# Joint High Performance Computing Exchange (JHPCE) Cluster Orientation



http://www.jhpce.jhu.edu/

Version: 20240102

### Schedule

- Introductions who are we, who are you?
- Terminology
- Logging in and account setup
- Basics of running programs on the cluster
- Details limits and resources
- Examples



### Who we are:

- JHPCE – Joint High Performance Computing Exchange

- Co-Director: Brian Caffo

- Co-Director: Mark Miller

Systems Engineer: Jiong Yang

Systems Engineer: Jeffrey Tunison

Application Developer: Adi Gherman

- Beyond this class, when you have questions:
  - http://www.jhpce.jhu.edu
    - lots of good FAQ info
    - use the search field
    - these slides
  - bitsupport@lists.johnshopkins.edu
    - System issues (password resets/disk space)
    - Monitored by the 5 people above
  - bithelp@lists.johnshopkins.edu
    - Application issues (R/SAS/perl...)
    - Monitored by dozens of application subject matter experts
    - All volunteers
  - Others in your lab
  - Web Search



# Who are you?

- Name
- Department
- How do you plan on using the cluster? What data or applications will you be using?
- Will you be accessing the cluster from a Mac or a Windows system?
- What is your experience with Unix?
- Any experience using other clusters?



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# Clusters – what and why?

### What is a cluster?

- A collection of many powerful computers (**nodes**) that can be shared with many users.

### Why would you use a cluster?

- Need resources not available on your local laptop
- Need to run a program (job) that will run for a long time
- Need to run a job that can make use of multiple computers simultaneously (parallel computing)
- Want to queue multiple jobs so they run ASAP without needing your attention to launch them (using a job scheduler)



## Node (Computer) Components

- Each computer is called a "node"
- Each node, just like a desktop/laptop has:
  - RAM
  - Intel/AMD CPUs
  - Disk space
- Unlike desktop/laptop systems, nodes do not make use of a connected display/keyboard/mouse they are used over a network, often from a command line interface (CLI) known as a "shell".
- **Graphical user interface** (GUI) programs can be run, displaying on your desktop/laptop.





# The JHPCE cluster components



- Fee for service nodes purchased by various Pls.
- Located at Bayview Colocation Facility (<u>ARCH</u>)

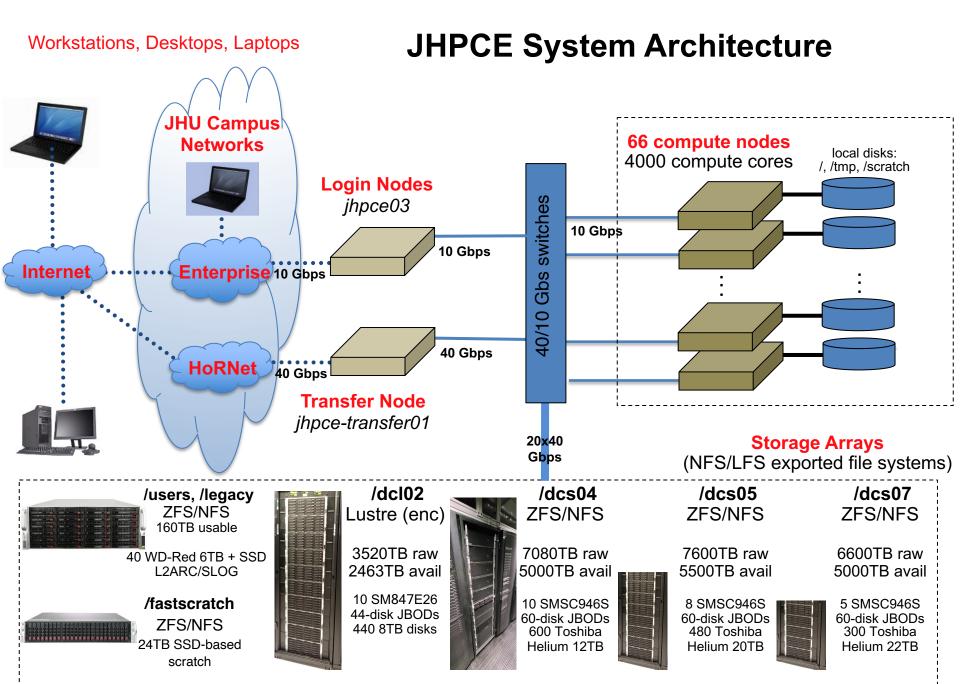


- 12 Racks of equipment 5 compute, 6 storage, 1 infra.
- 70 Nodes 66 compute, 2 transfer, 2 login
  - 4000 Cores Nodes have 2 4 CPUs, 24 to 128 cores per node
  - 30 TB of RAM Nodes ranges from 128 GB to 2048 GB RAM.
  - Range in size from a large pizza box to a long thin shoe box
- 21,000 TB of Disk space 18,000 TB of project storage,
   2000 TB of backup, 500TB of scratch/home/other storage.
  - Storage is network-attached, available to all cluster nodes.

#### Software:

- Based on Rocky Linux 9
- Used for a wide range of Biostatistics gene sequence analysis, population simulations, medical treatment.
- Common applications: R, SAS, Stata, python, Jupyter ...





### JHPCE 3.0

In fall 2023 we upgraded the JHPCE cluster

- from CentOS 7.9 (RHEL 7.9) to Rocky 9.2 (RHEL 9.2).
- Migrated scheduler from SGE (Sun Grid Engine) to SLURM (Simple Linux Utility for Resource Management)

JHPCE web site documentation has not entirely been updated for SLURM.



# SLURM Terminology

- Partitions: The queues used to schedule jobs
- Memory: The amount or RAM your job/program needs
- **CPU/core**: The number of cores your job/program needs



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# How do you use the cluster?

- The JHPCE cluster is accessed using SSH (Secure SHell), so you will need an ssh client.
- Use ssh to login to "jhpce03.jhsph.edu"



For Mac and Linux users, you can use ssh from a Terminal application window.



 For MS Windows users, you need to install an ssh client – such as MobaXterm (strongly recommended) or Cygwin, Putty and Winscp:

http://mobaxterm.mobatek.net/

http://www.chiark.greenend.org.uk/~sgtatham/putty/download.html

http://www.cygwin.com

http://winscp.net

# Quick note about graphical programs

To run graphical programs on the JHPCE cluster, you will need to have an X11 server running on your laptop.



- For Microsoft Windows, MobaXterm has an X server built into it.
- For Windows, if you are using Putty, you will need to install an X server such as Cygwin.



- For Macs:
- 1) You need to have the Xquartz program installed on your laptop. This software is a free download from Apple, and does require you to reboot your laptop <a href="http://xquartz.macosforge.org/landing/">http://xquartz.macosforge.org/landing/</a>
- 2) You need to add the "-X" option to your ssh command:

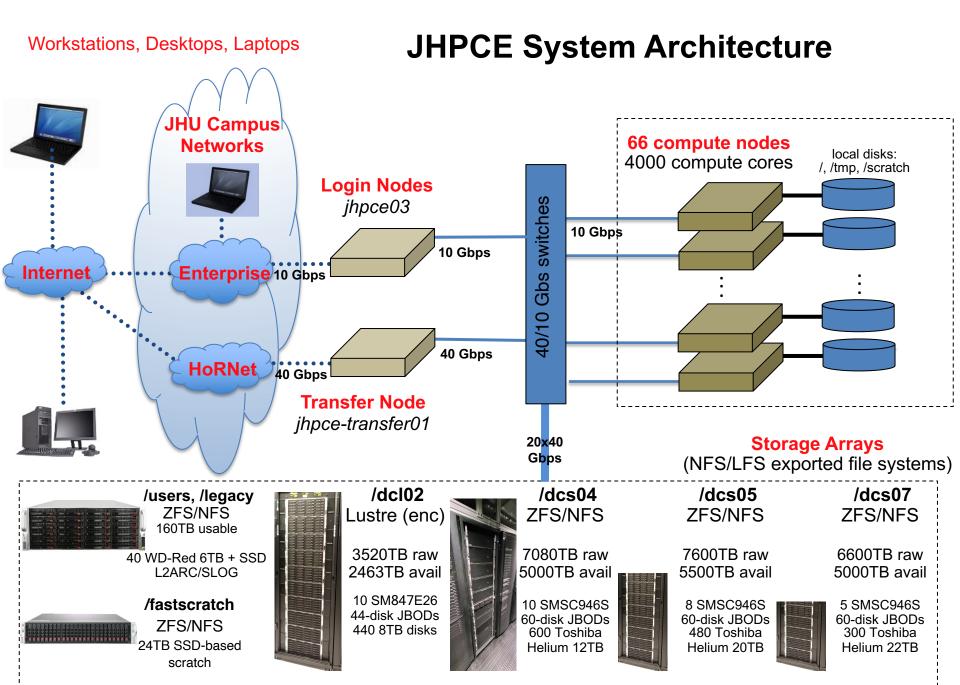
```
$ ssh -X mmill116@jhpce03.jhsph.edu
```



- For Linux laptops, you should already have an X11 server install. You will though need to add the –X option to ssh:

\$ ssh -X mmill116@jhpce03.jhsph.edu





# Example 1 – Logging in



- Bring up Terminal
- Run: ssh -x userin@jhpce03.jhsph.edu
- 2 Factor authentication
  - When you type your password, the cursor will not move. This is a security mechanism so that someone looking over your shoulder won't be able to see your password.
  - The first time you login, you will use the Initial Verification Code and Initial Password sent to you.
  - Google Authenticator will be set up after you login the first time
  - Going forward you'll use Google Authenticator when prompted for "Verification Code"
- Shell prompt



# Lab 1 - Logging In

### - For Mac/Linux laptop Users:

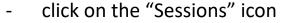
- Bring up a Terminal
- Run: ssh -X USERID@jhpce03.jhsph.edu
- Login with the initial Verification Code and Password that were sent to you

### For PC Users:

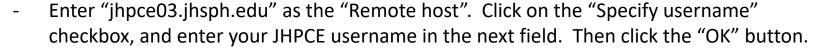
Launch MobaXterm







On the "Session settings" screen, click on "SSH"



in the upper left corner

- Login with the initial Verification Code and Password that were sent to you.
- If dialog windows pop up, click "Cancel" when prompted for another Verification Code, or click "No" or "Do not ask this again" when prompted to save your password.



# Lab 1 - Logging In - cont

- Change your password with the "kpasswd" command. You will be prompted for your current (initial) password, and then prompted for a new password.

### - Setup 2 factor authentication

- http://jhpce.jhu.edu/knowledge-base/how-to/2-factor-authentication/
- 1) On your smartphone, bring up the "Google Authenticator" app
- 2) On the JHPCE cluster, run "auth util"
- 3) In "auth\_util", use option "5" to display the QR code (you may need to resize your ssh window "view->terminal unzoom" in MobaXterm)
- 4) Scan the QR code with the Google Authenticator app. You should see a 6 digit number with a "jhpce" title in the Google Authenticator app.



# Lab 1 - Logging In - cont

5) Next, in "auth\_util" use option 2 to display your Scratch Codes

You should record these Scratch Codes in a file for now, but print them out or store them in an encrypted file on your laptop. Don't keep them in an unencrypted file on your laptop.

Normally when logging in you will use the 6 digit number from the Google Authenticator app on your phone when prompted for "Verification Code:" during the login process. But if you don't have access to your phone, you can use one of these Scratch Codes. Each code is good for one login, so if you have these printed on a sheet of paper, you would scratch it off of the list once you use it.

The most frequent time we see these needed is when someone either breaks or trades in their phone, and they don't have Google Authenticator set up on their old phone. You would need to use one of these Scratch Codes to login to the cluster, and follow steps 1-4 above to set up the Google Authenticator app on your new phone.

- 6) In " auth\_util", use option "6" to exit from "auth\_util"
- Log out of the cluster by typing "exit".
- Log into the cluster again with 2 factor authentication



# Lab 1 - Logging In - cont

- 100 GB limit on home directory. Home directories are backed up, but other storage areas are probably not.
- 1 TB of intermediate "fastscratch" storage for temporary storage (less than 30 days)

https://jhpce.jhu.edu/knowledge-base/fastscratch-space-on-jhpce https://jhpce.jhu.edu/policies/current-storage-offerings

(optional) Setup ssh keys

https://jhpce.jhu.edu/knowledge-base/authentication/ssh-key-setup https://jhpce.jhu.edu/knowledge-base/mobaxterm-configuration



## General Linux/Unix Commands 💍



#### Navigating Unix: Commands in example script:

- ls
- ls -1
- ls -al
- pwd
- cd
- . and ..

- date
- echo
- hostname
- sleep
- control-C

### Looking at files: Changing files with editors:

- more/less

nano

- vi/emacs

#### Good resources for learning Linux:

http://korflab.ucdavis.edu/Unix and Perl/unix and perl v3.1.1.html https://www.digitalocean.com/community/tutorials/a-linux-command-line-primer https://files.fosswire.com/2007/08/fwunixref.pdf



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#### Unix/Linux Command Reference



#### File Commands

ls - directory listing **ls -al** - formatted listing with hidden files cd dir - change directory to dir cd - change to home pwd - show current directory mkdir dir - create a directory dir rm file - delete file

rm -r dir - delete directory dir

rm -f file - force remove file rm -rf dir - force remove directory dir \*

cp file1 file2 - copy file1 to file2 cp -r dir1 dir2 - copy dir1 to dir2; create dir2 if it doesn't exist

mv file1 file2 - rename or move file1 to file2 if file2 is an existing directory, moves file1 into directory file2

In -s file link - create symbolic link link to file touch file - create or update file cat > file - places standard input into file

more file - output the contents of file head file - output the first 10 lines of file

tail file - output the last 10 lines of file tail -f file - output the contents of file as it grows, starting with the last 10 lines

#### **Process Management**

ps - display your currently active processes top - display all running processes kill pid - kill process id pid killall proc - kill all processes named proc \* ba - lists stopped or background jobs: resume a stopped job in the background fq - brings the most recent job to foreground **fg** n - brings job n to the foreground

#### **File Permissions**

**chmod** octal file - change the permissions of file to octal, which can be found separately for user. group, and world by adding:

- 4 read (r)
- 2 write (w) • 1 - execute (x)

Examples:

chmod 777 - read, write, execute for all chmod 755 - rwx for owner, rx for group and world For more options, see man chmod.

#### SSH

ssh user@host - connect to host as user ssh -p port user@host - connect to host on port ssh-copy-id user@host - add your key to host for

#### user to enable a keyed or passwordless login Searching

grep pattern files - search for pattern in files grep -r pattern dir - search recursively for pattern in dir

command | grep pattern - search for pattern in the output of command

locate file - find all instances of file

#### System Info

date - show the current date and time cal - show this month's calendar uptime - show current uptime w - display who is online whoami - who you are logged in as finger user - display information about user uname -a - show kernel information cat /proc/cpuinfo - cpu information cat /proc/meminfo - memory information man command - show the manual for command df - show disk usage du - show directory space usage **free** - show memory and swap usage whereis app - show possible locations of app which app - show which app will be run by default

#### Compression

tar cf file.tar files - create a tar named file.tar containing files tar xf file.tar - extract the files from file.tar tar czf file.tar.gz files - create a tar with Gzip compression tar xzf file.tar.gz - extract a tar using Gzip tar cjf file.tar.bz2 - create a tar with Bzip2 compression tar xjf file.tar.bz2 - extract a tar using Bzip2 qzip file - compresses file and renames it to file.az gzip -d file.gz - decompresses file.gz back to file

#### Network

ping host - ping host and output results whois domain - get whois information for domain dig domain - get DNS information for domain dia -x host - reverse lookup host waet file - download file wget -c file - continue a stopped download

#### Installation

Install from source: ./configure make make install dpkg -i pkg.deb - install a package (Debian) rpm -Uvh pkq.rpm - install a package (RPM)

#### **Shortcuts**

Ctrl+C - halts the current command Ctrl+Z - stops the current command, resume with fg in the foreground or bg in the background Ctrl+D - log out of current session, similar to exit Ctrl+W - erases one word in the current line Ctrl+U - erases the whole line Ctrl+R - type to bring up a recent command !! - repeats the last command exit - log out of current session

\* use with extreme caution.

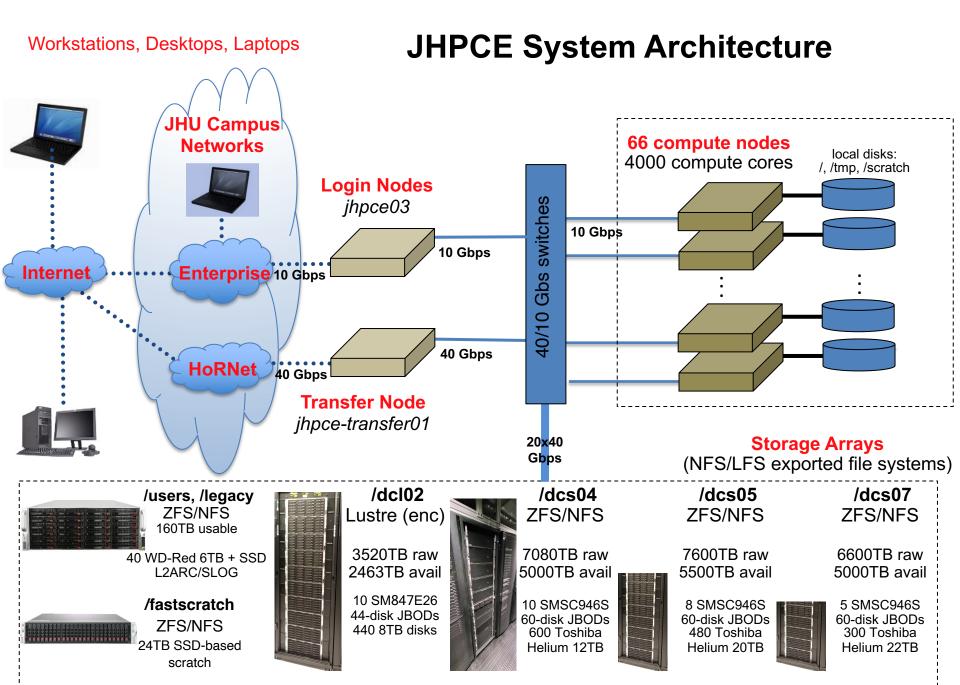




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# Primary Commands – SLURM (Simple Linux Utility for Resource Management)

- sbatch submit a batch job to the cluster
- srun --pty --x11 bash establish an interactive session
- scancel cancel or pause a job
- squeue see the status of running & pending jobs
- sacct see the status of past (& running) jobs
- sinfo see status of the compute nodes
- sstat see statistics from running jobs
- qmem show summary of RAM usage for running jobs
- slurmpic show table of compute node usage



# Lab 2 - Using the SLURM cluster

Example 2a – using an batch session

```
cd class-scripts
sbatch script1
squeue --me
sstat -j JOBID
```

examine results file with the more command more slurm-JOBID.out

**Example 2b** – submitting a **interactive** job

```
srun --pty --x11 bash
cd class-scripts
bash script1
```

Note that output is displayed on the screen rather than saved in a file



### Difference between Batch and Interactive

#### **Batch Jobs:**

- Running long-running jobs
- Batch Jobs continue to run even if you log off or get disconnected from the cluster

#### Interactive Sessions:

- Running short jobs
- Writing and debugging programs
- Running test on subset of data prior to submitting longrunning batch job on full dataset
- Running graphical programs
- An interactive session ends and your jobs is terminated if your connection to the cluster is disconnected (laptop reboot, network drops)
  - any unsaved changes may be lost
  - programs will be terminated and may leave truncated results



### Modules

Modules are sets of configuration information which change your environment to suite a particular software package.

We have modules for R, SAS, Mathematica, python, . . .

- module list
- module avail
- module avail stata
- module load
- module unload
- module describe



# Never run a job on the login node!

Login nodes have many fewer resources than the compute nodes. They are a shared resource.

- Always use "sbatch" or "srun" to make use of the compute nodes
- Jobs that are found running on the login node may be killed at will
- If you are going to be compiling programs, do so on a compute node via srun.
- Even something as simple as copying large files should be done via srun or sbatch



### Useful Slurm commands

### squeue - shows information about running & pending jobs

```
squeue # defaults to all jobs for all users
squeue --me -t r,pd # just my running & pending jobs
```

### sstat – shows detailed information about running jobs

```
sstat -j JOBID
sstat --helpformat # lists avail info fields
```

### sacct - shows information about completed jobs

```
sacct -j JOBID
sacct --helpformat # lists avail info fields
sacct --units=M -j JOBID -o JobID, JobName, MaxVMSize, Elapsed, TotalCPU
```

### scance1 – deletes your job (you can also can pause them)

scancel JOBID



### Summary of SLURM Commands

- sbatch submit a <u>batch</u> job to the cluster
- srun --pty --x11 bash establish an interactive session
- scancel cancel or pause a job
- squeue see the status of running & pending jobs
- sacct see the status of past (& running) jobs
- sstat see statistics from running jobs
- sinfo see status of the compute nodes

### Helpful scripts we have written:

- qmem show summary of RAM usage for running jobs
- slurmpic show table of compute node usage



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# Requesting additional RAM

- By default, when you submit a job with sbatch, or run srun, you are allotted 5GB of RAM and 1 core for your job.
- You can request more RAM by setting the "--mem" or "--mem-per-cpu" options
  - --mem: memory per node (for all cores used)
  - -mem-per-cpu: memory per core (harder to accurately estimate)

### - Examples:

```
sbatch --mem=10G job1.sh
Of
srun --mem-per-cpu=5G --cpus-per-task=2 --pty --x11 bash
```



# Estimating RAM usage

- No easy formula. Running an example job best.
- A good place to start is the size of the files you will be reading in. Add a bit extra, as a starting point.
- You can run sacct to gather info on a completed job:

sacct -o JobID, JobName, ReqTRES%40, MaxVMSize, MAXRSS, State%20 -j JOBID



# Requesting additional Cores

- By default, when you submit a job with sbatch, or run srun, you are allotted 5GB of RAM and 1 core for your job.
- You can request more cores with the --cpus-per-task option to sbatch and srun.
- Examples:

```
sbatch --cpus-per-task=4 job1.sh
Of
srun --mem=10G --cpus-per-task=6 --pty --x11 bash
```



# Types of parallelism on JHPCE

- 1. Embarrassingly (obviously) parallel ... <a href="http://en.wikipedia.org/wiki/Embarrassingly parallel">http://en.wikipedia.org/wiki/Embarrassingly parallel</a>
- 2. Multi-core (or multi-threaded) a single job using multiple CPU cores via program threads on a single machine (cluster node). Also see discussion of fine-grained vs coarse-grained parallelism at <a href="http://en.wikipedia.org/wiki/Parallel computing">http://en.wikipedia.org/wiki/Parallel computing</a>



### Email notification on sbatch job completion

 Rather than checking on your long-running job from time to, you can add options to sbatch to receive an email when your job completes or fails by adding the mail-type and mail-user options:

```
$ sbatch --mail-type=FAIL,END --mail-user=john@jhu.edu script2
```

- Note that email notification is a great option for a **handful** of long running jobs. This is a **horrible** option for 1000s of jobs, and has caused users to have their email accounts suspended as it has appeared that they were getting spammed.



### Supplying options to your sbatch job

- You can supply SLURM directives to sbatch in 4 ways:
- Order of precedence:
  - 1. On the command line

```
\$ sbatch --mem=10G --cpus-per-task=6 --mail-type=FAIL,END --mail-user=john@jhu.edu script2
```

- 2. Environment variable
- 3. Embedding them in your batch job script
  Lines which start with "#SBATCH" are interpreted as options to sbatch. Such lines must:
  - start at the very beginning of a line
  - come <u>after</u> the interpreter line #!/bin/bash
  - come <u>before</u> any commands
  - There is an example in the class-scripts directory:

```
[login-31 /users/mmill116/class-scripts]$ more script1-resource-request
#!/bin/bash
#
#SBATCH --mem=10G
#SBATCH --cpus-per-task=6
#SBATCH --mail-type=FAIL,END
#SBATCH --mail-user=marcus@jhu.edu

date
. . .
```



### Supplying options to your sbatch job (cont'd)

#### 4. In your ~/.slurm/defaults file

```
Syntax is: [<command>:][<cluster>:] <option> = <value>
Where [ ] indicates an optional argument
Command can be one of (at least): srun, sbatch, salloc
(But perhaps other commands also refer to the file.)
You need to specify an asterisk in between colons
We have not tested blank or commented lines.
```

#### Example contents:

```
mem=2GB
mail-user=franksmith@jh.edu
srun:*:partition=debug
sbatch:*:mail-type=FAIL,END
```



# "How many jobs can I run?"

If you anticipate the need to submit more than 1,000 jobs, please email us at <a href="mailto:bitsupport@lists.jhu.edu">bitsupport@lists.jhu.edu</a> as there are mechanisms and strategies for efficiently handling 1000s of jobs using array jobs.

More importantly, we impose a per-user limit on the number of cores and RAM for running jobs on the shared queue. Currently, the limit is set to **100 cores per user** and **1024GB of RAM per user**.

So, if a user submits 1,000 single-core jobs, the first 100 will begin immediately (assuming the cluster has 100 cores available on the shared queue), and the rest will remain in the 'PD' state until the first 100 jobs start to finish. As jobs complete, the cluster will start running 'PD' jobs, and keep the number of running jobs at 100.

Similarly, if a user's job requests 100GB of RAM to run, the user would only be able to run 10 jobs before hitting their 1024 GB limit, and subsequent jobs would remain in 'qw' state until running jobs completed.

The maximum number of slots per user may be temporarily increased by submitting a request to <a href="mailto:bitsupport@lists.jhu.edu">bitsupport@lists.jhu.edu</a>. We will increase the limit, depending on the availability of cluster resources. There are also dedicated queues for stakeholders which may have custom configurations and limits.



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### Lab 3

# R

#### Running R on the cluster:

- In \$HOME/class-scripts/R-demo, note 2 files — Script file and R file

- Submit Script file
  - sbatch plot1.sh
- Run R commands interactively
  - srun --pty --x11 bash
  - module load R
  - R --no-save -f plot1.r
- Look at pdf from example 4 via xpdf



# Lab 4 – Transfering data

Data can be transferred to and from the cluster through the transfer node using sftp. To use the text version of sftp you would run the following **from your local laptop or desktop**:

```
$ sftp mmill116@jhpce-transfer01.jhsph.edu
```

Login with the came credentials used for ssh. From within the "sftp" session, you can use "ls" and "cd" commands as well as "get" and "put" to upload/download files.

```
sftp> cd class-scripts/R-demo
sftp> ls
plot1.r plot1-R-results.pdf plot1.r.Rout plot1.sh slurm-1344981.out
sffp> get plot1-R-results.pdf
```

Once you have the file on your laptop, you can look at it with the PDFviewer on your laptop.

You can also use graphical sftp programs like Cyberduck on Mac or MobaXterm on Windows. From within the JHPCE cluster, you can access the transfer node by running:

```
$ srun --pty --partition=transfer bash
```

This can be used if you need to download large files from the internet or some external source to the JHPCE cluster (wget, curl, git clone).

More info on transferring files on JHPCE can be found at:

https://jhpce.jhu.edu/knowledge-base/file-transfer/

https://jhpce.jhu.edu/knowledge-base/file-transfer/mobaxterm-file-transfers/

https://www.digitalocean.com/community/tutorials/how-to-use-sftp-to-securely-transfer-files-with-a-remote-server



### Lab 5

### Running RStudio

#### - X Windows Setup

- For Windows, MobaXterm has an X server built into it
- For Mac, you need to have the Xquartz program installed (which requires a reboot), and you need to add the "-X" option to ssh:

```
$ ssh -X yourusername@jhpce03.jhsph.edu
```

#### - Start up Rstudio

```
$ srun --pty --x11 --mem=10G bash
$ module load R
$ module load rstudio
$ rstudio
$ exit # log out of your srun session
```



# Lab 6 – Running Stata



#### **Batch:**

```
$ cd $HOME/class-scripts/stata-demo
$ ls
$ less stata-demo1.sh  # see contents of the batch script
$ cat stata-demo1.do  # see contents of the stata program
$ sbatch stata-demo1.sh
$ cat stata-demo1.log  # see the output
```

#### Interactive:

```
$ srun --pty --x11 --cpus-per-task=4 bash
$ module load stata
$ stata-mp
or
$ xstata-mp # starts the GUI interface
```

#### Notes:

- The program and script do not need to be named the same, but it is good practice to keep them the same when possible.
- File extensions are sometimes meaningful in Linux. SAS doesn't care, but Stata programs need to have ".do" as the extension. It is good practice for human readability.
- By default "stata" runs a single thread. For faster results when running on real data, request 2 or more cores and use the command "stata-mp" instead of "stata"
- By default stata stores temporary files in /tmp. You may need to define an environmental variable to avoid job failure due to lack of space. export STATATMP=\$HOME



# Lab 7 – Running SAS



#### - SAS example:

#### Batch:

```
$ cd $HOME/class-scripts/SAS-demo
$ ls
$ cat sas-demo1.sh
$ cat class-info.sas
$ sbatch sas-demo1.sh
```

#### Interactive:



## Other Queues/Partitions

- "shared" queue default queue
- "dedicated" queues Queues that are for PIs who have purchased nodes on the cluster.
- "transfer" partition
  - srun --pty --x11 -p transfer bash
    (jhpce-transfer01.jhsph.edu)
- "sas" partition
  - srun --pty --x11 -p sas bash
- "gpu" partition
  - srun --pty --x11 -p gpu bash



# Summary

#### Review

- Get familiar with Linux
- Use ssh to connect to JHPCE cluster
- Use rsun and sbatch to submit jobs
- Never run jobs on the login nodes
- Helpful resources
  - http://www.jhpce.jhu.edu/
  - <u>bitsupport@lists.johnshopkins.edu</u> System issues
  - <u>bithelp@lists.johnshopkins.edu</u> Application issues

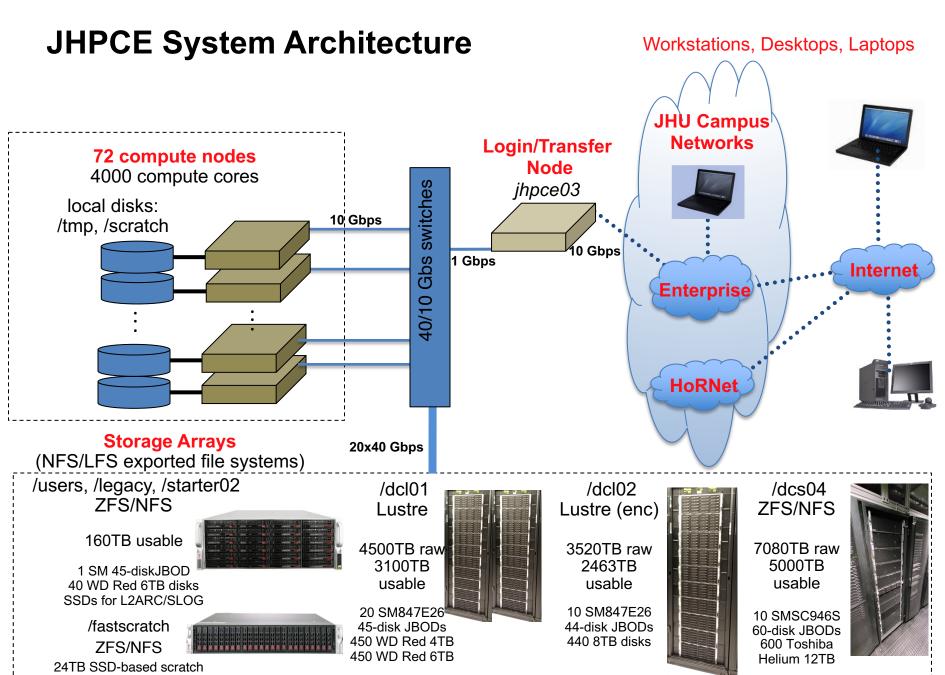
#### What to do next

- Make note of your Google Authenticator scratch codes (option 2 in "auth\_util")
- Set up ssh keys if you will be accessing the cluster frequently <a href="https://jhpce.jhu.edu/knowledge-base/authentication/login/">https://jhpce.jhu.edu/knowledge-base/authentication/login/</a>
- Play nice with others this is a shared community-supported system.



# Thanks for attending! Questions?





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