Introduction to High Performance Computing (HPC)

QLS 612 - 2023
Brent McPherson, PhD

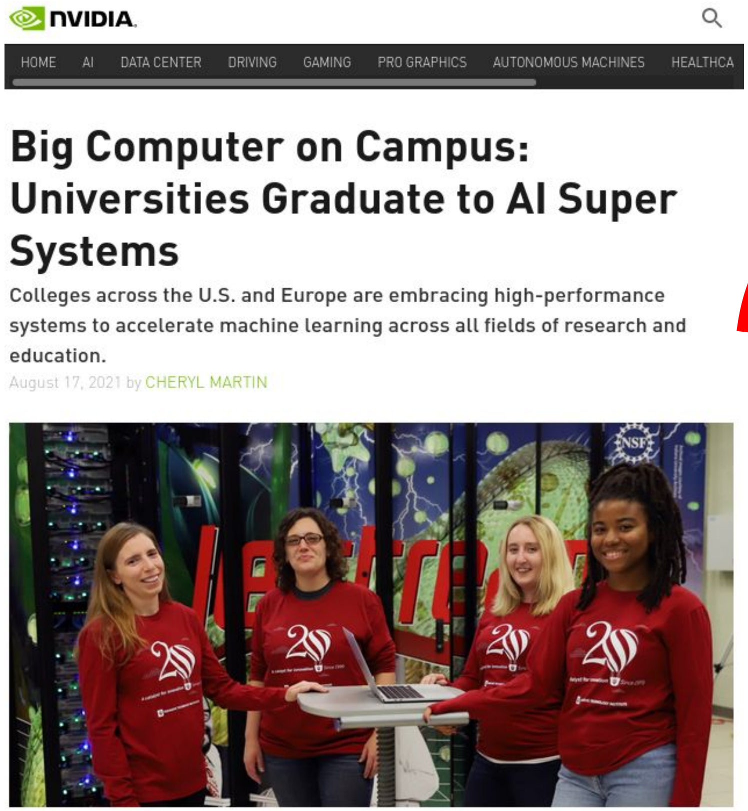
The goals of this lecture are to:

- Describe the structure of HPCs and how they differ from other traditional computers and common approaches.
    - Laptops / Desktops
- Introduce the concepts of using High Performance Computing (HPCs).
- How to begin effectively using HPC clusters in your work.

This will reference concepts covered in the “Introduction to the Terminal and Bash” and “Containerization” lectures.

Modern NeuroData Science Requires Computers

- No part of our research can progress without access to useful computing resources.
  - Data is acquired and stored on computers.
  - Data preparation and curation is performed on computers.
  - Analysis and modeling require computers.
  - Visualization and reporting or results require computers.
  - The distribution and reporting of results require computers.
- If at any point our work cannot continue in a digital space, it has effectively ended.
- In order to maximize our ability to perform innovative work in a field dependent on modern computational advances, a useful understanding of these machines is necessary.



Big Computer on Campus: Universities Graduate to AI Super Systems

Colleges across the U.S. and Europe are embracing high-performance systems to accelerate machine learning across all fields of research and education.

August 17, 2021 by CHERYL MARTIN

The Concepts of High Performance Computing (HPC)

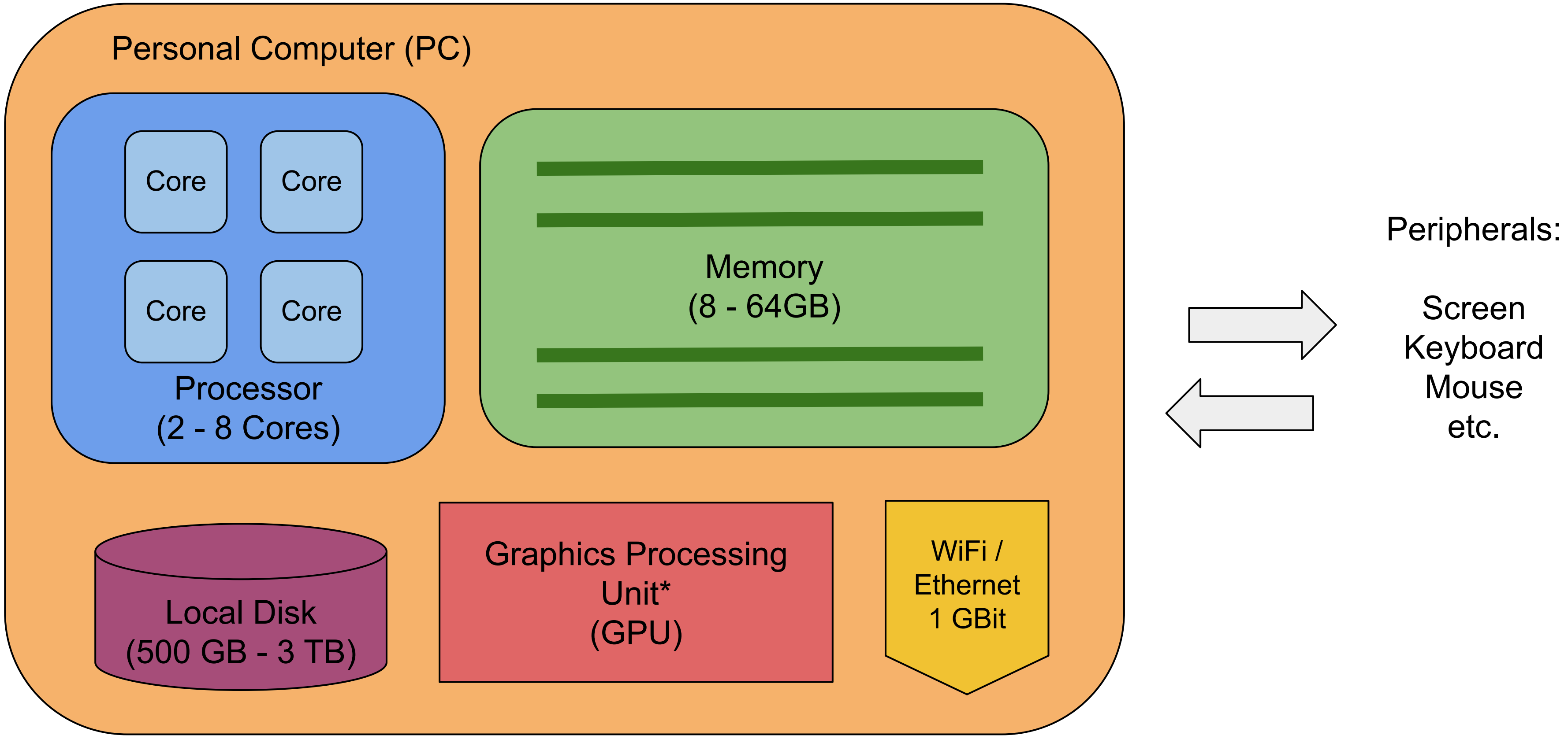
Working on a personal computer (PC)

- Everyone is familiar with this.
  - You’re using one now.
- These machines are designed to facilitate the most common needs of the most people.
- However, the limits of these machines can be easily reached when performing modern neuroscience analysis.

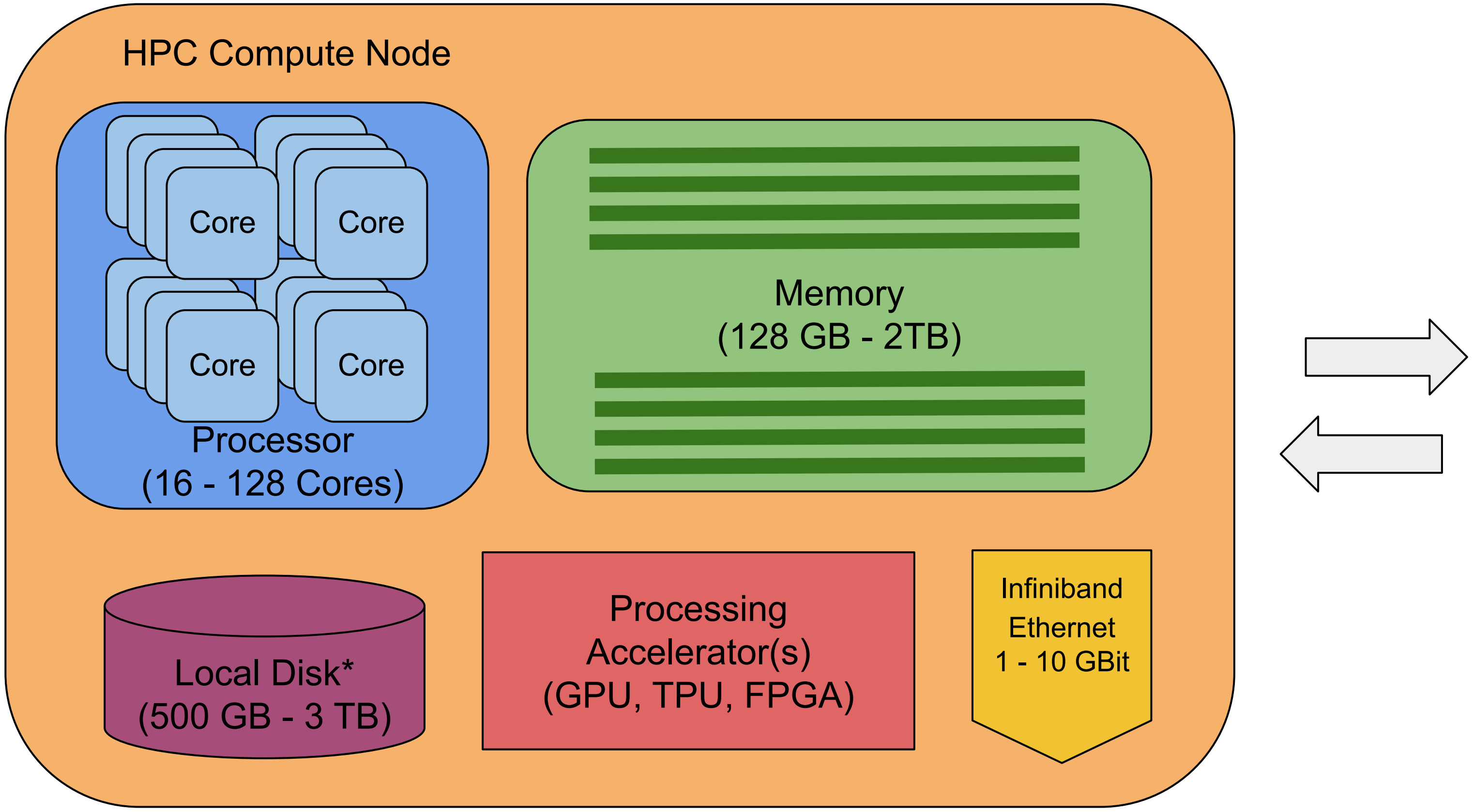
Working on an HPC

- These are not “personal” systems, they are multi-user.
- You do not interact with them directly, but over a network connection.
- The interaction with your analysis entails:
  - Transferring data / results.
  - Managing your analysis “jobs”.
- There is minimal “interactive” computing performed on a HPC.
  - Typically little to no visualization is performed on HPC systems.
- They almost exclusively run Linux.

The Schematic of a Computer



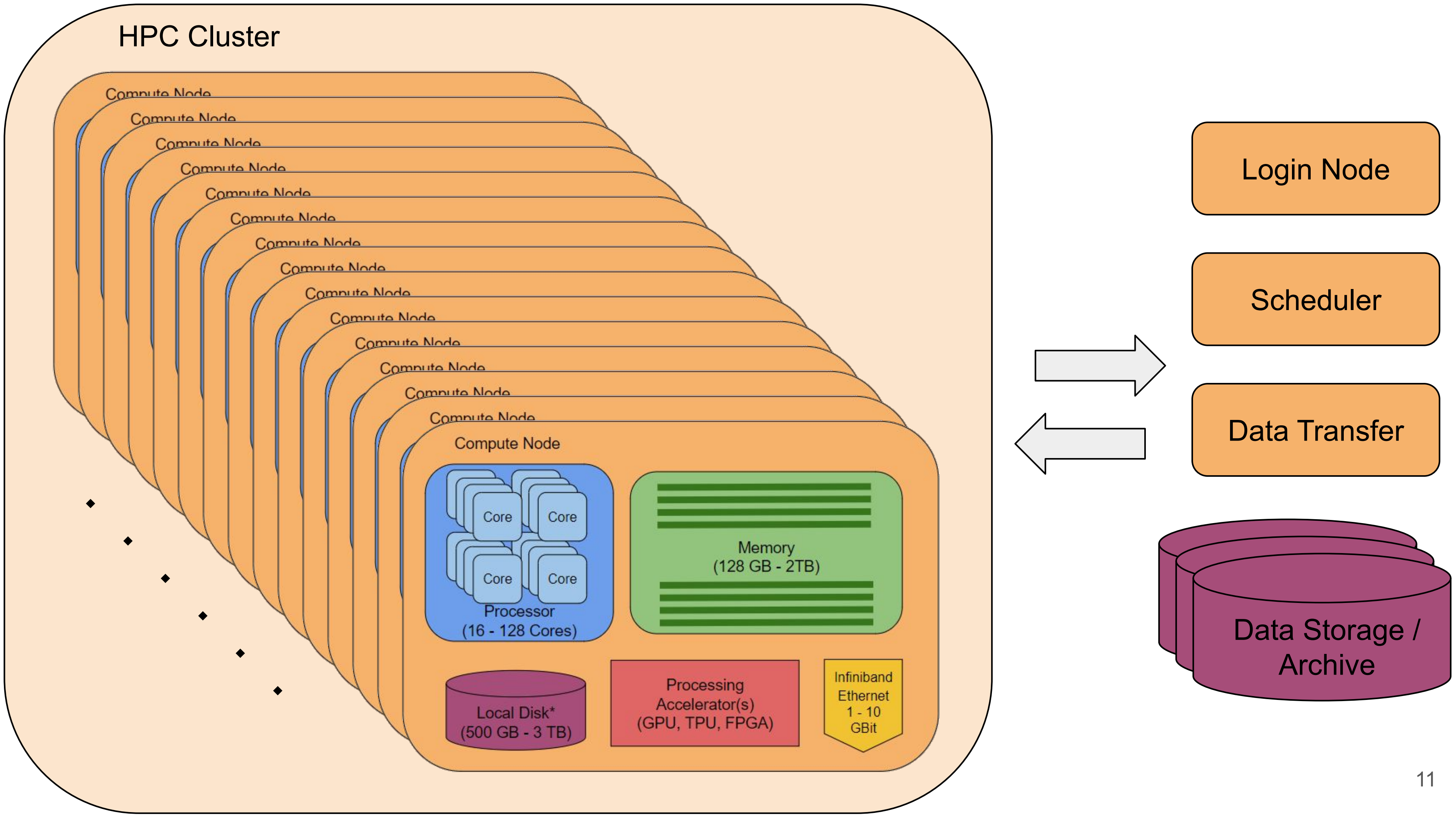
* not necessarily present in all systems (laptops)



Peripherals:
None

Connects to the rest of the compute cluster.

* it may be less and / or have higher access speed


HPC Cluster
Compute Node
Core
Core
Core
Core
Processor
(16 - 128 Cores)
Memory
(128 GB - 2TB)
Local Disk*
(500 GB - 3 TB)
Processing
Accelerator(s)
(GPU, TPU, FPGA)
Infiniband
Ethernet
1 - 10
GBit
Login Node
Scheduler
Data Transfer
Data Storage /
Archive

Other important things to keep in mind

- For a single, small process, an HPC may be slower than your laptop
  - The clock speed of processors is often slower when more cores are present.
  - There is also the overhead of moving / staging data, waiting for walltime, etc.
- Some HPCs have a different system architecture
  - Most PCs are 64-bit (x86) system architectures.
    - ARM is also common for some laptops (Apple M1)
  - Some HPCs do not have an x86 architecture
    - Big Red II (Cray), Longhorn (PPCx64)
  - This may cause challenges for deploying your code.

The Anatomy of a Computer

PCs

- 1 CPU
  - 2 - 8 cores
  - 3.5 - 4.5 GHz
- 8 - 64 GB RAM
- 500 GB - 3 TB Storage
- 1 GPU
  - This may be built into the CPU
- WiFi / 1 GBit Ethernet
- x86 (maybe ARM) architecture
- Single-User System
- Good for most general usage
  - This is likely where you will develop your analysis.

HPCs

- Multiple CPUs
  - 16 - 128 cores per CPU
  - 2.4 - 3.5 GHz
- 128 GB - 2 TB RAM
- 500 GB - 3 TB Storage
  - Not for long term storage
- 0 - 4 Processor Accelerators
  - GPUs w/ double precision CUDA
  - TPUs, FPGAs, Coprocessors, etc.
- 1 - 10 GBit Ethernet, Infiniband
- Different architectures (x86, PPC, Cray)
- Multi-User System
- Good for high throughput / large models.

Working on the Cloud - An expensive middle ground

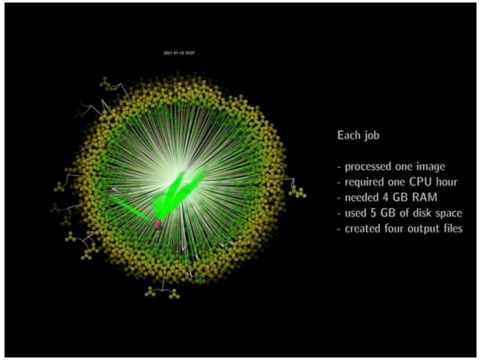
- This is most often an option through dedicated research proposals.
- The cloud system can be tailored to fit your specific analysis and data requirements.
    - A large virtual analysis computer
    - Your own dedicated cluster
- The data may be distributed on the cloud already.
    - Many open datasets are already on AWS.
- This will be *very* expensive for long term use.

The advantages of a HPC over a PC

- The ability to handle large datasets in a more time efficient manner.
- The option to “**Scale Out**” or “**Scale Up**” an analysis.
  - **Scale Out**: the ability to analyze independent parts of a dataset simultaneously
    - Independent permutations / cross-validations / simulations.
    - Different subjects through the same preprocessing preparations.
      - “Embarrassingly Parallel”
      - High Throughput Computing
  - **Scale Up**: create a larger single instance of computing resources to run a larger model, estimation, or analysis.
- We’ll be introducing you to “**Scaling Out**” your analysis in the example today.

Scaling Out

biobank uk

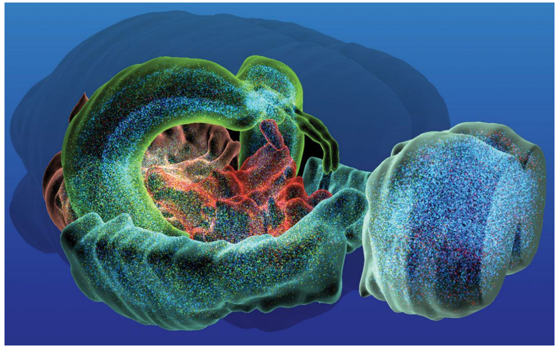


Each job

- processed one image
- required one CPU hour
- needed 4 GB RAM
- used 5 GB of disk space
- created four output files

Scaling Up

Blue Brain Project

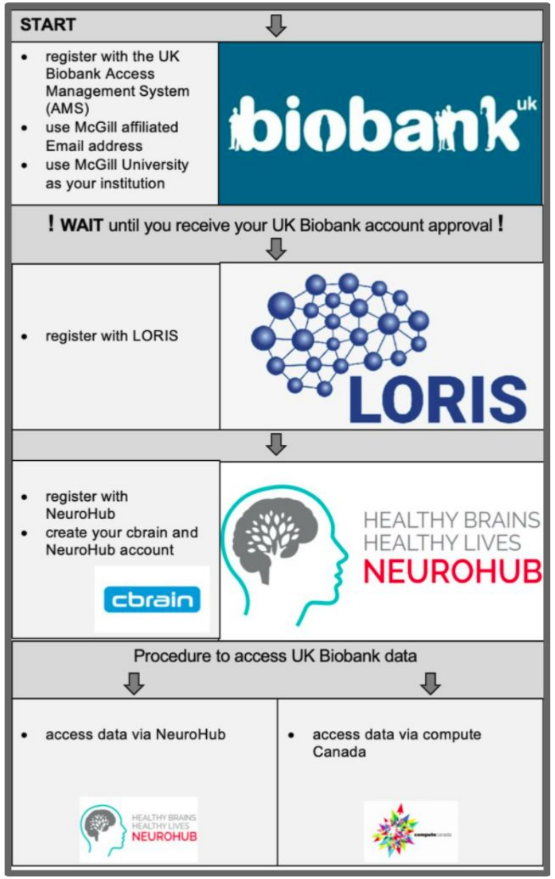


UKBB high-throughput replication of over 40K subjects

UKBB Data Access

Multi-step process!

1. Register with UKBB AMS
2. Register with LORIS
   a. Project and data management platform
3. Get a NeuroHub account
   a. Data and compute management platform
4. Get a Compute Canada account
   a. High performance compute cluster



START

- register with the UK Biobank Access Management System (AMS)
- use McGill affiliated Email address
- use McGill University as your institution

! WAIT until you receive your UK Biobank account approval !

- register with LORIS

- register with NeuroHub
- create your cbrain and NeuroHub account

Procedure to access UK Biobank data

- access data via NeuroHub

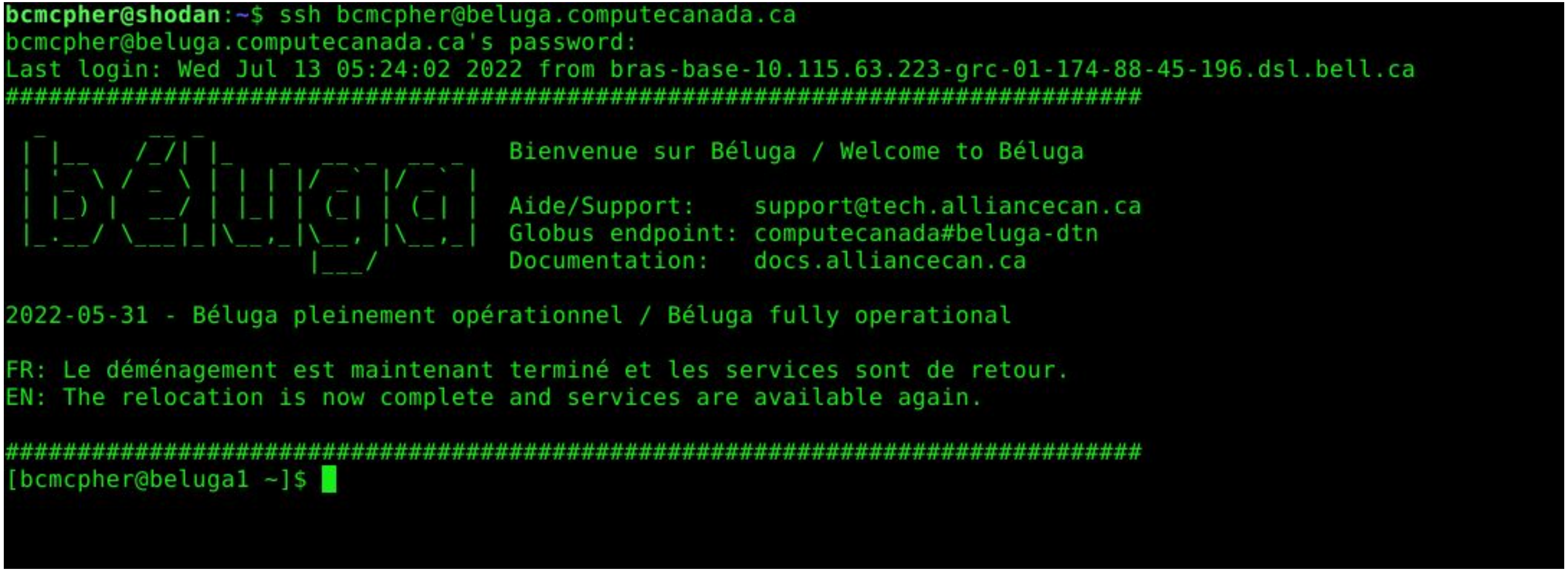
- access data via compute Canada

Thanks Nikhil!

Beginning to use a Cluster Computer

Accessing the Cluster

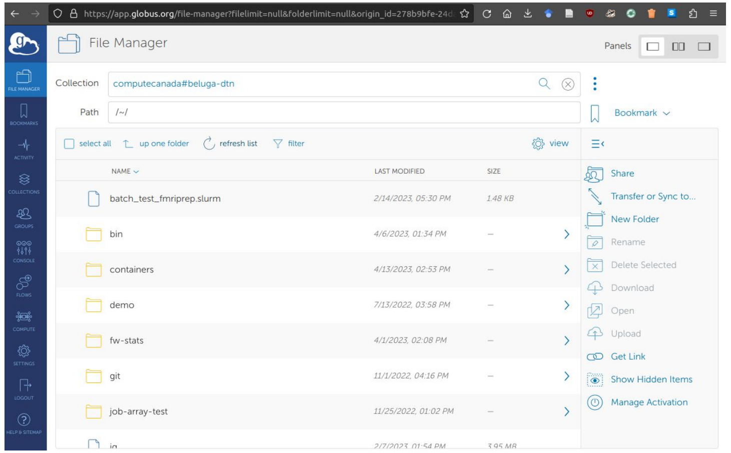
- This is done exclusively through a remote connection.
  - `ssh`, a remote desktop client, etc.
- You will connect to the **Login Node** of the cluster.
  - The login in node manages the coordination of user processes on the cluster
  - It also reports the overall status of the system.
- You will submit your jobs and query their status from the Login Node.
  - DO NOT run analyses or do other work on the Login Node.



```
bcmcpher@shodan:~$ ssh bcmcpher@beluga.computecanada.ca
bcmcpher@beluga.computecanada.ca's password:
Last login: Wed Jul 13 05:24:02 2022 from bras-base-10.115.63.223-grc-01-174-88-45-196.dsl.bell.ca
###############################################################################

 _        __ _
| |__   /_/| |_   _  __ _  __ _    Bienvenue sur Béluga / Welcome to Béluga
| '_ \ / _ \ | | | |/ _` |/ _` |
| |_) |  __/ | |_| | (_| | (_| |   Aide/Support:    support@tech.alliancecan.ca
|_.__/ \___|_|\__,_|\__, |\__,_|   Globus endpoint: computecanada#beluga-dtn
                    |___/          Documentation:   docs.alliancecan.ca

2022-05-31 - Béluga pleinement opérationnel / Béluga fully operational

FR: Le déménagement est maintenant terminé et les services sont de retour.
EN: The relocation is now complete and services are available again.

###############################################################################
[bcmcpher@beluga1 ~]$ 
```

Getting your data on the cluster

- I assume your data is on a computer not accessible by the cluster.
- You will use a file transfer tool to move your data from where it is to the data server.
    - `scp`, sftp, rsync, FileZilla, mobaXterm, etc.
    - This data server will be accessible to the compute nodes
- This may be done through the Login Node, but there may be a specific Data Transfer Node to move data.
    - Check with the system administrators.


https://app.globus.org/file-manager?filelimit=null&folderlimit=null&origin_id=278b9bfe-24d

File Manager

Collection: computecanada#beluga-dtn

Path: /~/

NAME	LAST MODIFIED	SIZE
batch_test_fmriprep.slurm	2/14/2023, 05:30 PM	1.48 KB
bin	4/6/2023, 01:34 PM	–
containers	4/13/2023, 02:53 PM	–
demo	7/13/2022, 03:58 PM	–
fw-stats	4/1/2023, 02:08 PM	–
git	11/1/2022, 04:16 PM	–
job-array-test	11/25/2022, 01:02 PM	–
iq	2/7/2023, 01:54 PM	3.95 MB

Getting your data on the cluster - Things to Remember

- Be aware of the policies of this server!
    - Files are often automatically removed after a (potentially short) window of inactivity.
    - Your analysis code, jobs, and data are probably not backed up on the HPC.
- It is your responsibility to make sure your data and code are securely backed up somewhere else.
- Once your analysis is complete you need to have a plan for storing your data long term.
    - OSF
    - OpenNeuro

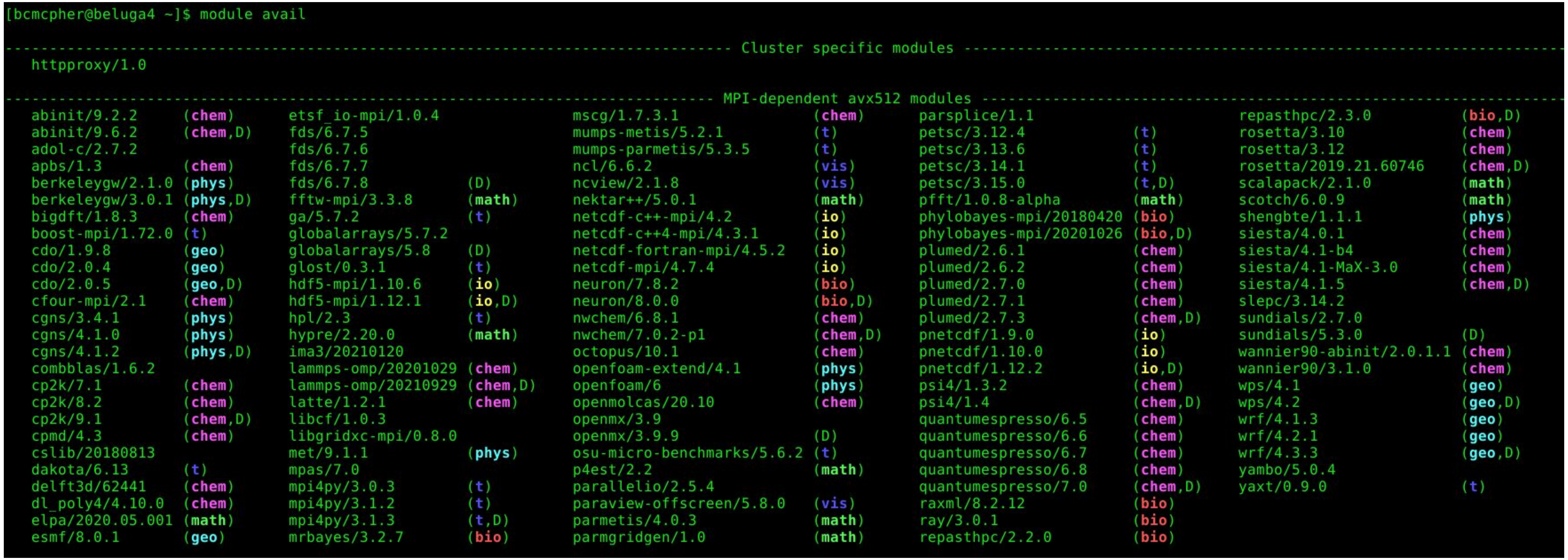
Getting your software on the cluster

- The cluster administrators will likely need to install it for you.
    - If you are confident you know how the tools works, you may be able to set it up yourself.
- Many tools will be readily available on the cluster through **modules**.
    - These are an efficient way to add and remove tools installed on the cluster to your session.
    - They are like an interactive `venv` for any tool.
    - They also allow for easier management of different versions of the same tool.
    - Hopefully, most of the tools you need will already be installed.
- Running your code in **containers** guarantees you have the tools you need to run your analysis.
    - You do have to a have (or be able to build) a working container of the tool.

Getting your software on the cluster - Modules

- How most software is made available to users on a HPC.
- A convenient way to set up basic development environments and change between versions.

```
> module avail
> module load python
> module load python/3.10.2
> module unload python
> module swap python/3.9.6
```



```
[bcmcpher@beluga4 ~]$ module avail

--------------------------------------------------------------------------------- Cluster specific modules ---------------------------------------------------------------------
   httpproxy/1.0

------------------------------------------------------------------------------- MPI-dependent avx512 modules -------------------------------------------------------------------
   abinit/9.2.2     (chem)      etsf_io-mpi/1.0.4               mscg/1.7.3.1               (chem)      parsplice/1.1                       repasthpc/2.3.0          (bio,D)
   abinit/9.6.2     (chem,D)    fds/6.7.5                       mumps-metis/5.2.1          (t)         petsc/3.12.4            (t)         rosetta/3.10             (chem)
   adol-c/2.7.2                 fds/6.7.6                       mumps-parmetis/5.3.5       (t)         petsc/3.13.6            (t)         rosetta/3.12             (chem)
   apbs/1.3         (chem)      fds/6.7.7                       ncl/6.6.2                  (vis)       petsc/3.14.1            (t)         rosetta/2019.21.60746    (chem,D)
   berkeleygw/2.1.0 (phys)      fds/6.7.8           (D)         ncview/2.1.8               (vis)       petsc/3.15.0            (t,D)       scalapack/2.1.0          (math)
   berkeleygw/3.0.1 (phys,D)    fftw-mpi/3.3.8      (math)      nektar++/5.0.1             (math)      pfft/1.0.8-alpha        (math)      scotch/6.0.9             (math)
   bigdft/1.8.3     (chem)      ga/5.7.2            (t)         netcdf-c++-mpi/4.2         (io)        phylobayes-mpi/20180420 (bio)       shengbte/1.1.1           (phys)
   boost-mpi/1.72.0 (t)         globalarrays/5.7.2              netcdf-c++4-mpi/4.3.1      (io)        phylobayes-mpi/20201026 (bio,D)     siesta/4.0.1             (chem)
   cdo/1.9.8        (geo)       globalarrays/5.8    (D)         netcdf-fortran-mpi/4.5.2   (io)        plumed/2.6.1            (chem)      siesta/4.1-b4            (chem)
   cdo/2.0.4        (geo)       glost/0.3.1         (t)         netcdf-mpi/4.7.4           (io)        plumed/2.6.2            (chem)      siesta/4.1-MaX-3.0       (chem)
   cdo/2.0.5        (geo,D)     hdf5-mpi/1.10.6     (io)        neuron/7.8.2               (bio)       plumed/2.7.0            (chem)      siesta/4.1.5             (chem,D)
   cfour-mpi/2.1    (chem)      hdf5-mpi/1.12.1     (io,D)      neuron/8.0.0               (bio,D)     plumed/2.7.1            (chem)      slepc/3.14.2
   cgns/3.4.1       (phys)      hpl/2.3             (t)         nwchem/6.8.1               (chem)      plumed/2.7.3            (chem,D)    sundials/2.7.0
   cgns/4.1.0       (phys)      hypre/2.20.0        (math)      nwchem/7.0.2-p1            (chem,D)    pnetcdf/1.9.0           (io)        sundials/5.3.0           (D)
   cgns/4.1.2       (phys,D)    ima3/20210120                   octopus/10.1               (chem)      pnetcdf/1.10.0          (io)        wannier90-abinit/2.0.1.1 (chem)
   combblas/1.6.2               lammps-omp/20201029 (chem)      openfoam-extend/4.1        (phys)      pnetcdf/1.12.2          (io,D)      wannier90/3.1.0          (chem)
   cp2k/7.1         (chem)      lammps-omp/20210929 (chem,D)    openfoam/6                 (phys)      psi4/1.3.2              (chem)      wps/4.1                  (geo)
   cp2k/8.2         (chem)      latte/1.2.1         (chem)      openmolcas/20.10           (chem)      psi4/1.4                (chem,D)    wps/4.2                  (geo,D)
   cp2k/9.1         (chem,D)    libcf/1.0.3                     openmx/3.9                             quantumespresso/6.5     (chem)      wrf/4.1.3                (geo)
   cpmd/4.3         (chem)      libgridxc-mpi/0.8.0             openmx/3.9.9               (D)         quantumespresso/6.6     (chem)      wrf/4.2.1                (geo)
   cslib/20180813               met/9.1.1           (phys)      osu-micro-benchmarks/5.6.2 (t)         quantumespresso/6.7     (chem)      wrf/4.3.3                (geo,D)
   dakota/6.13      (t)         mpas/7.0                        p4est/2.2                  (math)      quantumespresso/6.8     (chem)      yambo/5.0.4
   delft3d/62441    (chem)      mpi4py/3.0.3        (t)         parallelio/2.5.4                       quantumespresso/7.0     (chem,D)    yaxt/0.9.0               (t)
   dl_poly4/4.10.0  (chem)      mpi4py/3.1.2        (t)         paraview-offscreen/5.8.0   (vis)       raxml/8.2.12            (bio)
   elpa/2020.05.001 (math)      mpi4py/3.1.3        (t,D)       parmetis/4.0.3             (math)      ray/3.0.1               (bio)
   esmf/8.0.1       (geo)       mrbayes/3.2.7       (bio)       parmgridgen/1.0            (math)      repasthpc/2.2.0         (bio)
```

Running your analysis - Working with a Scheduler

- With your data and `env` ready you can run your analysis.
- You will do this by submitting your work as a **Job**.
- **Jobs** are submitted to the Scheduler to be run.
    - This deploys the analysis onto the compute nodes.
- Your entire analysis will need to be scripted.
    - You cannot interact with or manually input information to a job when it’s running.
- Once your analysis script is complete, you create your job script for the analysis.
    - This script describes the resources needed to successfully run your analysis on the cluster.

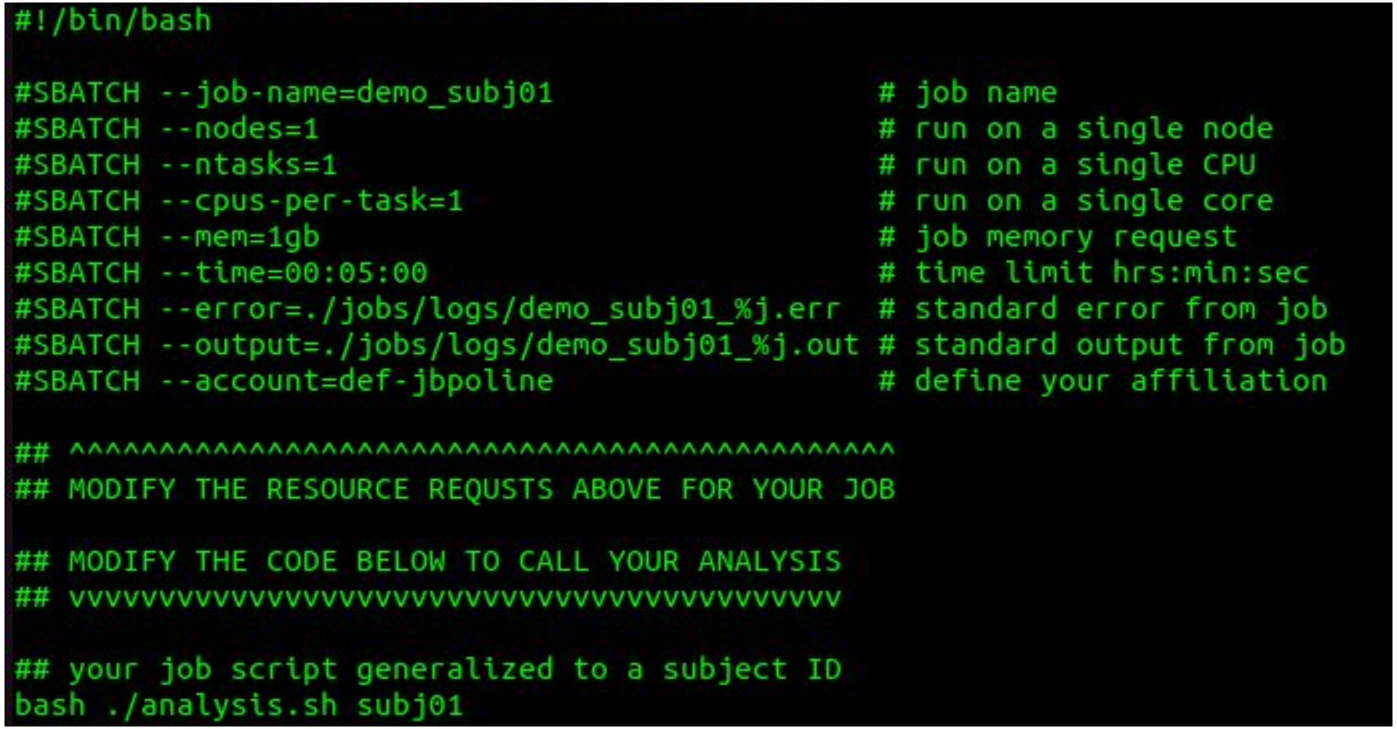
Running your analysis - Available Resources / Queues

- You will need to submit your work to a compute cluster that can accommodate your resource request.
- Specifically, this means you may have to submit your jobs to the GPU queue if you analysis requires a GPU to execute.
    - This will be in addition to requesting the GPU cores / memory
- Similar queues exist for jobs that are:
    - Expected to run for a long time (> 24 hours)
    - High memory requirement (> 256GB)
- The queues available on a cluster reflect the hardware available.
    - Often you will select the cluster you will work on based on the queues you plan to use.

Running your analysis - Creating Job Scripts

- Your job scripts define the system resources required by your analysis.
- The job script will be submitted to the scheduler from the login node to be added to the queue.
  - The scheduler uses your resource requests and your priority to determine what runs when.
- Your outputs, along with logs, will be created for each job you submit.
- The example today will assume you are **Scaling Out** your analysis.
  - You want to run a common process across many subjects.
  - i.e. fMRIPrep, FreeSurfer, etc.

demo_subj01.slurm



```
#!/bin/bash

#SBATCH --job-name=demo_subj01                        # job name
#SBATCH --nodes=1                                     # run on a single node
#SBATCH --ntasks=1                                    # run on a single CPU
#SBATCH --cpus-per-task=1                             # run on a single core
#SBATCH --mem=1gb                                     # job memory request
#SBATCH --time=00:05:00                               # time limit hrs:min:sec
#SBATCH --error=./jobs/logs/demo_subj01_%j.err        # standard error from job
#SBATCH --output=./jobs/logs/demo_subj01_%j.out       # standard output from job
#SBATCH --account=def-jbpoline                        # define your affiliation

## ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
## MODIFY THE RESOURCE REQUSTS ABOVE FOR YOUR JOB

## MODIFY THE CODE BELOW TO CALL YOUR ANALYSIS
## vvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvv

## your job script generalized to a subject ID
bash ./analysis.sh subj01
```

Commands for working with Jobs

- `sbatch`
  - Submit a job to the scheduler.
  - `> sbatch job.slurm`
- `squeue`
  - Monitor the status of jobs on the cluster.
  - `> squeue -u USERNAME`
- `scancel`
  - Cancels a job that hasn’t completed.
  - `> scanel JOBID`
- `sacct`
  - Provides a summary of the jobs your have recently submitted.
  - `> sacct`
- `srun`
  - Start an interactive job to test that your job will work correctly.
  - `> srun --nodes=1 --ntasks-per-node=1 --time=01:00:00 --pty bash -i`

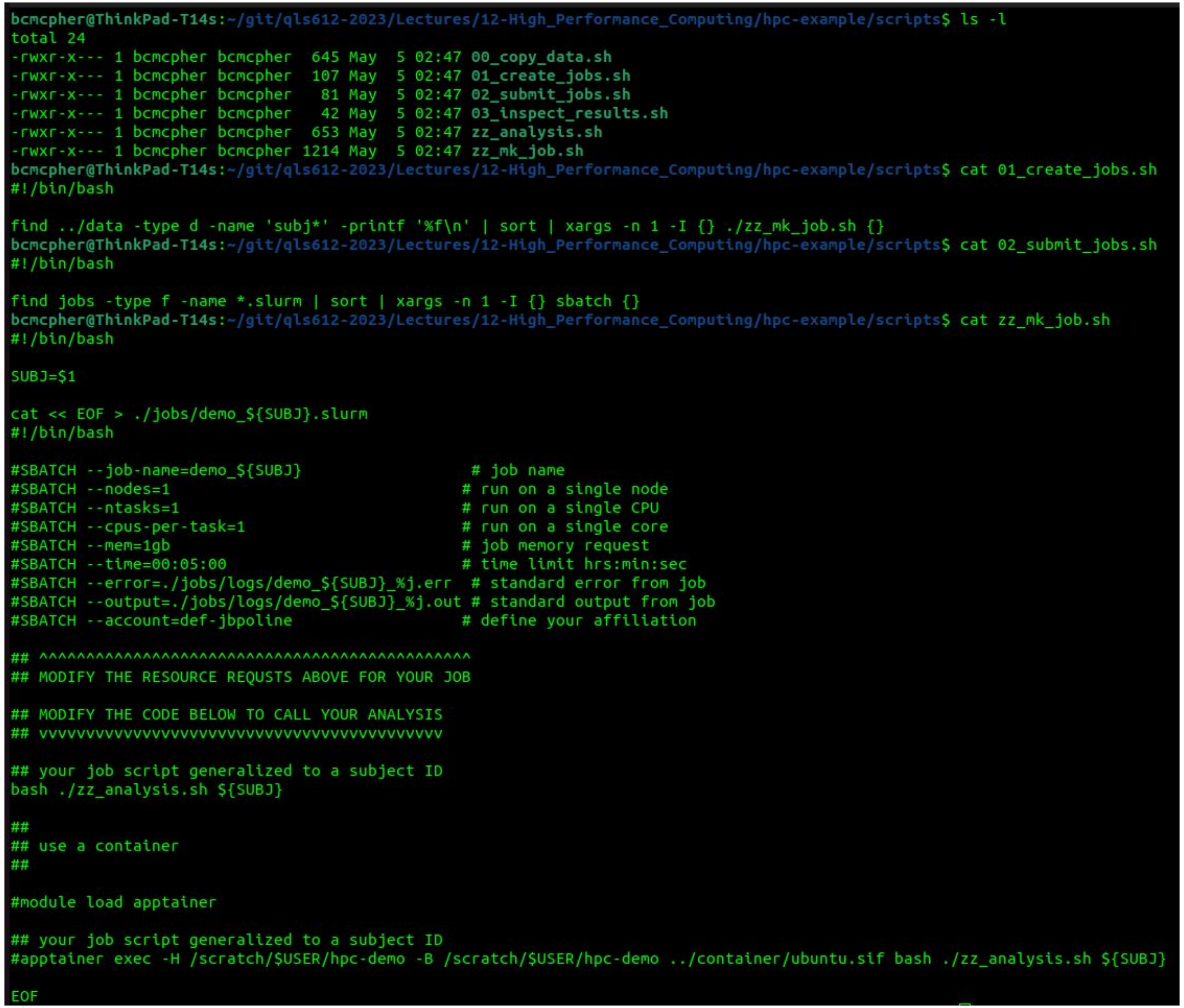
There are a lot of resources available for learning about HPCs online and in your lab. Find a process that works for you and ASK how others have solved similar problems!

Running your analyses - be efficient

- For every job you run, you will have:
    - The input data - *the same files for each subject*
    - The analysis script - *the same analysis for each subject*
    - The job script and logs - *a separate job for every subject with logs for each attempt*
    - The results - *whatever output your analysis produces that you intend to keep*
- Just like your analyses, you should script as much of your cluster work as possible.
    - You should never be individually making or modifying job files for subjects.
    - Having scripts for moving and backing up data is a good idea, too.

The Example

- The example today reports back a short log about the system status of the node before waiting.
  - This will let you see the different nodes your jobs ran on.
- The analysis input wants a subject ID as an input
  - This is is likely how you would set up a symmetric analysis across your subjects.
- The goal is to provide a basic working template for your job scripts that you can modify.



```
bcmcpher@ThinkPad-T14s:~/git/qls612-2023/Lectures/12-High_Performance_Computing/hpc-example/scripts$ ls -l
total 24
-rwxr-x--- 1 bcmcpher bcmcpher  645 May  5 02:47 00_copy_data.sh
-rwxr-x--- 1 bcmcpher bcmcpher  107 May  5 02:47 01_create_jobs.sh
-rwxr-x--- 1 bcmcpher bcmcpher   81 May  5 02:47 02_submit_jobs.sh
-rwxr-x--- 1 bcmcpher bcmcpher   42 May  5 02:47 03_inspect_results.sh
-rwxr-x--- 1 bcmcpher bcmcpher  653 May  5 02:47 zz_analysis.sh
-rwxr-x--- 1 bcmcpher bcmcpher 1214 May  5 02:47 zz_mk_job.sh
bcmcpher@ThinkPad-T14s:~/git/qls612-2023/Lectures/12-High_Performance_Computing/hpc-example/scripts$ cat 01_create_jobs.sh
#!/bin/bash

find ../data -type d -name 'subj*' -printf '%f\n' | sort | xargs -n 1 -I {} ./zz_mk_job.sh {}
bcmcpher@ThinkPad-T14s:~/git/qls612-2023/Lectures/12-High_Performance_Computing/hpc-example/scripts$ cat 02_submit_jobs.sh
#!/bin/bash

find jobs -type f -name *.slurm | sort | xargs -n 1 -I {} sbatch {}
bcmcpher@ThinkPad-T14s:~/git/qls612-2023/Lectures/12-High_Performance_Computing/hpc-example/scripts$ cat zz_mk_job.sh
#!/bin/bash

SUBJ=$1

cat << EOF > ./jobs/demo_${SUBJ}.slurm
#!/bin/bash

#SBATCH --job-name=demo_${SUBJ}                  # job name
#SBATCH --nodes=1                               # run on a single node
#SBATCH --ntasks=1                              # run on a single CPU
#SBATCH --cpus-per-task=1                       # run on a single core
#SBATCH --mem=1gb                               # job memory request
#SBATCH --time=00:05:00                         # time limit hrs:min:sec
#SBATCH --error=./jobs/logs/demo_${SUBJ}_%j.err  # standard error from job
#SBATCH --output=./jobs/logs/demo_${SUBJ}_%j.out # standard output from job
#SBATCH --account=def-jbpoline                  # define your affiliation

## ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
## MODIFY THE RESOURCE REQUSTS ABOVE FOR YOUR JOB

## MODIFY THE CODE BELOW TO CALL YOUR ANALYSIS
## vvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvv

## your job script generalized to a subject ID
bash ./zz_analysis.sh ${SUBJ}

##
## use a container
##

#module load apptainer

## your job script generalized to a subject ID
#apptainer exec -H /scratch/$USER/hpc-demo -B /scratch/$USER/hpc-demo ../container/ubuntu.sif bash ./zz_analysis.sh ${SUBJ}

EOF
```

1. Connect to the HPC.
2. Move the example scripts to the HPC.
3. Make and submit your jobs.
4. Monitor the job status.
5. Cancel a job.
6. Run an interactive job.
7. Modify your resource requests / Explore documentation.
8. Run the script in a container.

Demo Redux

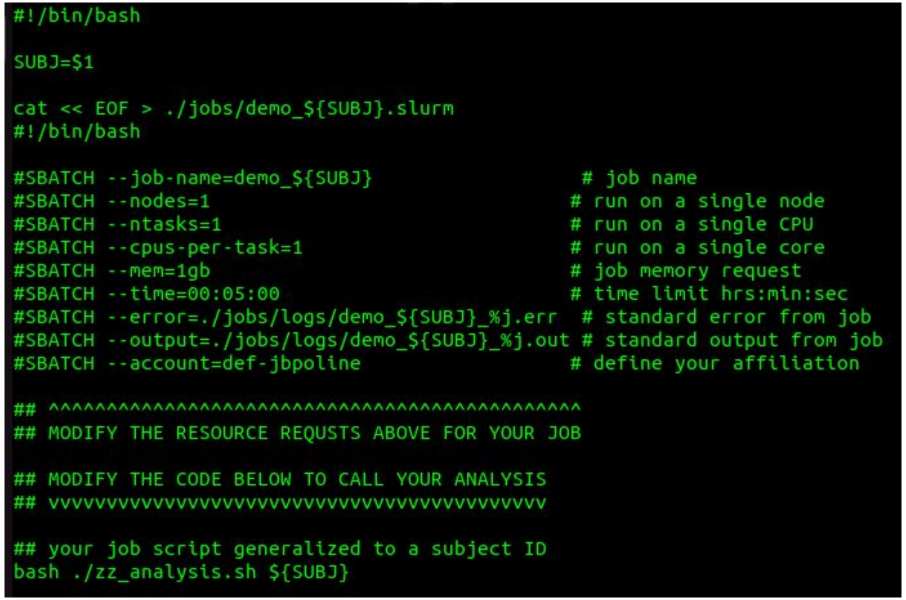
Step 0: Create a container

```
module load singularity
singularity build ../container/ubuntu.sif docker://ubuntu:latest
```

- From the login node, load the singularity module
  - Interactive sessions may not have internet access to download an image
- Call the build function pointing to the docker image you want to import
  - `docker://` - look on dockerhub
  - Ubuntu:latest for the most recently tagged ubuntu image
- This will create the singularity container you can use on Compute Canada

Step 1.1 - Make a template job script for your process

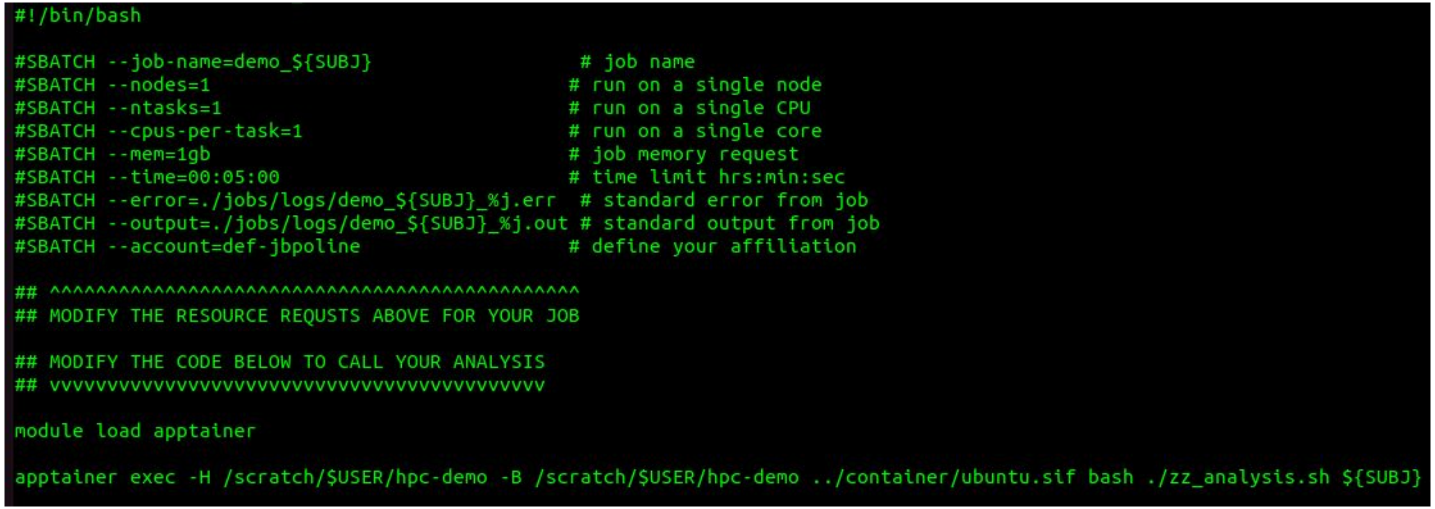
- `SUBJ=$1` assigns the first argument of the shell script to `$SUBJ`
- `cat << EOF > ./jobs/demo_${SUBJ}.slurm`
  `…`
  `…`
  `EOF`
  - This syntax will output everything immediately below it until `EOF` into the text file: `./jobs/demo_${SUBJ}.slurm`
- This allows you to define the resource allocation and other parameters that are common for each subject.
- This file can be versioned or modified for each job your need to run across subjects.



```
#!/bin/bash

SUBJ=$1

cat << EOF > ./jobs/demo_${SUBJ}.slurm
#!/bin/bash

#SBATCH --job-name=demo_${SUBJ}                   # job name
#SBATCH --nodes=1                                # run on a single node
#SBATCH --ntasks=1                               # run on a single CPU
#SBATCH --cpus-per-task=1                        # run on a single core
#SBATCH --mem=1gb                                # job memory request
#SBATCH --time=00:05:00                          # time limit hrs:min:sec
#SBATCH --error=./jobs/logs/demo_${SUBJ}_%j.err   # standard error from job
#SBATCH --output=./jobs/logs/demo_${SUBJ}_%j.out # standard output from job
#SBATCH --account=def-jbpoline                   # define your affiliation

## ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
## MODIFY THE RESOURCE REQUSTS ABOVE FOR YOUR JOB

## MODIFY THE CODE BELOW TO CALL YOUR ANALYSIS
## vvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvv

## your job script generalized to a subject ID
bash ./zz_analysis.sh ${SUBJ}
```

Step 1.1 - Make a template job script w/ Singularity

- You will also be able to call your jobs with a singularity container.
- You can call multiple scripts or functions within your job.
- Don’t forget to load the module!



```
#!/bin/bash

#SBATCH --job-name=demo_${SUBJ}                   # job name
#SBATCH --nodes=1                                # run on a single node
#SBATCH --ntasks=1                               # run on a single CPU
#SBATCH --cpus-per-task=1                        # run on a single core
#SBATCH --mem=1gb                                # job memory request
#SBATCH --time=00:05:00                          # time limit hrs:min:sec
#SBATCH --error=./jobs/logs/demo_${SUBJ}_%j.err  # standard error from job
#SBATCH --output=./jobs/logs/demo_${SUBJ}_%j.out # standard output from job
#SBATCH --account=def-jbpoline                   # define your affiliation

## ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
## MODIFY THE RESOURCE REQUSTS ABOVE FOR YOUR JOB

## MODIFY THE CODE BELOW TO CALL YOUR ANALYSIS
## vvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvv

module load apptainer

apptainer exec -H /scratch/$USER/hpc-demo -B /scratch/$USER/hpc-demo ../container/ubuntu.sif bash ./zz_analysis.sh ${SUBJ}
```

Step 1.2 - Make a job file for each subject

```
find ../data -type d -name 'subj*' -printf '%f\n' | sort | xargs -n 1 -I {} ./zz_mk_job.sh {}
```

- `find ../data`
    - Find in the data folder
- `-type d -name *.slurm`
    - All directories named `subj*`
- `-printf '%f\n'`
    - Only print the directory name. This is each subject ID for this study.
- `| sort | xargs -n 1 I {} zz_mk_job.sh {}`
    - Then sort the subject IDs and pass each ID as an input to `zz_mk_job.sh` to create a job script from your template for each subject.

Step 2 - Submit your job scripts

```
find jobs -type f -name *.slurm | sort | xargs -n 1 -I {} sbatch {}
```

- `find jobs`
    - Find in the jobs folder
- `-type f -name *.slurm`
    - All files named *.slurm
- `| sort`
    - Sort them in ascending order
- `| xargs -n 1 I {} sbatch {}`
    - Then pass each file as an input to `sbatch` to launch the job

Step 3 - Extract your results

- Once the jobs are done, you can extract your results
    - This may mean moving the data off the compute cluster to visualize
- For the tutorial your outputs are text. So you can
    - `grep -r ‘error’ ./logs/*`
        - To look for errors (or other messages) in the logs
    - `grep -r ‘compute’ ../results/*`
        - To look for the result the “analysis” returned.

Step 4 - Make it your own!

- The steps outlined here are a good starting point of some best practices, but there is so much you can do with HPCs.
  - There are many different ways to effectively use these tools and manage your jobs.
    - Job Arrays, for example
  - This is a wide domain to explore
- Learn what you can from others and try your best to understand these kinds of systems, they'll be an invaluable tool for the rest of your career.

Thanks