=http://10.8.0.1:8080 pip  
pip3 install --proxy=http://10.8.0.1:8080 numpy ipython jupyter  
pip3 list - to check installed packages  
  
qsub <pbs_script.sh>
```

PBS script – detailed discussion

- PBS directives used in the script
- man qsub
 - discuss environment variables
- <https://docs.adaptivecomputing.com/torque/4-0-2/Content/topics/commands/qsub.htm>

qstat -an

-a - all jobs

-n - display nodes allocated to jobs

qstat -q

qstat <jobid> -f - full detail

qdel jobid

qdel all

```
Qsub -I <pbs_script.sh>
```

Exercise 1

1. Login to the cluster
2. Copy the `mysqrt.py` file to `wd`
3. Copy a sample serial PBS script from the HPC website and edit it to calculate the square root of 2.0 with the debug mode on. The output should not be redirected into a file. See where it goes.
4. Launch the script on CPUHPC. Also, try with a different queue.
5. Launch the script on GPUHPC. Take care that the queues are different on the two clusters.
6. Also, try using the interactive mode in `qsub`
7. Try `qstat` options, and `pbsnodes` to check node mapping.
8. Copy the output file and error files back to your PC
9. Added challenge: can you write a bash conditional in your PBS script that runs the code only if the job is sent to `n121`. Use `--l nodes=n121.cluster.iitmandi.ac.in` to test it.

Exercise 2 - advanced

- Copy the `mysqrt.py` module to the HPC home
- Write a python script called `root.py` that calculates the sqrt of number using `mysqrt` module and prints it. The number should be passed to the script through bash using `sys.argv` variable
- Write a bash loop that calls `root.py` for the first 1000 even numbers, i.e. 2,4,6,...
- The results should be appended into a file in the following format:
 - Sqrt of 2 is 1.414xxx, time taken xx seconds
 - Sqrt of 4 is 2.0, time taken xx seconds
- Run the bash loop over the HPC cluster in the serial queue