Using GACRC HPC Computing Facility

Sapelo2 Cluster

Georgia Advanced Computing Resource Center (GACRC)

Enterprise Information Technology Services(EITS)

The University of Georgia

Outline

- GACRC
- Sapelo2 Cluster and Workflow
- Request Computing Resources
- Run MPI Job
- Run GPU Job
- Obtain Job Details
- Guideline and Practical Tips

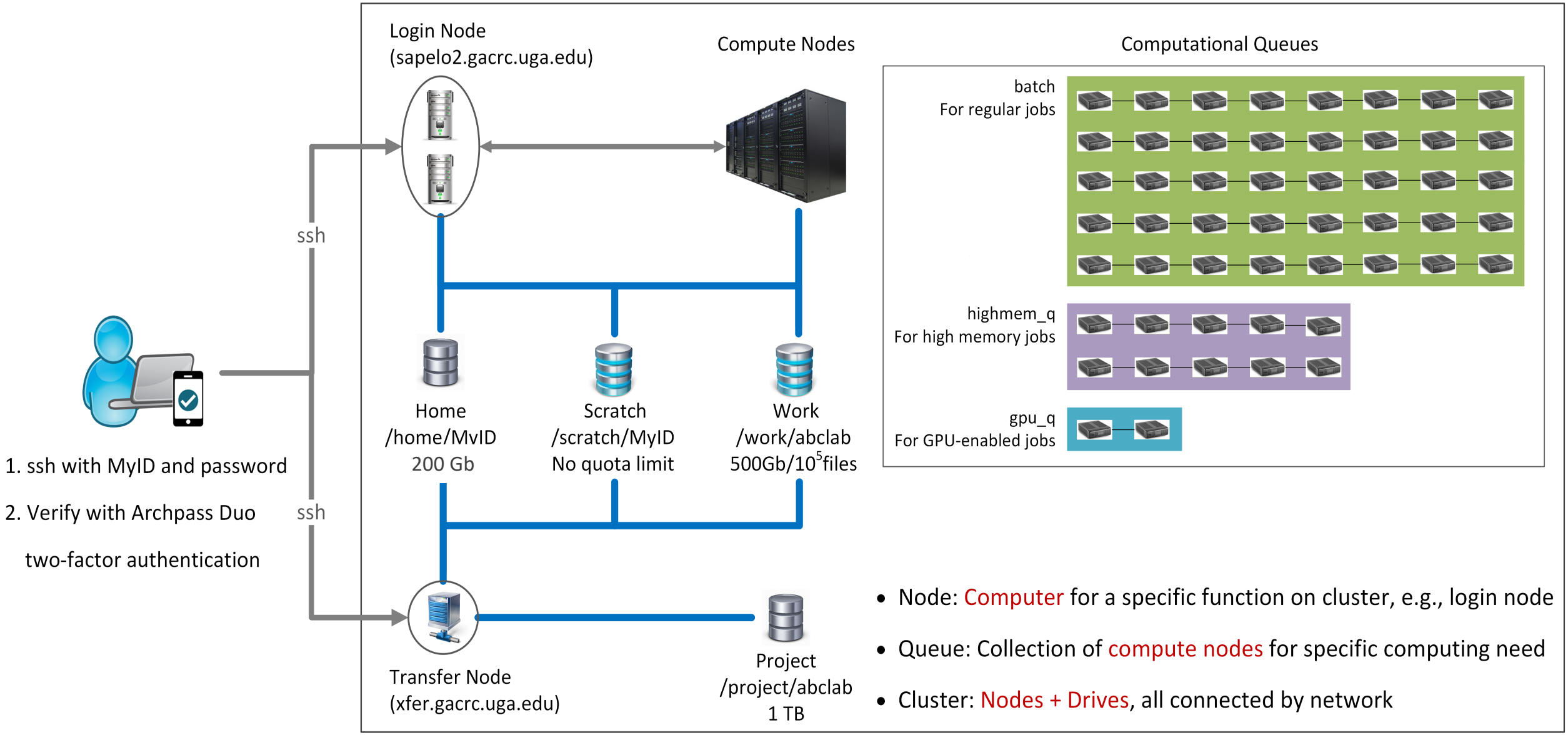
GACRC

- A high-performance-computing (HPC) center at the UGA
- Provide to the UGA research and education community an advanced computing environment:
  - HPC computing and networking infrastructure located at the Boyd Data Center
  - Comprehensive collection of scientific, engineering and business applications
  - Consulting and training services

Wiki: http://wiki.gacrc.uga.edu

Support: https://uga.teamdynamix.com/TDClient/Requests/ServiceCatalog?CategoryID=11593

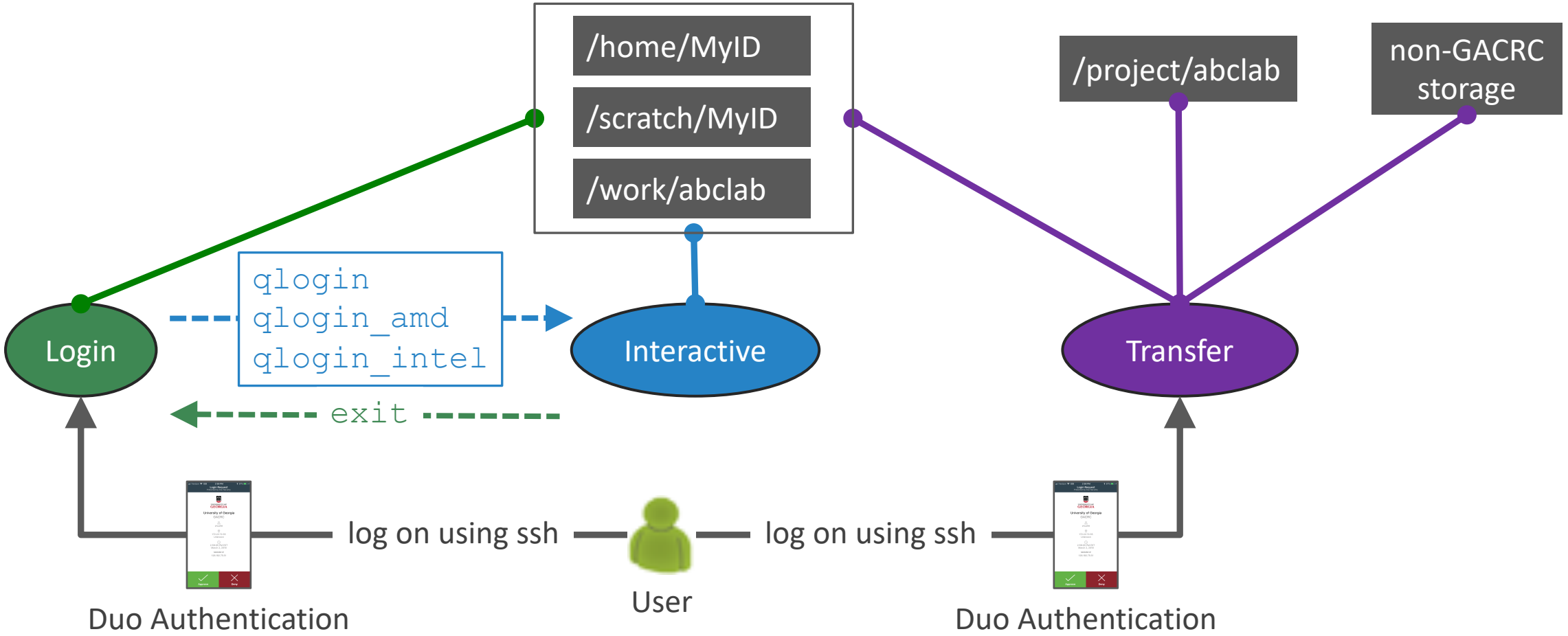
Web Site: http://gacrc.uga.edu



- Node: Computer for a specific function on cluster, e.g., login node
- Queue: Collection of compute nodes for specific computing need
- Cluster: Nodes + Drives, all connected by network

Please Note: You need to connect to the UGA network using VPN when accessing from outside of the **UGA main campus**.
UGA VPN: https://eits.uga.edu/access_and_security/infosec/tools/vpn/

3 nodes and 4 Directories



Queue	Total Nodes	RAM(GB) /Node	Max Mem(GB) /Single-node job	Cores /Node	Processor Type	GPU Cards /Node	InfiniBand
batch	42	192	184	32	Intel Xeon Skylake	N/A	Yes
	32	64	58	28	Intel Xeon Broadwell		
	106	128	120	48	AMD Opteron		
	53			32	AMD EPYC		
highmem_q	9	1024	990	28|48|64	Intel Xeon Broadwell (4) AMD Opteron (1)|EPYC (4)		
	18	512	502	32|32|48	Intel Xeon Nehalem (1) AMD EPYC (8)|Opteron (6)		
gpu_q	4	192	184	32	Intel Xeon Skylake	1 NVDIA P100	
	2	128	120	16	Intel Xeon	8 NVIDIA K40m	
	4	96	90	12		7 NVIDIA K20Xm	
groupBuyin_q	variable						

"30-day purge" Policy on Scratch

https://wiki.gacrc.uga.edu/wiki/Disk_Storage#Scratch_file_system

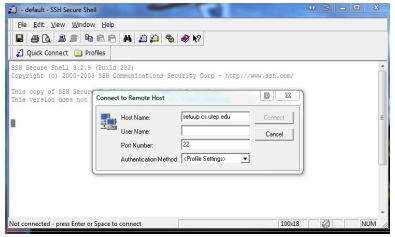
Any file that is not accessed or modified in over 30 days will be automatically deleted off the /scratch file system. Measures circumventing this policy will be monitored and actively discouraged.

- You have a list of those purgeable files located at /usr/local/var/lustre_stats/$USER.over30d.files.lst
- You are suggested to copy files from /scratch to /project or outside of GACRC
- You should first move all unnecessary files and folders to /scratch/trash/$USER
- The fastest way to save your old files is to copy them to /project area, using the fpsync utility on xfer.gacrc.uga.edu
- If you want to first create a tar archive of your /scratch area, DO NOT compress the archive when creating the archive

Job Submission Workflow

1. Linux/Mac user:
`ssh MyID@sapelo2.gacrc.uga.edu`

Windows user:



Login

2. `cd /scratch/MyID`

3. `mkdir ./workDir`
4. `cd ./workDir`

6. `nano ./sub.sh`

```
#PBS -S /bin/bash
#PBS -q batch
#PBS -N bowtie2_test
#PBS -l nodes=1:ppn=1
#PBS -l mem=2gb
#PBS -l walltime=1:00:00

#PBS -M yourMyID@uga.edu
#PBS -m ae

cd $PBS_O_WORKDIR

module load Bowtie2/2.3.3-
foss-2016b……
```

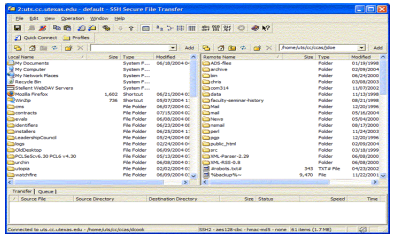
7. `$ qsub sub.sh`

8. `$ qstat_me or qdel JobID`

lustre1

5. Linux/Mac user:
`scp file MyID@xfer.gacrc.uga.edu:/scratch/MyID/workDir`

Windows user:



Computing Resources Requesting

- What are computing resources for a job?

1. Queue: batch, highmem_q, gpu_q
2. Node Feature: AMD (Opteron or EPYC), Intel (Broadwell or Skylake), EPYC, Skylake, K40, P100, etc.
3. Node Number : Serial/Threaded Job ➔ 1 node ; MPI Job ➔ N nodes (N ≥ 1)
4. Core Number :

   Serial Job ➔ 1 core

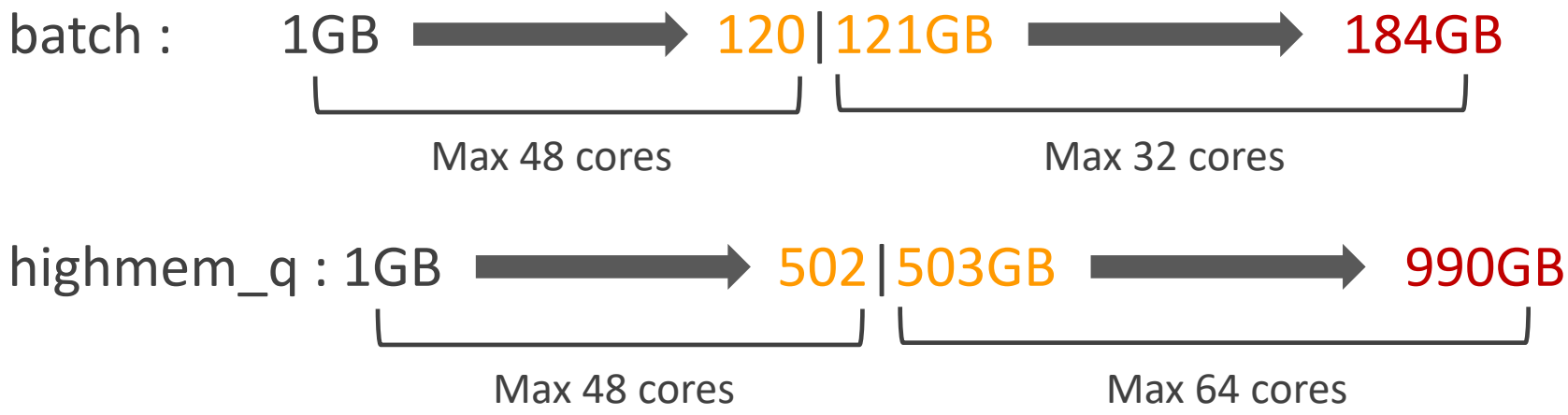
   Threaded Job ➔ Threads number t = Core number n (1≤n≤48 for batch)

   MPI Job ➔ Process number p < Core number n (`-np p` option to mpirun/mpiexec is needed!)

   p = n (1≤n≤48*N for batch, `-nq p` option is not needed)

Computing Resources Requesting

4. Maximum Memory Requestable for Serial/Threaded Job on Compute Node:



5. Wall-Clock Time: Time requested for a job running from starting to finishing:
   - Job pending time is NOT included
   - Default 1 hour, if not requested specifically

Computing Resources Requesting

- How to request computing resources for a job?

1. Request in your Sapelo2 job submission script
2. Include PBS header lines in script, e.g.:

```
#PBS -l queue=batch
#PBS -l nodes=1:ppn=24
#PBS -l mem=20gb
#PBS -l walltime=60:00:00
```

➔ Use Sapelo batch queue

➔ Request 24 cores from 1 node (AMD or Intel)

➔ Request 20GB memory

➔ Request 60 hours wall-clock time

Computing Resources Requesting

- How to know node details on queues?

mdiag -v -n | head -n 2; mdiag -v -n | grep batch

mdiag -v -n | head -n 2; mdiag -v -n | grep batch | grep Intel

mdiag -v -n | head -n 2; mdiag -v -n | grep batch | grep AMD

mdiag -v -n | head -n 2; mdiag -v -n | grep highmem

mdiag -v -n | head -n 2; mdiag -v -n | grep highmem | grep Intel

mdiag -v -n | head -n 2; mdiag -v -n | grep highmem | grep AMD

Computing Resources Requesting

- Why do my jobs have to wait so long in the queue?

  If you request computing resources incorrectly, your jobs will pend forever!

  I. You requested invalid resources, e.g., ppn=96 or mem=192gb from a batch queue node

  II. You requested too large resources which are not actually needed by a job, e.g., nodes=1, ppn=48 for a serial job; nodes=3, ppn=24 for a threaded job; walltime=480:00:00 for a short job actually needs 48 hours

  III. You requested resources which are occupied by other jobs running on cluster

Note: Jobs that cannot run across multiple nodes will not run faster if more than one node requested

Computing Resources Requesting

- How to estimate the computing resources needed, before you run the job?

  Option1: Refer to sample scripts on GACRC Wiki Software page:

  https://wiki.gacrc.uga.edu/wiki/Software

  Option2: Do computing resource scaling-up by running testing job (suggested!)

Computing Resources Requesting

- How to do computing resource scaling-up by running testing job?

1. Reduce your computational scale to a smaller testing one:

   E.g. 1: Actual 20 threads ➔ Testing 4 threads : scaling factor f ~ 5

   E.g. 2: Actual 10GB input data ➔ Testing 2GB input data : scaling factor f ~ 5

2. Make testing job submission script requesting smaller computing resources, and submit it
3. After job finished successfully, `qstat -j JobID` gives `resources_used.vmem` and `resources_used.walltime` numbers, e.g., 4GB and 5 hours
4. Do computing resources scaling-up for actual job using f and the above two numbers:

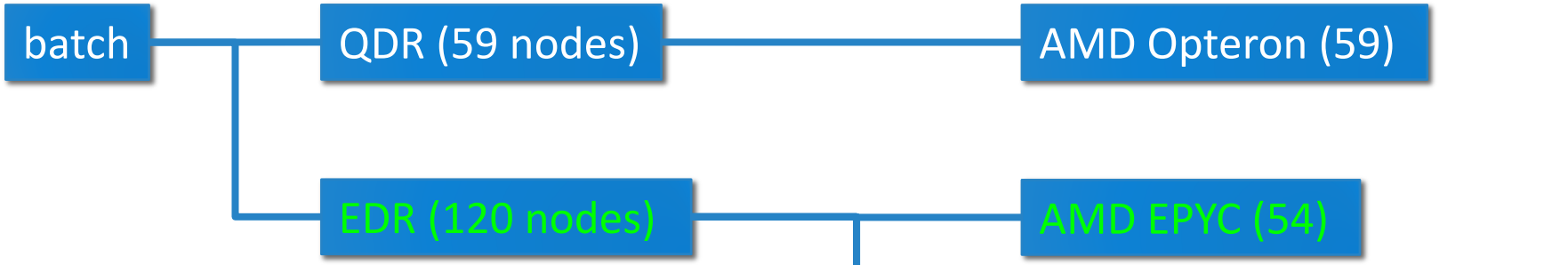
   E.g. 1: f ~ 5 ➔ Actual ~20 GB and ~1 hours

   E.g. 2: f ~ 5 ➔ Actual ~20GB and ~25 hours

Note: Scaling may not be linear

Run MPI Job

Sapelo2 nodes Sapelo2 nodes communicate via InfiniteBand (IB): QDR and EDR




```
mdiag -v -n | grep batch | grep QDR
mdiag -v -n | grep batch | grep EDR
```

Run MPI Job – PBS headers for running MPI job

Scenario 1: Request multiple nodes; use ALL cores from each node

#PBS -l queue=batch	➔ Use batch queue
#PBS -l nodes=2:ppn=32:EPYC	➔ Request 64 cores from 2 AMD EPYC nodes (EDR)
#PBS -l pmem=2gb	➔ Request 2GB memory for each MPI process, so 64GB/node ✓
#PBS -l walltime=60:00:00	➔ Request 60 hours wall-clock time

#PBS -l queue=batch	➔ Use batch queue
#PBS -l nodes=4:ppn=32:Skylake	➔ Request 128 cores from 4 Intel Skylake nodes (EDR)
#PBS -l pmem=4gb	➔ Request 4GB memory for each MPI process, so 128GB/node ✓
#PBS -l walltime=60:00:00	➔ Request 60 hours wall-clock time

Run MPI Job – PBS headers for running MPI job

Scenario 2: Request multiple nodes; does NOT use all cores from each node

#PBS -l queue=batch	➔ Use batch queue
#PBS -l nodes=5:ppn=12:EDR	➔ Request 60 cores from 5 EDR nodes (AMD or Intel)
#PBS -l pmem=2gb	➔ Request 2GB memory for each MPI process, so 24GB/node ✓
#PBS -l walltime=60:00:00	➔ Request 60 hours wall-clock time

#PBS -l queue=batch	➔ Use batch queue
#PBS -l nodes=5:ppn=12:AMD:EDR	➔ Request 60 cores from 5 AMD EDR nodes (AMD EPYC)
#PBS -l pmem=5gb	➔ Request 5GB memory for each MPI process, so 60GB/node ✓
#PBS -l walltime=60:00:00	➔ Request 60 hours wall-clock time

Run MPI Job – MPI libraries installed on Sapelo2

https://wiki.gacrc.uga.edu/wiki/MPI

When run MPI software using MVAPICH2, you will need to differentiate EDR from QDR;

But it is not necessary for OpenMPI

module spider MVAPICH2

QDR Versions:	EDR Versions:
MVAPICH2/2.2-GCC-5.4.0-2.26	MVAPICH2/2.3-GCC-5.4.0-2.26-EDR
MVAPICH2/2.2-GCC-6.4.0-2.28	MVAPICH2/2.3-GCC-6.4.0-2.28-EDR
MVAPICH2/2.2-iccifort-2013_sp1.0.080	MVAPICH2/2.3-iccifort-2013_sp1.0.080-EDR
MVAPICH2/2.2-iccifort-2015.2.164-GCC-4.8.5	MVAPICH2/2.3-iccifort-2015.2.164-GCC-4.8.5-EDR
MVAPICH2/2.2-iccifort-2018.1.163-GCC-6.4.0-2.28	MVAPICH2/2.3-iccifort-2018.1.163-GCC-6.4.0-2.28-EDR

Run MPI Job – Memory request for MPI job

Memory request for MPI job: using pmem, instead of mem, in your job script

For example:

#PBS -l pmem=2gb

pmem: maximum memory for each MPI process

Run MPI Job – sample scripts running MPI jobs

```
#PBS -S /bin/bash
#PBS -q batch
#PBS -N testmpi4py
#PBS -l nodes=1:ppn=12:EDR
#PBS -l pmem=1gb
#PBS -l walltime=4:00:00
cd $PBS_O_WORKDIR
ml Python/2.7.14-foss-2016b
mpirun python ./testmpi4py.py
```

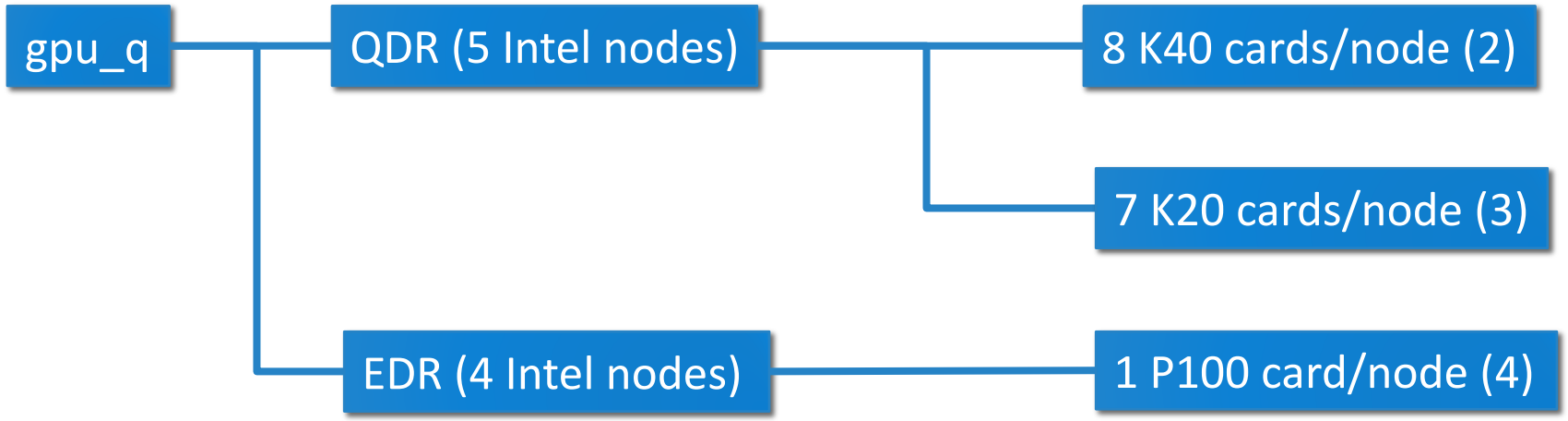
```
#PBS -S /bin/bash
#PBS -q batch
#PBS -N testraxml
#PBS -l nodes=2:ppn=48:EDR
#PBS -l walltime=48:00:00
#PBS -l pmem=2g
 #PBS -j oe
#PBS -M MyID@uga.edu
#PBS -m ae
cd $PBS_O_WORKDIR
ml RAxML/8.2.11-foss-2016b-mpi-avx
mpirun raxmlHPC-MPI-AVX [options]
```

Run GPU Job

https://wiki.gacrc.uga.edu/wiki/Running_Jobs_on_Sapelo2#GPU.2FCUDA

- How to know node details on gpu_q?

mdiag -v -n | head -n 2 ; mdiag -v -n | grep gpu_q



Run GPU Job – PBS headers for running GPU job

https://wiki.gacrc.uga.edu/wiki/Running_Jobs_on_Sapelo2#GPU.2FCUDA

Scenario 1: Request one or more CPU cores with one or more GPU devices

#PBS -l queue=gpu_q	➔ Use gpu_q queue
#PBS -l nodes=1:ppn=1:gpu=1	➔ Request 1 CPU core with 1 GPU card from 1 node (EDR or QDR)
#PBS -l mem=10gb	➔ Request 10GB total memory
#PBS -l walltime=60:00:00	➔ Request 60 hours wall-clock time

#PBS -l queue=gpu_q	➔ Use gpu_q queue
#PBS -l nodes=1:ppn=4:gpu=2	➔ Request 4 CPU cores with 2 GPU cards from 1 node (EDR or QDR)
#PBS -l mem=20gb	➔ Request 20GB total memory
#PBS -l walltime=60:00:00	➔ Request 60 hours wall-clock time

Run GPU Job – PBS headers for running GPU job

Scenario 2: Request one or more GPU devices with specific device selection

#PBS -l queue=gpu_q	➔ Use gpu_q queue
#PBS -l nodes=1:ppn=4:gpu=1:K20	➔ Request 4 CPU cores with 1 K20 GPU card from 1 node (QDR)
#PBS -l mem=20gb	➔ Request 20GB total memory
#PBS -l walltime=60:00:00	➔ Request 60 hours wall-clock time

#PBS -l queue=gpu_q	➔ Use gpu_q queue
#PBS -l nodes=1:ppn=4:gpu=1:P100	➔ Request 4 CPU cores with 1 P100 GPU card from 1 node (EDR)
#PBS -l mem=20gb	➔ Request 20GB total memory
#PBS -l walltime=60:00:00	➔ Request 60 hours wall-clock time

Run GPU Job – PBS headers for running GPU job

Scenario 3: Run more than one process at a time on the GPU node by selecting "Default" compute mode

#PBS -l queue=gpu_q	➔ Use gpu_q queue
#PBS -l nodes=1:ppn=4:gpu=1:default	➔ Request 4 CPU cores with 1 GPU card from 1 node (QDR)
#PBS -l mem=20gb	➔ Request 20GB total memory
#PBS -l walltime=60:00:00	➔ Request 60 hours wall-clock time

#PBS -l queue=gpu_q	➔ Use gpu_q queue
#PBS -l nodes=1:ppn=4:gpu=1:P100:default	➔ Request 4 CPU cores with 1 P100 GPU card from 1 node (EDR)
#PBS -l mem=20gb	➔ Request 20GB total memory
#PBS -l walltime=60:00:00	➔ Request 60 hours wall-clock time

Run GPU Job – Useful environment variable for GPU job

https://wiki.gacrc.uga.edu/wiki/Running_Jobs_on_Sapelo2#GPU.2FCUDA

1. PBS_GPUFILE : The name of a file storing GPU devices allocated to your GPU job:

   ```
   echo $PBS_GPUFILE
   ```

2. To get a list of the numbers of the GPU devices allocated to your job, separated by a blank space, use the command:

   ```
   CUDADEV=$(cat $PBS_GPUFILE | rev | cut -d"u" -f1)
   echo "List of devices allocated to this job:"
   echo $CUDADEV
   ```

Run GPU Job – GPU utilization of a GPU job

E.g. a job is running on gn164 (a K20 node), from login node:

```
ssh  gn164  nvidia-smi
```

```
Thu Jan 9 21:35:33 2020
+-----------------------------------------------------------------------------+
| NVIDIA-SMI 410.48 Driver Version: 410.48 |
|-------------------------------+----------------------+----------------------+
| GPU Name Persistence-M| Bus-Id Disp.A | Volatile Uncorr. ECC |
| Fan Temp Perf Pwr:Usage/Cap| Memory-Usage | GPU-Util Compute M. |
|===============================+======================+======================|
| 0 Tesla K20Xm On | 00000000:0C:00.0 Off | 0 |
| N/A 38C P0 70W / 235W | 883MiB / 5700MiB | 32% Default |
+-------------------------------+----------------------+----------------------+
| 1 Tesla K20Xm On | 00000000:0D:00.0 Off | 0 |
| N/A 43C P0 90W / 235W | 3211MiB / 5700MiB | 65% Default |
+-------------------------------+----------------------+----------------------+
| 2 Tesla K20Xm On | 00000000:11:00.0 Off | 0 |
| N/A 46C P0 81W / 235W | 3211MiB / 5700MiB | 64% Default |
+-------------------------------+----------------------+----------------------+
.....
```

Obtain Job Details

https://wiki.gacrc.uga.edu/wiki/Monitoring_Jobs_on_Sapelo2

Option 1:

`qstat -n1 -u MyID` for running/pending/completed jobs on cluster

`qstat -n1r -u MyID` for running jobs on cluster

`qstat -n1rt -u MyID` for running jobs on cluster, showing each array job element

Option 2:

`qstat -f JobID` for detail info of a running jobs or finished job within 24 hours

Option 3:

Email notification from finished jobs (completed, canceled, or crashed), if using:

```
#PBS -M MyID@uga.edu
#PBS -m ae
```

Guideline Tips

- Do NOT use Login Node to run jobs ➔ Interactive Node OR submit job to queue
- Do NOT use Login Node upload or download data to/from cluster ➔ Transfer Node
- Do NOT use Login Node to transfer data on cluster
- NO large memory job running on batch queue ➔ highmem_q
- NO small memory job running on highmem queue ➔ batch
- As a general rule, thread number for running software = core number requested

Practical Tips

- Each directory should not have too many files inside! A rule of thumb would be to try to keep no more than a few tens of thousands of files (<10000 would be even better) in any single directory which is accessed frequently.

All files are in ONE single dir!

Files are organized in subdirs!

Practical Tips

- Job name should have a specific computational meaning.

  Good Examples: `#PBS -N blastn_dataSet1_trail2 ; #PBS -N M-10-1121`

  Bad Examples: `#PBS -N job1 ; #PBS -N bowtie ; #PBS -N 20160930`

- Redirect standard output and error of the application to a log file, instead of letting it be written in the stdout .o file and stderr .e file of the job, e.g.:

  ```
  time application >log 2>&1
  ```

- Monitor job progress from time to time, to catch if a job gets stuck

Thank You!

Telephone Support

EITS Help Desk: 706-542-3106

Monday – Thursday: 7:30 a.m. – 7:30 p.m.

Friday: 7:30 a.m. – 6 p.m.

Saturday – Sunday: 1 p.m. – 7 p.m.

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