

An Introduction to Supercomputing at IU

Nils Hjortnæs

- 1. Systems available at IU
 - 1.1 Carbonate
 - 1.2 Big Red 200
 - 1.3 Quartz
 - 1.4 Acknowledgements
- 2. Accessing the Machines
 - 2.1 Getting Accounts
 - 2.2 Logging In
 - 2.3 The File System
- 3. Setting Up your Environment
- 4. Running your Jobs
 - 4.1 The Queue
 - 4.2 Interactive Jobs
 - 4.3 Batch Jobs

Changes (i.e. why to do this presentation again)

- Carbonate is gone
- Quartz is useful now
- HPC Everywhere is gone
- Found nice visualization
- Added huge slurm cheatsheet

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Carbonate



Big Red 200

- bigred200.uits.iu.edu
- 640 compute nodes
 - 256 GB RAM
 - 2 64-core CPUs
 - 4 day time limit
- 64 GPU nodes
 - 256 GB RAM
 - 4 NVIDIA A100 GPUs (~\$9000 each)
 - 2 day time limit
- https://kb.iu.edu/d/brcc

Quartz

- quartz.uits.iu.edu
- large amounts of processing capacity over long periods of time
- 92 General Compute Nodes
 - 2 64 Core CPUs
 - 512GB RAM
 - 4 day time limit
- 22 GPU Nodes
 - 4 Nvidia V100s
 - 768GB RAM
 - 2 day time limit

Slate

- Slate offers additional storage attached to the supercomputers if needed
- You can create a Slate account at https://access.iu.edu/Accounts/Create
- When on the supercomputer, slate storage is available at /N/slate/[username]
- You can see how much space you have used with the quota command

Acknowledgements

Important Note

When using any of the IU supercomputers for research, you must include a blurb in your acknowledgements section of the paper.

https://kb.iu.edu/d/anwt

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Command Line Cheatsheet

- Is Show what is in this folder/directory
- cd [directory] Change directory to [directory]
- cd .. Go to the parent directory
- ssh [servername] Connect to [servername]
- scp [file] [server]:[directory] Copy [file] to [directory] on [server]
- scp -r [folder] [server]:[directory] Copy a folder instead of a file
- mkdir [name] Make a new directory named [name]
- rm [file] Delete [file]
- rm -r [folder] Delete [folder]

Getting your Accounts

There are 2 kinds of accounts:

Personal:

- 1. Visit https://access.iu.edu/Accounts/Create
- 2. Select the accounts you'd like to add
- 3. Fill in the form
- 4. They usually respond within a business day

Getting your Accounts

There are 2 kinds of accounts:

Lab:

- 1. After you get the confirmation email of your personal account
- Ask Fran or Sandra to add you to their lab "project"
- Fran/Sandra: Visit https://hpcprojects.uits.iu.edu/
- 4. Note the project id, you will need it later!

Logging In

- All of the computers have a terminal interface (shell)
- On Macs and Linux, use ssh
- On Windows you can use PuTTy https://www.chiark. greenend.org.uk/~sgtatham/putty/latest.html
- Use your iu network id as the username
 - \$ ssh [username]@bigred200.uits.iu.edu

The File System

- Use git, scp, or sftp to down/upload files/folders
 - \$ scp file.file [username]@bigred200.uits.iu.edu:
 - \$ scp -r folder [username]@bigred200.uits.iu.edu:
- For Windows, use winSCP

```
https://winscp.net/eng/index.php
```

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The Module System

- module list List loaded modules
- module avail Show available (compatible) modules
 - On Big Red 200: module spider show all modules
- module load [module] Load [module]
- module swap [old module] [new module] Unload [old module] and load [new module]
 - If add fails because of a module conflict, use this
- module unload [module] Unload [module]

The Module System

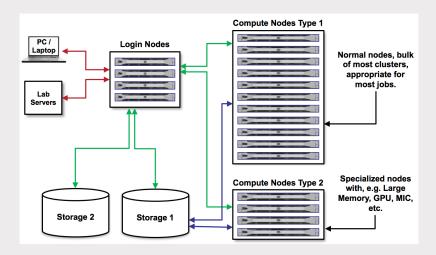
- You can edit the .modules file in your home directory to set up modules every time you log in
 - Just type the commands you want to run
- Only Professors can request new software be installed
- There are Python GPU modules use these for DL

my .modules file

module swap python deeplearning/1.13.1 module load libsndfile/1.0.28

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Visualization



The Queue

- When you log onto the supercomputer, you're on a login node.
 These are for configuring your environment and up/downloading data, not running code
- Jobs that run on the login nodes are limited to 20 minutes of cpu time. After that you'll get booted
- To use the high performance nodes, you enter the queue

Slurm Cheatsheet

- sinfo View partition information
- squeue View queue info
 - -u [username]
 - p [partition]
- srun Run an interactive session
- sbatch [job script] Submit [job script] as a batch job
- scancel [jobid] Cancel a job with id [jobid]
- And so much more

Submitting Interactive Jobs

- Interactive Jobs let you open a terminal on a compute node
- srun -p general --time=00:05:00 -A [project id] --pty bash
 - 'srun' : submit a job
 - '-p general' : open on the general partition
 - '--time=00:05:00' : request 5 minutes
 - '--pty': keeps the terminal open
 - 'bash': run bash on the terminal
 - '-A': required, the project ID to use
 - » Fran's lab's: r00027
- More options available here https://kb.iu.edu/d/awrz

Batch Jobs

- Batch Jobs send a job to Slurm without opening a terminal
- To run them, you have to prepare a script
- To submit the script, type 'sbatch <script>'
- More options available here https://kb.iu.edu/d/awrz

Example batch script

#!/bin/bash

#SBATCH -J [job_name] #SBATCH -p general #SBATCH -o filename_%j.txt #SBATCH -e filename %j.err #SBATCH -- mail - type = ALL #SBATCH -- mail - user = [username]@iu.edu #SBATCH -- nodes = 1 #SBATCH -- ntasks - per - node = 1 #SBATCH --time=2-02:00:00 #SBATCH --mem=16G #SBATCH -A [slurm - account - name] #Load any modules that your program needs module load modulename

```
#Run your program
srun ./my_program my_program_arguments
```

Sources

- Supercomputers Overview https://kb.iu.edu/d/alde
- Big Red 200 https://kb.iu.edu/d/brcc
- Slate https://kb.iu.edu/d/aqnk
- Modules https://kb.iu.edu/d/bcwy
- Slurm https://kb.iu.edu/d/awrz