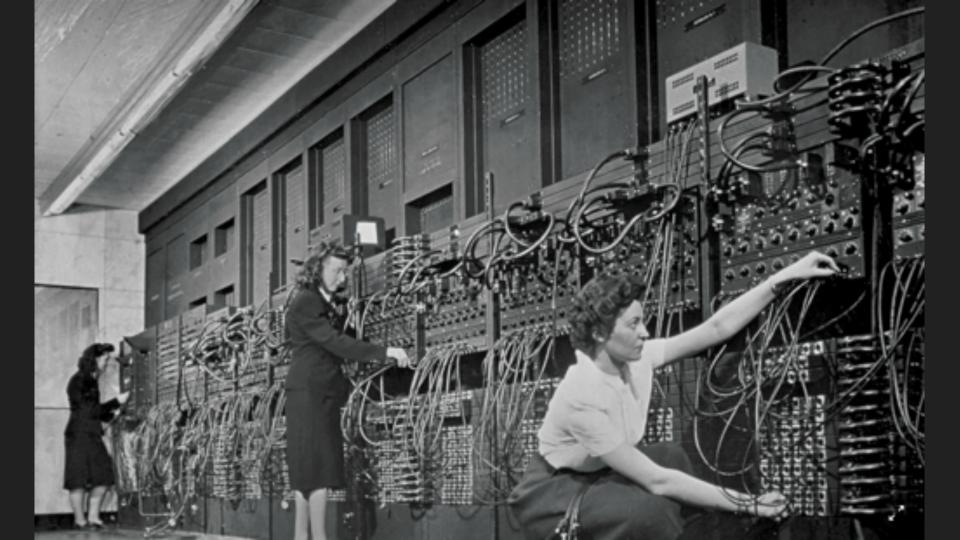


What is a super computer?

- AKA High Performance Computing (HPC) cluster
- AKA a cluster or clustered computing or a grid or process server
- A collection of computing resources working together as one!
- Kind of like having a bunch of computers that you can control from a single interface.



Important Terminology

Node: a computing unit that is comprised of a CPU, RAM, and maybe GPU

- Like a single computer
- Different nodes might have different specs

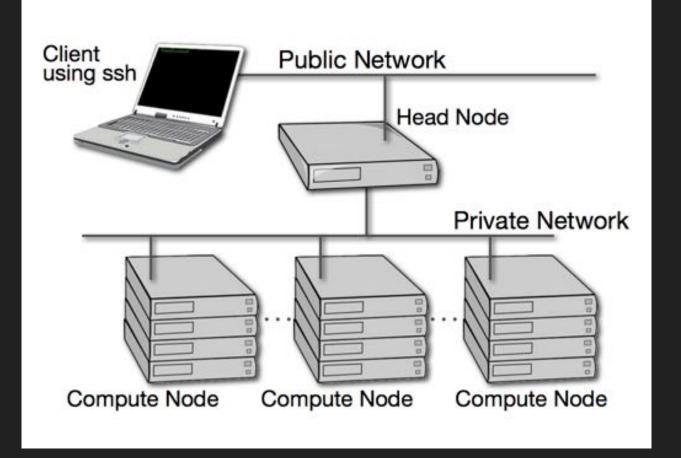
Head node: Where you (and everyone else) login & submit jobs from

- Master node that decides which node jobs are submitted to
- Shared resource, so DON'T run any jobs here

Job: A single process or script or program that you want to run on a node

- Can be comprised of subprocesses
- must run with no interaction (more on this later)

Important Terminology



Pros

More processing power >= Sum of it's parts!



- Parallel and distributed processing (a lot of data all at once).
- High specification nodes (e.g. nodes with crazy amounts of RAM)

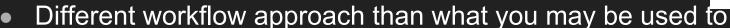
Centralized data that is maintained and backed up

Sign in from anywhere

Potentially free!

Cons

Requires grid commands to harness parallelization

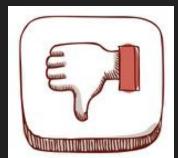


A little bit of a learning curve

No virtual desktop environment (no VNC) or SMB

- Requires comfort with the terminal/command line
- But there are some work around for graphic user interface

Requires some level of conscientious use





Getting started

Find the right HPC for you, and get an allocation:

http://hpcc.umd.edu/

https://oacs.umd.edu/oacs-cloud/bsoshigh-performance-computing-cluster

You might need to have certain affiliations for different clusters



Getting started

Figure out the node specifications you need for your processing:

http://hpcc.umd.edu/

https://oacs.umd.edu/facilities/bswifthigh-performance-computing-clusterspecifications

Different nodes have different specifications. If you need really high specs, you might have to wait.

Getting started: Find your specs

The following table lists the hardware on the Deepthought2 cluster:

Description	Processor	Number of nodes	Cores/node	Memory/node GB	-	Scratch space per node, GB	GPUs/node	Interconnect
C8220	Ivy Bridge, 2.8 GHz	444	20	128	6.4	750	0	FDR Infiniband
C8220X	Ivy Bridge, 2.8 GHz	40	20	128	6.4	750	2	FDR Infiniband
Poweredge R820	Ivy Bridge, 2.2 GHz	4	40	1024	25.6	750	0	FDR Infiniband

All of the nodes except for the 1 TB RAM nodes have dual Intel by Bridge E5-2680v2 processors running at 2.80 GHz. Memory is DDR3 at 1866 MHz.

The 1 TB RAM nodes require a different processor in order to support that much memory. These have quad Intel Xeon Ivy Bridge E5-4640v2 processors running at 2.20 GHz. The memory is DDR3 at 1333 MHz in these nodes.

The nodes containing GPUs have dual Nvidia Tesla K20m (GK110GL) GPUs (supporting Cuda compute capability 3.5).

The cluster has over 1 PB of file storage, and has FDR infiniband interconnects between the nodes with a theoretical maximum throughput of about 56 Gb/s.

- Compute Nodes
 - 40 compute nodes (760 cores)
 - compute-4-1 to compute-4-30:
 - Dual Intel X5650 6C 2.66GHz 12MB cache 1333MHz 95w processors
 - 24 GB RAM
 - 250 GB 7200 RPM 3.5"SATA II storage (single drive)
 - compute-4-31 to compute-4-33 and compute-5-1 to compute-5-7:
 - Dual Intel E5-2680v2 10C 2T 2.80GHz 25MB cache 115w processors
 - 256 GB RAM (compute-5-1 to compute-5-7 have additional 1.0 TB NVRAM via NVMe Solid-State Drives (Sa 960))
 - 1 TB 7200 RPM 3.5" SATA III storage (single drive)
 - GPU slots (only one GPU installed on compute-4-33: NVIDIA TESLA M2090 (6GB, GDDR5, 1.8GHz PCI-ex1)
 - Infiniband via Mellanox Connect X-3 VPI Single-port QSFP QDR IB/10GbE PCI-E 3.0 HCA
 - Redundant power supply
- Login Node (login.bswift.umd.edu)
 - Dual Intel X5650 6C 2.66GHz 12MB cache 1333MHz 95w processors
 - 48 GB RAM
 - Dual 500GB 7200 NL SATA 2.5" SFF Slim-HS HDD (RAID 1 at root partition) via on board RAID controller.
 - Infiniband via Mellanox Connect X-3 VPI Single-port QSFP QDR IB/10GbE PCI-E 3.0 HCA
 - 10 Gb Ethernet via Chelseo T420-CR (SFP+) dual-port 10GbE PCI-E 3.0 HCA

Getting started: connecting to your server

Once you have an account, you can shell in through a terminal; for example:

```
ssh jmerch@login.bswift.umd.edu
ssh <user name>@<server address>
```

Enter your password when prompted

Now you're on the head node of the HPC, where you can run basic commands, explore the directory structure, and submit jobs

Do NOT run big jobs on the head node

Getting started: connecting to your server

Last login: Thu Feb 28 18:52:38 on ttys888 training5s-HBP:- junaid\$ ssh -Y jmerch@login.bswift.umd.edu

* * * VARNING * * *

Unauthorized access to this computer is in violation of Md. Annotated Code. Criminal Law Article sections 8-606 and 7-302 and the Computer Fraud and Abuse Act, 18 U.S.C. sections 1838 et seg. The University may monitor use of its computing resources as permitted by state and federal law, including the Electronic Communications Privacy Act. 18 U.S.C. sections 2518-2521 and the Md. Annotated Code. Courts and Judicial Proceedings Article, Section 18, Subtitle 4. Anyone using this system acknowledges that all use is subject to University of Maryland Policy on the Acceptable Use of Information Technology Resources available at http://www.umd.edu/aup.

By logging in I acknowledge and agree to all terms and conditions regarding my access and the information contained therein.

To report problems or request assistance call the Help Desk at 301-405-1500

Password: P



Getting started: connecting to your server

```
* * * WARNING * * *
   Unauthorized access to this computer is in violation of Md.
   Annotated Code, Criminal Law Article sections 8-686 and 7-382 and the
   Computer Fraud and Abuse Act, 18 U.S.C. sections 1838 et seg. The University
   may monitor use of its computing resources as permitted by state
   and federal law, including the Electronic Communications Privacy Act,
   18 U.S.C. sections 2518-2521 and the Md. Annotated Code, Courts and Judicial
   Proceedings Article, Section 10, Subtitle 4. Anyone using this system
   acknowledges that all use is subject to University of Maryland Policy
   on the Acceptable Use of Information Technology Resources available at
   http://www.uad.edu/aup.
   By logging in I acknowledge and agree to all terms and conditions
   regarding my access and the information contained therein.
To report problems or request assistance call the Help Desk at 301-405-1500
Password:
Warning: No xauth data: using fake authentication data for X11 forwarding.
DISPLAY is login-1.bswift.umd.edu:21.8
login-1:-:
login-1:-:
login-1:-:
```

Getting started

More help on getting started:

https://oacs.umd.edu/facilities/getting-started-bswift

I cannot do a comprehensive tutorial of bash commands, so you'll have to do your homework on that end, or HPC will not work out for you.

However, there are plenty of good guides if you're unfamiliar with bash:

https://lifehacker.com/a-command-line-primer-for-beginners-5633909

http://swcarpentry.github.io/shell-novice/

Alternatively, if you are more familiar with another programming language, you can shell in, load your preferred flavor of python, for example, and work in that language. I'm more proficient at bash, so I'll be showing you everything in bash.

Here are a list of commands to get familiar with to get started:

- Is list; list items in current directory if no other options are given.
- cd change directory; change your current working directory.
- mkdir make directory; create a new directory
- cp copy; you can copy files or directories with this command.
- mv move; you can move files or directories with this command.
- pwd present working directory; find out what directory you are in.
- rm remove; delete files or folders.

Here are a list of commands to get familiar with to get started:

- for for loops; really useful! (We'll look at a for loop later as a way of submitting a bunch of job files)
- if/then if-then statements really useful for bash scripting!
- tar compress/archive files or folders; really useful for copying files to/from HPC (really speeds up transfers). To compress and archive an entire directory:

tar -zcvf /path/to/create/Folder.tar.gz /path/to/folder/

Here are a list of commands to get familiar with to get started:

scp – secure copy; copy files to/from the HPC server.

You can use FileZilla for a graphical interface transfer: https://filezilla-project.org/, but I've occasionally gotten corrupted files using FileZilla.

Here are a list of commands to get familiar with to get started:

nano – Command line text editor. There are others, but this is the easiest to use. This will allow you to easily create new scripts, or edit existing ones without having to copy the scripts/code/text files back and forth to/from HPC.

To create a new script in your current directory:

nano NewScript.sh

And enter or copy/paste in whatever code you want. Hit control+x to exit, and type 'y' to save the edits.

Getting started: Software

MRI analysis software: MATLAB and SPM (and whatever related toolboxes you upload), FSL, AFNI, FreeSurfer, ANTS etc.

All basic Linux/Unix bash commands

Other languages/software: Python, R, Perl, code compilers, containers and literally 100s more applications

For a full list: https://www.glue.umd.edu/hpcc/help/software.html

Or, you can type the following to get the full list: module avail

Getting started: Software

```
logim-1:-: module sysil
                                     ...../usr/local/Modules/verstons
3.2.10
             3.2.9
                           3.2.9+flavours
                                    ····· /usr/local/Modules/3.2.18/aodulefiles ·····
          module-git module-info modules
                                                      use.own
                         ...../cell_root/system/common/modulefiles/sys
BESST/2.1
                                                               leveldb/1.18
                                                              libdatrie/0.2.12/gnu/4.9.3
BESST/2.2.6
GapCloser/1.12-r6
                                                               libdatrie/gnu/4.9.3/8.2.12
R/3.0.3
                                                              libdatrie/hold
R/3.1.2
                                                               libint/2.4.2/gnu/6.1.8/nosiad/openap
R/3.2.2
                                                               libint/gnu/6.1.8/nosimd/openmp/2.4.2
R/3.3.2
                                                               liboglytewer/2.6.3
8/3.5.1
                                                               libreoffice/3.3
RAxML/8.1.22/hybrid/avx
                                                               libreoffice/5.1.3
RAxML/8.1.22/hybrid/sse3
                                                               librs/3.1.0
RAxML/8.1.22/ap1/avx
                                                              11bsx/2.84
RAxML/8.1.22/sp1/sse3
                                                              libsc/4.2.3/gmu/6.1.0
                                                               libic/gnu/6.1.8/4.2.3
RAxML/8.1.22/pthreads/avx
RAxML/8.1.22/pthreads/sse3
                                                              11ge/20120612
50#Pdenovo/2.84-r248
                                                               lis/7.1rp7/eswf/5.2.8rp3
acigs/staff
                                                               lis/7.1rp7/intelspi-st
afm1/16.0.00
                                                              11s/7.1rp7/nomp1
afm1/17.2.10
                                                              11vs/4.0.1
agalma/0.5.0/python/2.7.0
                                                              IncRMAp1pe/1.0.7
ags1ss/1.0.0
                                                               154/1.7.5
```

Getting started: Software

Now, unlike your personal workstation, the software is not ready to run.

You have to load it first using the following command:

```
module load <application name>
```

Make sure you type the application name exactly how it's specified in module list.

If there are multiple versions available, make sure you specify. For example:

```
module load matlab/2018b
```

Now you can launch the application by typing the name of the software or use this in your job submission code!

SLURM



SLURM

Simple Linux Utility for Resource Management (SLURM)

Workload manger, job scheduler, & queuing system for running processes on an HPC

Figures out what specifications you need, finds the available node that meets the requirements, and allocates your job to that node!

Runs multiple jobs in parallel at once.

Use in conjunction with the job script you want to run

https://slurm.schedmd.com/quickstart.html

SLURM Commands: sbatch

sbatch – probably the most important thing in this entire presentation

Allows you to submit a job to the appropriate node

Use with job script for whatever sort of process you want to run

Things you absolutely MUST specify when using sbatch to submit a job:

- # of Nodes
- Amount of RAM
- Time to process the job

You can specify a lot of other things: https://slurm.schedmd.com/sbatch.html

SLURM Commands: sbatch

sbatch https://slurm.schedmd.com/sbatch.html

Usage: sbatch [options] <job script>

For example: sbatch RunSimulation.sh

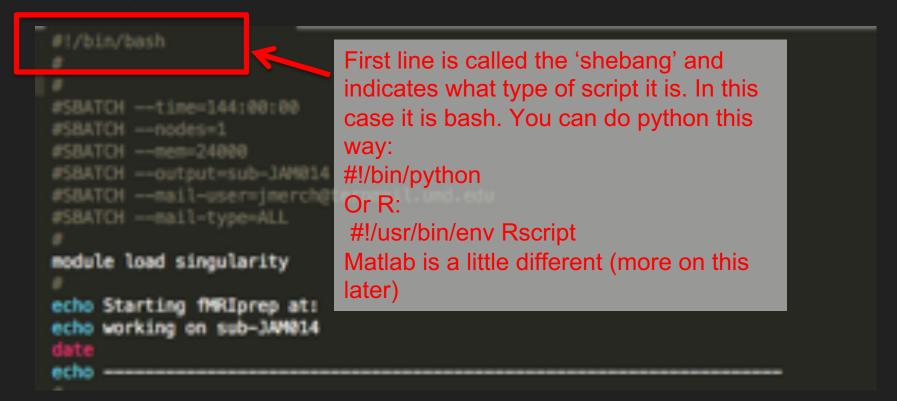
This will give you a job number that you can check in on later

```
[login-1:~: sbatch example.sh
Submitted batch job 82581
login-1:~:
```

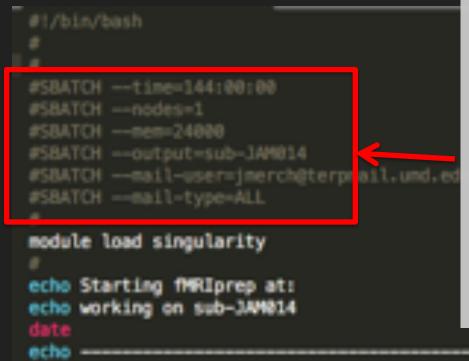
Before going too much further, we should look inside a job script

```
#1/bin/bash
#SBATCH --time=144:00:00
#SBATCH --nodes=1
#SBATCH ---mem=24000
#SBATCH ---output-sub-JAM014
#SBATCH --mail-user=jmerch@terpmail.umd.edu
#SBATCH --mail-type=ALL
module load singularity
echo Starting fMRIprep at:
echo working on sub-JAM814
```

Before going too much further, we should look inside a job script



Before going too much further, we should

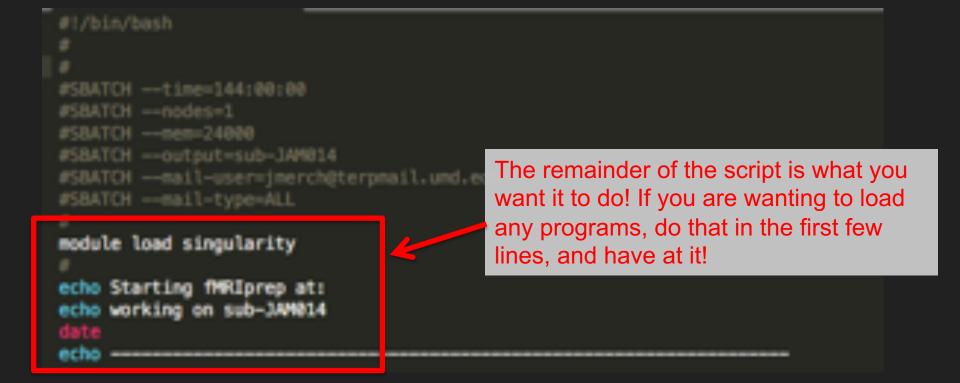


The next few lines are sbatch options.
These options can be specified within
the job script, or outside of the script as I
described before:

sbatch [options] <job script>

- -Time is the amount of time you want allocated in hours:minutes:seconds
- -Nodes is # of nodes
- -Mem is amount of RAM in megabytes
- -Output is the name of the output log file that contains what would be printed to terminal and any errors that occurred
- -Mail-you can give your email so it sends you a message when the job starts and ends!

Before going too much further, we should look inside a job script



Now, let's look at the special case of creating a job script with a MATLAB process.

For this, you want to create a bash script that looks the same as the previous example, but then calls matlab

```
#!/bin/bash
#SBATCH --time=144:00:00
#SBATCH --nodes=1
#SBATCH ---mem=24800
#SBATCH --output=sub-JAM014
#SBATCH --mail-user=jmerch@terpmail.umd.edu
#SBATCH --mail-type=ALL
module load matlab/2018b
matlab -nosplash -nodisplay -nodesktop -r "clear; addpath('/share/apps/spm/spm12');
spm_jobman('initcfg'); load $1; spm_jobman('run',matlabbatch); exit"
```

Now, let's look at the special case of creating a job script with a MATLAB process.

For this, you want to create a bash script that looks the same as the previous example, but then calls matlab

```
#!/bin/bash
#SBATCH --time=144:00:00
                                                   First, load the version of
#SBATCH ---nodes=1
#SBATCH ---mem=24000
                                                   matlab that you want
#SBATCH --output=sub-JAM014
#SBATCH --mail-user=jmerch@terpmail.umd.
module load matlab/2018b
matlab -nosplash -nodisplay -nodesktop -r "clear; addpath('/share/apps/spm/spm12');
    jobman('initcfg');    load $1;    spm_jobman('rum',matlabbatch);    exit"
```

Now, let's look at the special case of creating a job script with a MATLAB process.

For this, you want to create a bash script that looks the same as the previous example, but then calls matlab

```
#!/bin/bash
                                          Next, you want to start
                                          matlab using the nodisplay
#SBATCH --time=144:00:00
                                          options because otherwise it
#SBATCH --nodes=1
                                          will try to launch the matlab
#SBATCH ---mem=24000
#SBATCH --output=sub-JAM014
                                          window
#SBATCH --mail-user=jmerch@terpmail.umd.e
#SBATCH --mail-type=ALL
   lab -nosplash -nodisplay -nodesktop -r "clear; addpath('/share/apps/spm/spm12');
   journamit initions ); todo si, sprijouman('run',matlabbatch); exit"
```

Now, let's look at the special case of cr

For this, you want to create a bash scri example, but then calls matlab

#!/bin/bash to using matlab interactively, so I recommend making sure you #SBATCH --time=144:00:00 have a set of working matlab that #SBATCH ---nodes=1 you test outside of a job #SBATCH ---mem=24000 #SBATCH --output=sub-JAM014 submission before starting this. #SBATCH --mail-user=jmerch@terpmail.umd.edu #SBATCH --mail-type=ALL module load matlab/2018b

matlab -nosplas i -nodisplay -nodesktop -r "clear;

Finally, you want to feed into the matlab command everything you brocess. want to do within matlab using the -r option, followed by all the lus matlab operations within quotes. This can be tricky if you're used

addpath('/share/apps/spm/spm12');

Matlab/SPM tricks

Note: If you are using Matlab, you must launch it with no graphical interface. The below example loads the default matlab (2017a), and launches it in the terminal with no display, desktop, or Java:

```
module load matlab
matlab -nodesktop -nodisplay -nojvm
```

You can also launch Matlab, and tell it to run the commands/scripts following the '-r' option, which will become useful when we go over job submission:

```
matlab -nodesktop -nodisplay -nojvm -r
"run('YourCommand.m'); exit"
```

Matlab/SPM tricks

Matlab from the command line:

```
matlab -nodisplay -nodesktop -nosplash -nojvm
```

Spm from the command line. If you already have SPM batch jobs created and saved as .mat:

```
% initiates spm configuration
spm_jobman('initcfg');
% load spm job .mat
load('path/to/spm/batchjob.mat');
% run job without GUI
spm jobman('run',matlabbatch);
```

Matlab/SPM tricks

Now, combining what we learned in the previous 2 slides, here's how to launch matlab, and have it start running a SPM batch job:

```
matlab -nodesktop -nodisplay -nojvm -r
"spm_jobman('initcfg'); load('path/to/spm/batchjob.mat');
spm jobman('run',matlabbatch); exit"
```

This will launch matlab with no interface, run the SPM batch job, and then exit out of matlab when it finishes. This is essentially what goes into job submission script so that it can be run on a non-interactive node. But, I'm getting ahead of myself..

SLURM Job Scripts

IMPORTANT THINGS TO REMEMBER WHEN WRITING JOB SCRIPTS

It's totally non-interactive, so make sure you write and test properly before submitting

Paths--when a job is submitted, it starts in your homes directory, so give full paths where ever you can

Make sure you specify the options correctly

You can specify a lot of other things: https://slurm.schedmd.com/sbatch.html

Now that we have the basics covered, now we can get into how this can make this useful

Loops --First learn how to do a simple loop in bash or tcsh

Now, if you have a number of job scripts you want to run, you can create a loop to submit all of them

Even more fancy, instead of creating individual job scripts, you can create a job script that takes an input (e.g. subject ID) which performs the process on the input

Even if you aren't trying to parallelize a bunch of jobs, HPCs are useful for jobs that require crazy amount of computational resources (e.g. node with 1 TB RAM)

For example, pretend you have EEG data for 50 subjects that you want to preprocess: /path/to/subject/dir/sub_001 sub_002 ...

First, you want to write a job script that takes subject ID as an input, which performs the process on the subject. PreprocessEEG.sh:

```
#!/bin/bash
CurrentSubject=$1
module load EEGprogram
Process $CurrentSubject
...
```

Now, you can loop this job script for all the subjects, and have them process simultaneously:

```
for sub in $(ls /path/to/subject/dir); do
sbatch PreprocessEEG.sh $sub
done
```

```
for sub in $(ls /path/to/subject/dir); do
sbatch PreprocessEEG.sh $sub
done
```

This should give you something like this:

Now go have a beer because you are

processing all the data simultaneously!

```
Submitted batch job 82588
Submitted batch job 82581
Submitted batch job 82582
Submitted batch job 82583
Submitted batch job 82584
Submitted batch job 82585
Submitted batch job 82586
Submitted batch job 82507
Submitted batch job 82588
Submitted batch job 82589
Submitted batch job 82510
Submitted batch job 82511
Submitted batch job 82512
Submitted batch job 82513
Submitted batch job 82514
Submitted batch job 82515
Submitted batch job 82516
Submitted batch job 82517
```

What and When to parallelize

25 Subjects: The data processing pipeline can be divided up in numerous ways. Can create full pipeline per person, or be more modular.

Hypothetical data processing section:

Run the full pipe-line for all participant serially
Or set up individual subject pipelines and distribute

Convert dicom to nifti: mcverter

Converting 25 subs serially or convert each sub on separate node

Skull strip niftis: bet

Realign and unwarp: spm

Bet 25 subs serially or bet each sub in parallel or bet each run of each sub or bet each nifti file!

squeue – to check the status of your jobs that are running. If you type this by itself, it will list all the jobs that are running/pending:

```
login-1:-$ squeue
                                                                        NODELIST(REASON)
                                                                          cospute: 4:26
                                                                          cospute-4-26
                                                                          compute: 4:25
                                                                          compute: 4:25
                                                                          compute: 4:25
                                                                          compute-4-25
                                                                          compute 4-26
                                                                          compute-4-26
                                                                          compute-4-27
                                                                          compute-4-4
                                                                          cospute-4-4
                                                                          cospute-4-4
                                                                          cospute-4-4
                                                                         compute-5-2
                                        mbotdorf
                                                                         compute-4-2
```

squeue – you can be more specific with this queue, and just list the jobs you have submitted using the –u option followed by your user ID. For example:

```
squeue -u jmerch
```

```
[login-1:~$ squeue -u jmerch

JOBID PARTITION NAME USER ST TIME NODES NODELIST(REASON)

82557 standard SingPrep jmerch R 7:31:08 1 compute-5-2
```

scancel – if you have a job running that you want to cancel, you can use this command followed by the job ID given by slurm; for example:

scancel 82557

sinteractive – if you want to shell into one of the compute nodes to do some interactive processing, you can use this. Remember how I said never do any big processing on the head node, well you can shell in to one of the compute nodes and do some big processing. Like sbatch, you have to specify the time (in minutes), memory (in mb), and cpus. For example, this will give you an interactive node for 120 minutes, with 8 gb of RAM, and 1 CPU:

```
sinteractive -t 120 -m 8<u>000 -c 1</u>
```

```
login-1:~$ sinteractive -t 120 -m 8000 -c 1 salloc: Granted job allocation 82584 salloc: Waiting for resource configuration salloc: Nodes compute-4-7 are ready for job DISPLAY is login-1.bswift.umd.edu:21.0 compute-4-7:~:
```

Questions?

I'm available for consulting on how to get you set up on an HPC for the price of some beer and/or food (or cash)!

#AlwaysLookingForASideHustle

merchantjs@gmail.com

828-301-3155

