HBIC COGNEURO WORKGROUP

HBIC COMPUTING RESOURCES

EXPANDING SYNAPSE CAPACITY



SYNAPSE CAPACITY ISSUES AND SOLUTIONS

- Slow applications due to high load
- Incomplete preprocessing jobs due to killed processes
- Increasing capacity:
 - Added new compute servers
 - KU-L HPC cluster
 - Lab-owned resources
 - Web services





24 CPU @ 2.40 GHz 64 GB RAM Physical hardware. Exceeded service life requiring decommission.

new hbic-synapse



12 CPU @ 2.40 GHz 24 GB RAM Virtual machine.
Perpetual support,
in-place hardware upgrades

NEW HBIC SERVER LINEUP

- Added four servers
 - 8 CPUs / 12 GB RAM
- Main server
 - hbic-synapse



- Data Visualization
 - Data management
 - Small/short processing jobs
 - Submit jobs to Compute nodes

- New Interactive terminals
 - hbic-alpha
 - hbic-beta



- Large interactive jobs
- Graphical applications

- New Compute nodes
 - hbic-gamma
 - hbic-delta



- Long processing scripts
- Dedicated CPU/RAM
- No ssh access

NEW TERMINALS: HBIC-ALPHA, HBIC-BETA

- Cloned hbic-synapse server: the same applications are on hbic-alpha and hbic-beta
- NB: No syncing is done of user home directories or configuration files across servers. Keep shared files on R-Drive
- Select a server after first checking current processing loads
- Connect the same way as on hbic-synapse: ssh hbic-alpha.kumc.edu ssh hbic-beta.kumc.edu
- These are an unmoderated shared resource be considerate of your use
- Not suited for jobs that depend on dedicated resources for their duration (e.g., AFNI's SSWarper, freesurfer's recon-all)

NEW COMPUTE NODES: HBIC-GAMMA, HBIC-DELTA

- Uses SLURM (Simple Linux Utility for Resource Management) for job scheduling and resource management
- Synapse acts as the host. Login to Synapse, specify the script to run and its required CPU/RAM and submit it to the scheduler.
 Those resources are dedicated to your process for the job's duration
- If the requested resources are not available, the scheduler will wait to run it until those resources are freed up
- Request only as much CPU/RAM as you need to minimize wait times

SLURM USAGE

- Login to synapse and create a job script specifying the required resources (CPUs, memory, time) and commands to run.
- Use sinfo to check node status
- Submit the job using sbatch
- Use squeue to check the status of submitted jobs
- SLURM ensures jobs are queued and only start when the requested resources are available, preventing conflicts and killed processes due to exhausted memory

myjob.sh

```
#!/bin/bash
#SBATCH --job-name=fs project
                                  # Job name
#SBATCH --output=fs %j.log
                                  #logfile name
#SBATCH --error=fs_%j_error.log
                                  #logfile name
#SBATCH --ntasks=1
                                     # Run a single task
#SBATCH --cpus-per-task=4
                                   # Number of CPU cores per task
#SBATCH --mem=8G
                                    # Memory for the whole job
#SBATCH --time=1-00:00:00
                                  # Time limit day-H:M:S
#SBATCH --mail-type=ALL
                                   # Mail events (NONE, BEGIN, END,
FAIL, ALL)
#SBATCH -mail-user=jbartolotti2@kumc.edu # mail address (kumc only)
load freesurfer
~/R-Drive/Bartolotti J/project/2 freesurfer recon.sh
```

```
[sa-j186b025@hbic-synapse ~]$ sinfo

PARTITION AVAIL TIMELIMIT NODES STATE NODELIST

hbic up infinite 1 idle hbic-delta.kumc.edu

hbic up infinite 1 idle hbic-gamma.kumc.edu

[sa-j186b025@hbic-synapse]$ sbatch myjob.sh
```

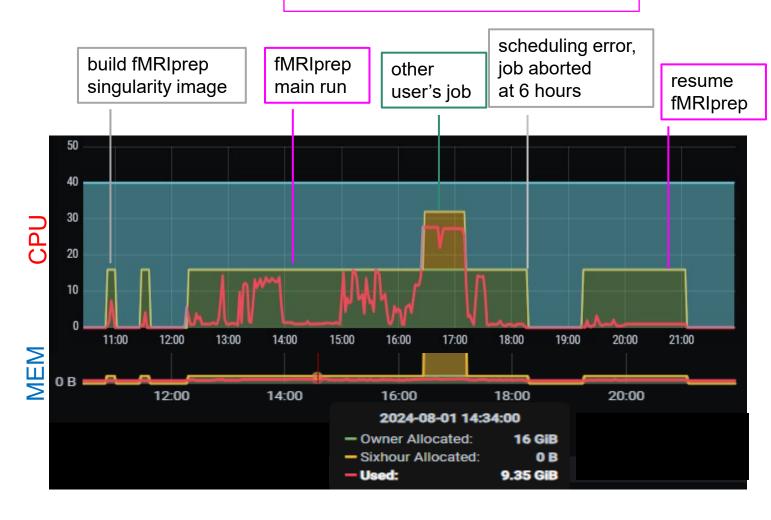
KUMC COMMUNITY CLUSTER

- High Performance Computing (HPC) Cluster that aggregates hardware purchased by different KU-L and KUMC researchers
- Hardware and software administered by the KU Center for Research Computing Staff with a 5year warranty, ~\$11,000 upfront cost
- Access is restricted to hardware owners or individuals sponsored by an owner
- Data processing jobs can be run on your own node, or a special "sixhour" time-limited partition comprising pooled inactive resources from all nodes
- Jobs submitted using SLURM

Example fMRIprep processing

- 16 CPU cores
- ~8 GB RAM (max 9.35)
- 7-8 hours runtime

Allocated: 16 CPU / 16 GB



KU CLUSTER AND KUMC SERVER SPECS

KU Cluster

~\$11,000 Standard Compute Unit (5 year warranty)

- 48 cores @ 2.6GHz Dual Intel Xeon 6442Y CPU
- 256GB RAM 4800MT/s DDR5
- 480GB SSD Hard Disk
- 1 Gb/s Ethernet & 100 Gb/s Infiniband
- 5 Year Hardware Warranty after 5 years owner pays for repairs; unit remains in cluster as long as space is available

KUMC Large Server (e.g., Synapse)

\$6,000 KUMC server (over 5 years)

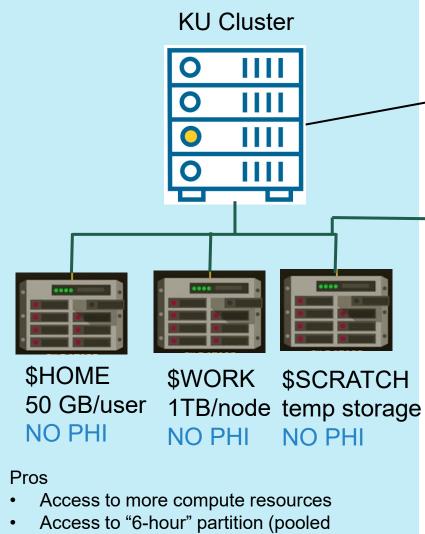
- 12 CPU @ 2.20 GHz
- 24 GB RAM
- 500 GB Hard Disk
- 10 Gb/s Ethernet
- \$1,200 annual fee hardware maintained by IT, no repair costs to VM owner

KUMC Typical Server

\$3,950 KUMC server (over 5 years)

- 8 CPU @ 2.20 GHz
- 12 GB RAM
- 500 GB Hard Disk
- 10 Gb/s Ethernet
- \$790 annual fee

hardware maintained by IT, no repair costs to VM owner



- resources from other nodes, 6 hour time limit per job)
- Guaranteed minimum CPU/RAM per job

Cons

- Limited interactive terminal / graphical apps
- Limited software installation (use containers)
- No PHI data storage or processing

Typical Workflow

USAGE

ssh

Copy Raw Data XNAT -> P-Drive

ssh

Synapse: De-identify data

Synapse: Copy De-id data

P/R Drive -> \$WORK

KU Cluster: Preprocess data

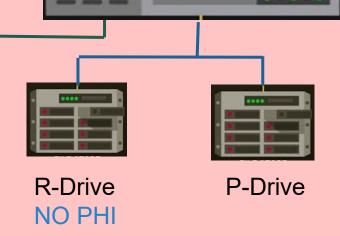
KU Cluster: Group analysis script

Synapse: Move processed

data \$WORK -> P/R Drive

Synapse: Interactive

data visualization



KUMC hbic-synapse

Pros

- Interactive terminal, no time limits
- Administrated by HBIC, flexible software installation
- Can mount and interact with P-Drive (PHI data)
- Can mount KU Cluster drives (HOME, WORK, SCRATCH)
- Run web servers (e.g., XNAT)

Cons

- Limited, shared compute resources
- Jobs killed if CPU/RAM exhausted partway through

OTHER RESOURCES

Lab-owned server

- KUMC IT supports Windows or Linux (RedHat) servers.
 IT provides secure access, backup, and security/OS updates.
- Application installation and support is performed by an application admin in your team, not IT
- https://kumed.sharepoint.com/sites/mykumc/catalog/tech/Lists/Services/DispForm.aspx?ID=85

Cloud computing (e.g. Amazon Web Services)

- Highly scalable
- Suitable for preprocessing very large datasets in parallel
- Current lack of KUMC/HBIC support

Typical Analysis Server

8 CPU @ 2.20 GHz
12 GB RAM
500 GB Hard Disk
Disk backed up by IT
\$65.91/month
\$790 annual
Disk not backed up by
IT
\$23.33/month
\$280 annual