# Intro to High-Performance Computing and the Smithsonian Hydra Cluster

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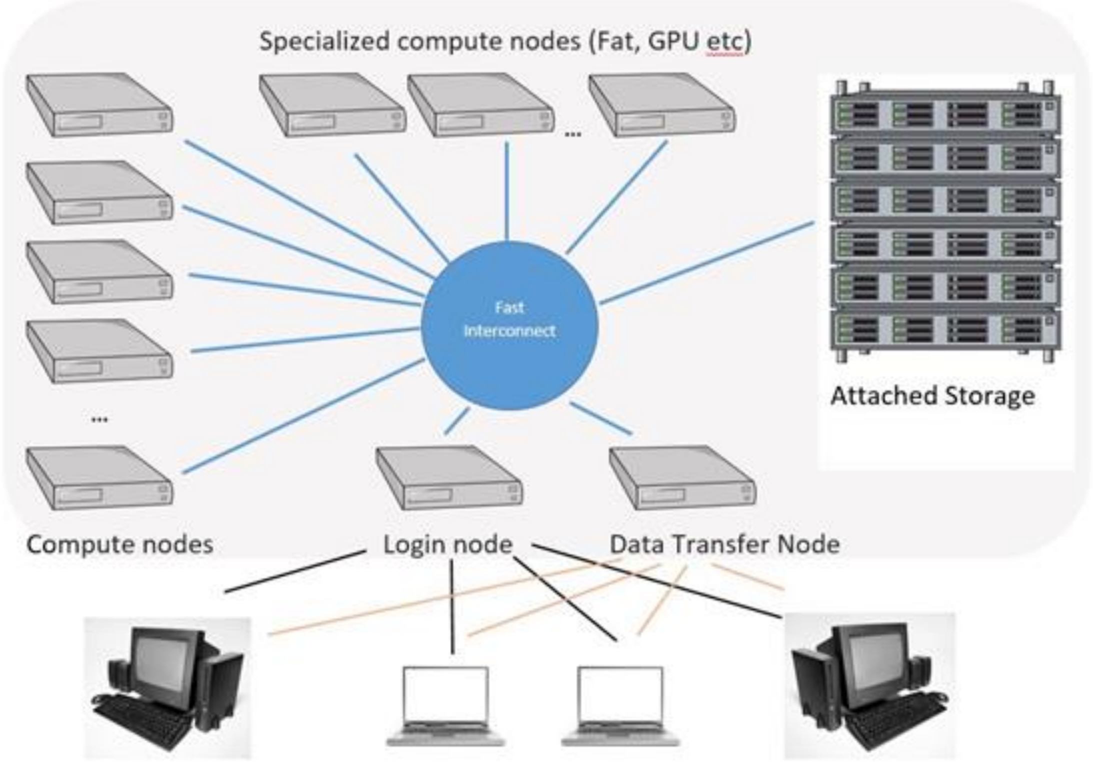
*Hydra vulgaris,* (c) Proyecto Agua
https://www.inaturalist.org/taxa/486293-Hydra-vulgaris

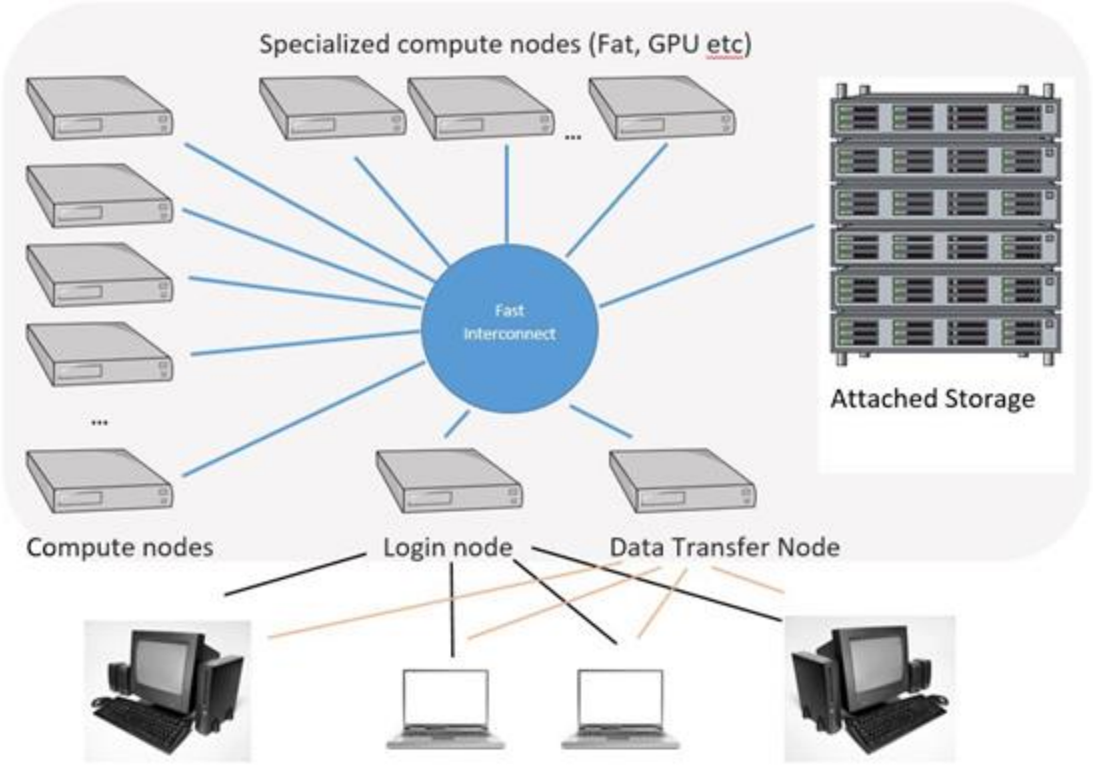
# What is a High-Performance Computing (HPC) cluster?

- Basically, just many individual computers linked together
- **Nodes** ~= individual computers
  - **Login node** = the central node that all users interact with when they log in
  - **Compute nodes** = nodes that run **jobs** (programs, code, scripts, etc) for users
- Each node has its own CPU with some number of cores and RAM



# Why use a HPC cluster?

- Access to way more computing power than any individual lab could afford
- Run analyses remotely so they won’t bog down your own computer
- Each user can run hundreds of computing jobs in parallel
- A “safe” environment to learn
  - Each user only has read/write access to their own files
  - Can’t accidentally delete someone’s data
- Hardware is maintained by professionals
- Tech support is available

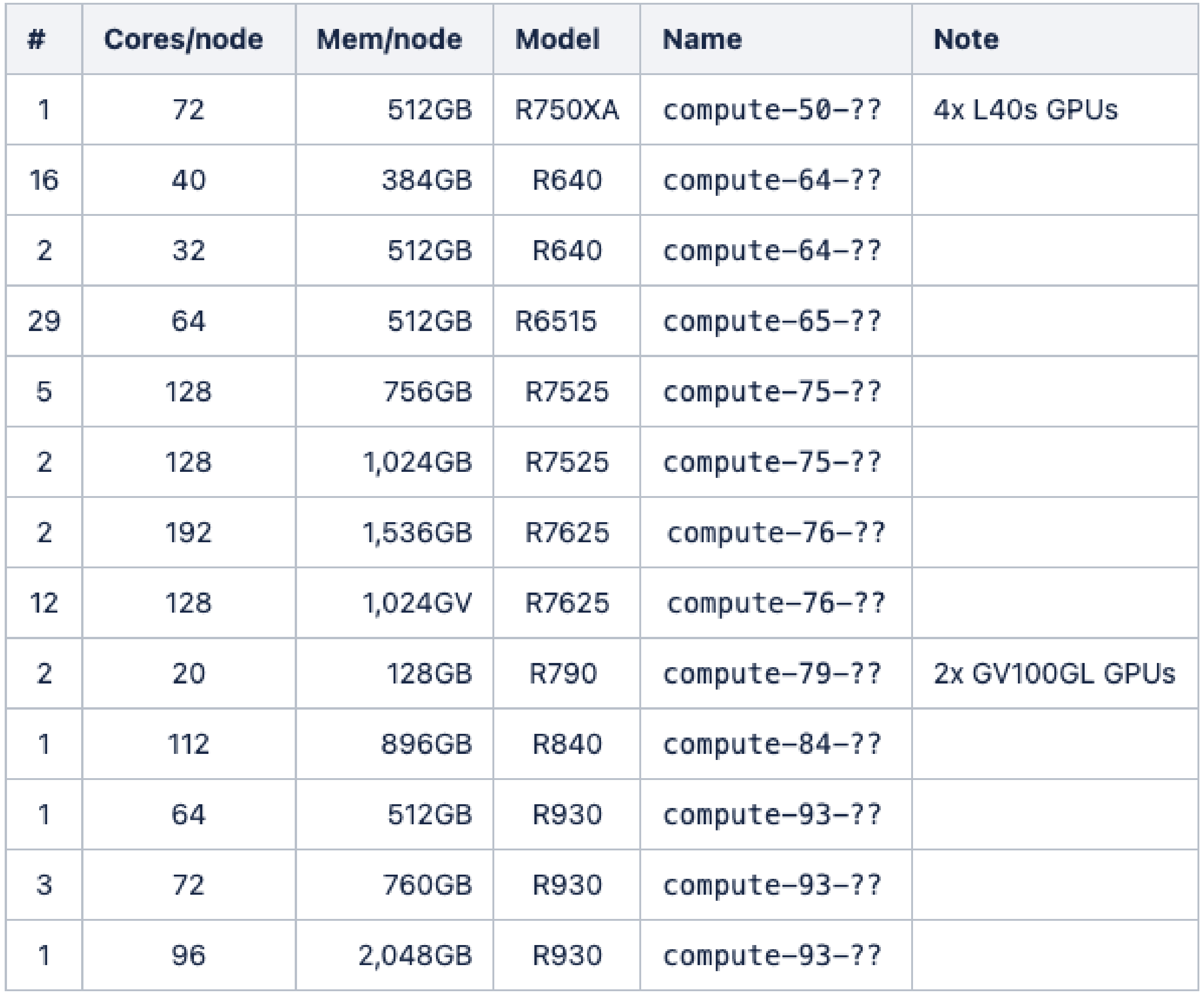


# The Hydra cluster

- Accessible to all Smithsonian researchers
- Must have an SI account and be on the “si-staff” wifi or an SI ethernet connection

# Hardware

- ~70 compute nodes
- ~6,000 CPUs
- 8 GPUs
- 45 TB RAM



| # | Cores/node | Mem/node | Model | Name | Note |
|---|---|---|---|---|---|
| 1 | 72 | 512GB | R750XA | compute-50-?? | 4x L40s GPUs |
| 16 | 40 | 384GB | R640 | compute-64-?? | |
| 2 | 32 | 512GB | R640 | compute-64-?? | |
| 29 | 64 | 512GB | R6515 | compute-65-?? | |
| 5 | 128 | 756GB | R7525 | compute-75-?? | |
| 2 | 128 | 1,024GB | R7525 | compute-75-?? | |
| 2 | 192 | 1,536GB | R7625 | compute-76-?? | |
| 12 | 128 | 1,024GV | R7625 | compute-76-?? | |
| 2 | 20 | 128GB | R790 | compute-79-?? | 2x GV100GL GPUs |
| 1 | 112 | 896GB | R840 | compute-84-?? | |
| 1 | 64 | 512GB | R930 | compute-93-?? | |
| 3 | 72 | 760GB | R930 | compute-93-?? | |
| 1 | 96 | 2,048GB | R930 | compute-93-?? | |

https://confluence.si.edu/display/HPC/Compute+Nodes

# Hydra resources

- Hydra Wiki
  - Login to Hydra
  - Transferring data to/from Hydra
  - Submitting a job
  - Hydra hardware
  - Hydra software
- Hydra Qsub generation tool
- Hydra status

# Hydra file system

| Location | Description | User storage space | Backed up? | Old files deleted? |
|---|---|---|---|---|
| **/home/USER_ID** | Your home directory, for your basic configuration files, scripts and job files | 512 Gb | Yes, every 4 weeks | No |
| **/pool/public/genomics/USER_ID** | For storing large files, fast disk R/W speed, good for analyses | 7.5 Tb | No | Yes, after 180 days |
| **/scratch/public/genomics/USER_ID** | For storing large files, fastest disk R/W speed, best for analyses | 15 Tb | No | Yes, after 180 days |

# Basic Linux commands

| command | description |
|---|---|
| **pwd** | Gives the full file path to your current directory. |
| **ls** | List the files and directories in my current location |
| **ls -l** | Nicer list format |
| **ls -la** | Nicer list format, show hidden files |
| **ls -lah** | Nicer list format, show hidden files, human-readable file sizes |
| **mkdir myNewDirectory** | Make a new directory. Important to avoid spaces or special characters. |
| **cd myNewDirectory** | Move into a directory |
| **cd ..** | Move up one directory |
| **cd /full/path/to/myNewDirectory** | Move to a directory using the full file path |
| **cd ~** | Move to your home directory |
| **touch myNewFile.txt** | Create a new, empty file |
| **nano myNewFile.txt** | Modify a file from the command line using the “nano” text editor |
| **cat my_new_file.txt** | Print the contents of a file to the screen |
| **clear** | Clean up your terminal window |

## USE WITH CAUTION

| command | description |
|---|---|
| **cp myNewFile.txt fileCopy.txt** | Copy a file |
| **cp –rf myNewDirectory directoryCopy** | Copy a directory |
| **mv myNewFile.txt newName.txt** | Rename a file |
| **rm myNewFileCopy.txt** | PERMANENTLY delete a file |
| **rm -r myNewDirectory** | PERMANENTLY delete a directory |

Many more commands:
https://phoenixnap.com/kb/linux-commands-cheat-sheet

# Tips for navigating on the command line

| Shortcut | Description |
|---|---|
| **~** | Your home directory |
| **.** | Your present directory |
| **..** | One directory above your current directory |
| **ctrl + arrow key (PC)**<br>**opt + arrow key (Mac)** | Move the cursor one word left or right |
| **fn + arrow key left (PC)**<br>**ctrl + a (Mac)** | Move the cursor to the beginning of the line. |
| **fn + arrow key right (PC)**<br>**ctrl + e (Mac)** | Move the cursor to the end of the line. |
| **control + c** | Cancel whatever is currently running on the command line |
| **tab** | Autocomplete the path or file name |
| **up and down arrows** | Scroll through your previous commands |
| **exit** | Close your connection to the cluster |