HPC at IU – Hands On

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How do I get access?

• I am sure you all already did this…
• Create an account:
  – https://itaccounts.iu.edu/
  – Graduate students with hourly positions may not see BRII listed, please contact us for an account!
• Login domain names:
  • bigred2.uits.iu.edu
  • quarry.uits.indiana.edu
  • mason.indiana.edu
  – IU network ID and pass phrase
  – Read the message of the day (MOTD)

https://kb.iu.edu/d/achr
Let’s get our hands dirty

- We will do the following on Big Red II today:
  - Copy something from your desktop to Big Red II
  - Change your environment to PrgEnv-gnu
  - Compile something
  - Submit a job to the queue to run something
  - Get an interactive node and launch a GUI application
SSH and SCP

• Sounds great, where do I login? Not in a browser 😞
• SSH is used to login to a remote machine
• SCP is used to copy files to and from a remote machine
• Example:
  ssh username@bigred2.uits.iu.edu

  scp local-file username@bigred2.uits.iu.edu:/path/to/remote/dir

https://kb.iu.edu/d/aelc
https://kb.iu.edu/d/agye
You need clients

• For SSH: Putty on Windows (http://www.putty.org/)
• For SCP: Winscp for windows (http://winscp.net/eng/index.php)
  • Filezilla is cross platform (https://filezilla-project.org/)
• On Mac and Linux: you can use the terminal for SSH
  • Use the terminal for SCP as well OR
  • Use Filezilla for GUI interface
Environment – in your login session

- **Home directory:**
  - `/N/u/<username>/BigRed2`

- **Scratch space for temporary files:**
  - `/N/dc2/scratch/<username>`

https://kb.iu.edu/d/avmj
Task 1: Login and copy something to BR 2

- ssh `username@bigred2.uits.iu.edu`
- Copy something from your desktop/laptop to BR 2

- Download something from the web onto BR 2:
  - `wget` lets you download from the web
How to find and use software

• module command for adding software to your environment
  - module avail
  - module list
  - module load <key>
  - module unload <key>

• Permanently configure your environment via the .modules file
• Modules arranged in groups, development, applications, life sciences, etc.

https://kb.iu.edu/d/bcwy
What does “module load” do?

- Makes the software ready for use
- Does not start or run the application
- There isn’t anything like this on Windows

https://kb.iu.edu/d/bcwy
Task 2: Play with modules

- Change your programming environment to PrgEnv-gnu
- Make this change permanent
  - Edit .modules in your $HOME
  - Edit a file on a remote machine
  - Common editors: vi, nano, emacs
Sample PBS script

• At the most basic level, on Quarry:

```bash
#!/bin/bash
#PBS -l nodes=2:ppn=6,walltime=30:00
cd /path/to/working/dir
mpirun -np 12 -machinefile $PBS_NODEFILE ~/bin/binaryname
```

• Put these lines in a text file and run “qsub script.sh”

https://kb.iu.edu/d/avmy
Queue commands

• Some other useful commands to see what’s going on with the queues:
  • qstat –Q #shows available queues
  • qstat –u username #shows the status of your queued jobs
  • showq –i #shows what’s going to run next

https://kb.iu.edu/d/avmy
On Quarry or Mason (non-Cray machines)

• There is a login node (s)
• There are compute nodes
• You build, install and setup your job environment on the login node
• Run the job on the compute node
• Using mpirun if parallel or just the binary if it is serial
  • That is:
    • mpirun –np 32 app_name
  • Or just:
    – ./app_name
On Big Red II and other Cray’s

- Login, aprun and compute nodes

https://kb.iu.edu/d/bdkt
ESM – Extreme Scalability Mode

- No compromise *scalability*
- Low-Noise Kernel for scalability
- Native Comm. & Optimized MPI
- Application-specific performance tuning and scaling

CCM – Cluster Compatibility Mode

- No compromise *compatibility*
- Fully standard x86/Linux
- Standardized Communication Layer
- Out-of-the-box ISV Installation
- ISV applications simply install and run

Launch everything with aprun or ccmrun, whether it is parallel or serial
Interactive jobs

- For graphical applications – you can launch GUIs
- For testing
- `qsub -l`
  - Followed by options to specify walltime, queue, etc.
  - `qsub -I -l walltime=00:30:00 -q debug`

- Straightforward on Quarry
- Will land on an aprun node on Big Red II
  - `module load ccm`
  - Need to `ccmlogin`

https://kb.iu.edu/d/bdsi
Compilers

- GNU, Cray, Intel, PGI

<table>
<thead>
<tr>
<th></th>
<th>GNU</th>
<th>Cray</th>
<th>Intel</th>
<th>PGI</th>
<th>MPI wrappers</th>
</tr>
</thead>
<tbody>
<tr>
<td>Big Red II</td>
<td>cc, CC, ftn</td>
<td>cc, CC, ftn</td>
<td>cc, CC, ftn</td>
<td>cc, CC, ftn</td>
<td>N/A</td>
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<tr>
<td>Quarry, Mason</td>
<td>gcc, g++, gfortran</td>
<td>N/A</td>
<td>icc, icpc, ifort</td>
<td>pgcc, pgCC, pgfortran</td>
<td>mpicc, mpic++, mpif77 or mpif90</td>
</tr>
</tbody>
</table>

https://kb.iu.edu/d/abby
Task 3: Submit a job to the queue

- Copy this directory to your scratch space on DC 2
  - Downloaded this from [http://go.iu.edu/g2H](http://go.iu.edu/g2H)
  - cp –r job-submission.tar /N/dc2/scratch/username
  - tar xvf job-submission.tar
- Compile the mpi_hello.c program
  - cc mpi_hello.c
- Edit the pbs.sh file to set the working directory and binary name
  - It will not work out of the box
- Submit the job to the queue
Launching GUI apps

• For X forwarding in SSH to work you must be running an X server program
• Most Linux systems have X server installed by default
• On Windows, can use Xming: http://sourceforge.net/projects/xming/
• On Mac, can use Xquartz: http://xquartz.macosforge.org/landing/
• Start these apps first before you launch SSH app
• Enable X11 forwarding by checking a box in your SSH app

https://kb.iu.edu/d/bdnt
Task 4: X forwarding exercise

1. On Big Red II and Quarry, login with X forwarding enabled
   1. Launch xclock

2. On Big Red II, start an interactive job with X forwarding enabled
   1. Launch xclock from the compute node

Hint: Find step by step instructions on the KB pages