High Performance Computing (HPC) on GACRC Sapelo2 Cluster

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Outline

- GACRC
- What is High Performance Computing (HPC)?
- What is a Cluster?
- How to Work on Cluster?

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

What is High Performance Computing?

1 worker

10 years later……

What is High Performance Computing? (cont.)

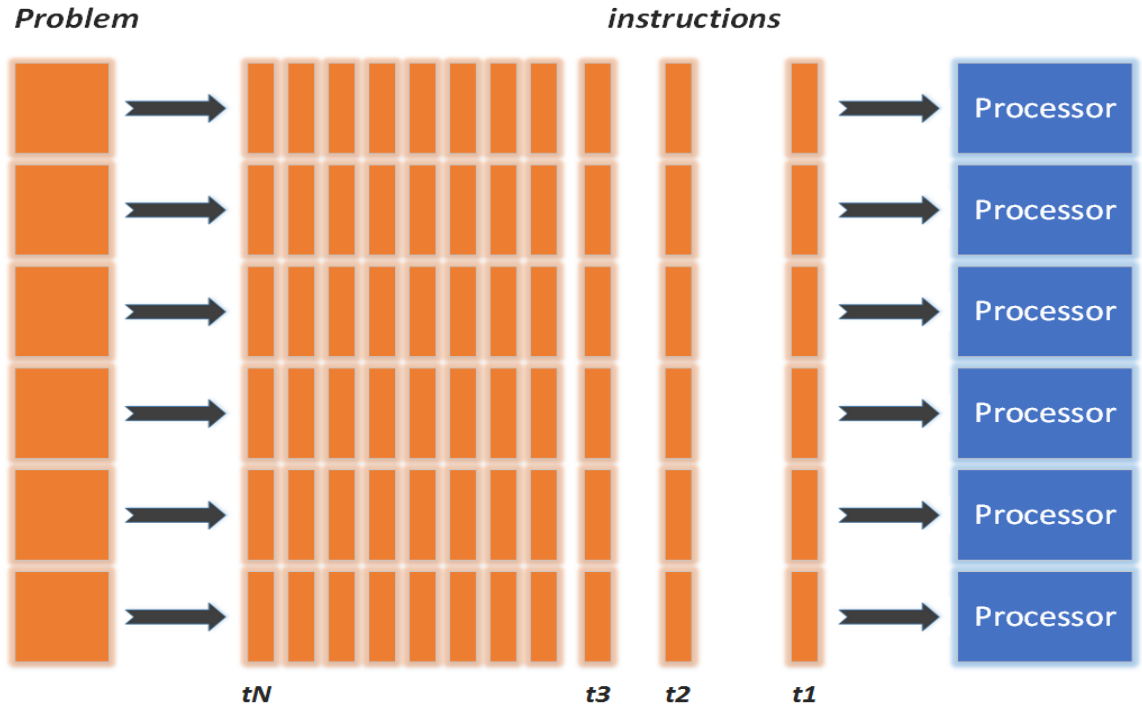
2 months later……

What is High Performance Computing? (cont.)

Serial Job with 1 worker

- ✓ Only 1 instruction executed at any time point on a single processor

Parallel Job with 6 workers

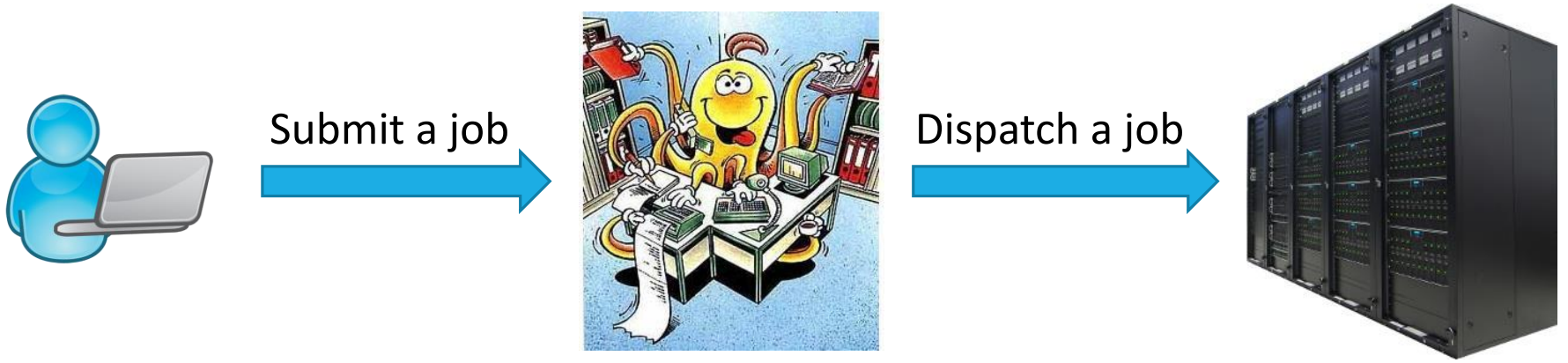


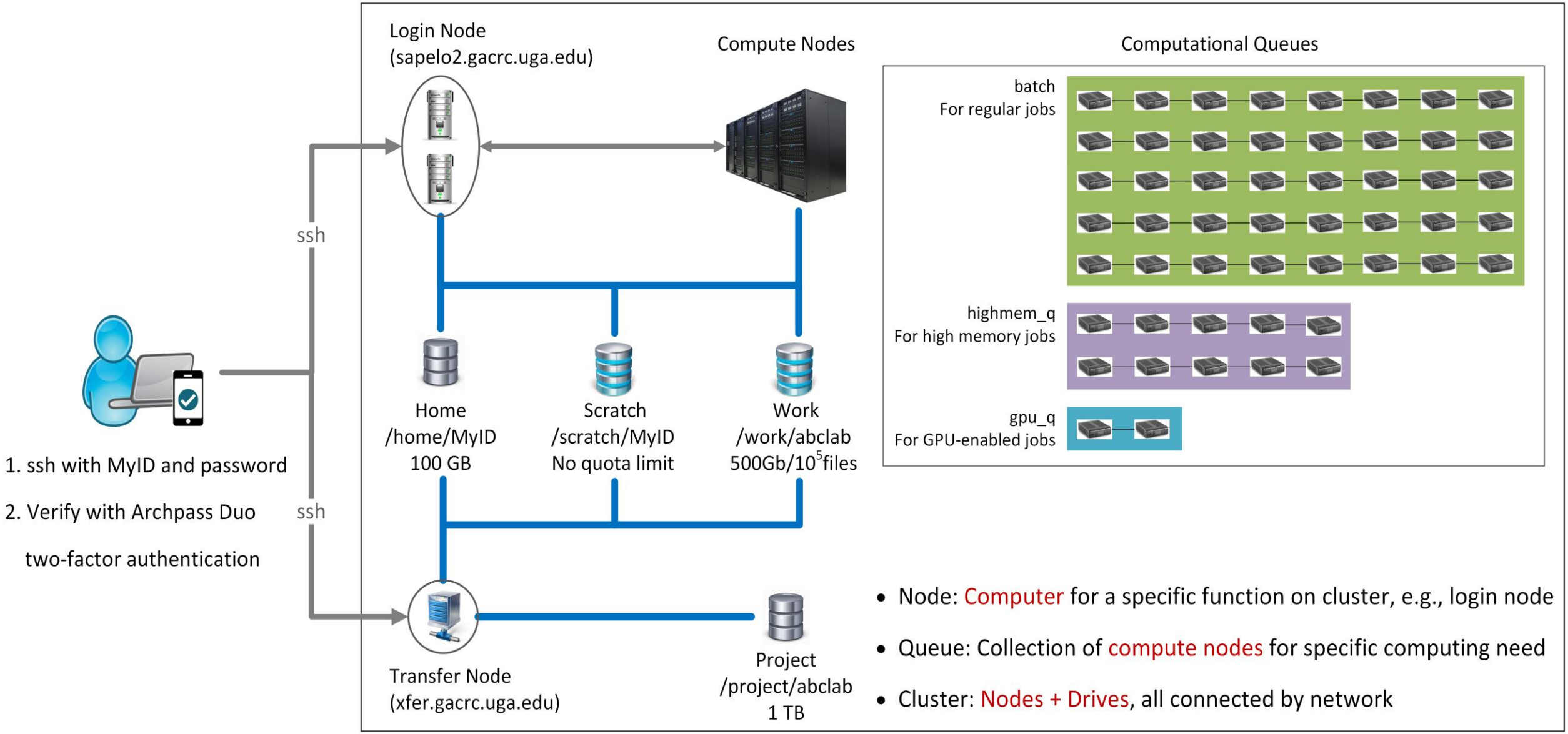
- ✓ 6 instructions executed *simultaneously* on *6* processors
- ✓ Shared-memory threaded parallel job or MPI distributed parallel job (Message Passing Interface)

What is a Cluster?

When you work on cluster, 3 roles are working:

- You: Who submit a job
- Queueing System: Who dispatch your job to run on cluster
- Cluster: Who run your job





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/

Overview https://wiki.gacrc.uga.edu/wiki/Systems#Sapelo2

- Two Nodes:
  1. Login node for batch job workflow: MyID@sapelo2.gacrc.uga.edu
  2. Transfer node for data transferring: MyID@xfer.gacrc.uga.edu
- Five Directories:
  1. Home: Login landing spot; 100GB quota; Backed-up
  2. Scratch: High-speed storage for temp files needed for current jobs; NO quota; NOT backed-up
  3. Work: High-speed storage for input files needed for repeated jobs; per group quota of 500GB and max 100,000 single files; NOT backed-up
  4. Project: Temporary data parking; per group quota of 1TB; Backed-up (ONLY accessible from Transfer node!)
  5. Local Scratch: Local storage on each individual compute node; 200GB quota; NOT backed-up
- Four Computational Queues: batch, highmem_q, gpu_q, groupBuyin_q

Overview (cont.)

- To connect to cluster, you need to have a user account:

1. Group PI request a user account for you: http://help.gacrc.uga.edu/userAcct.php
2. You need to pass new user training: https://wiki.gacrc.uga.edu/wiki/Training
3. We send you a welcome letter with detailed info about your Sapelo2 user account

- Once your account is provisioned, use SSH Secure Shell program to open connection: https://wiki.gacrc.uga.edu/wiki/Connecting

How to work on cluster?

Your job working space is global scratch folder /scratch/MyID/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- Why?

  High-performance filesystem with the fastest I/O!

- How to access?

  From Login node, `cd /scratch/MyID`

- What do you need?

  Software! We installed ~1000 software on cluster for you. Check if the software you need is already installed at https://wiki.gacrc.uga.edu/wiki/Software

- What do you need to pay attention to?

  Clean up data you will not need after your job is finished!

Workflow Diagram

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`

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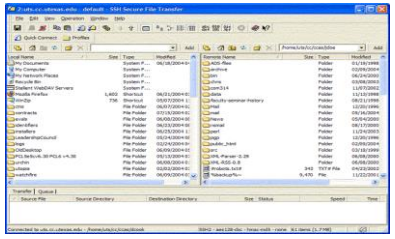
5. Linux/Mac user:
`scp file MyID@xfer.gacrc.uga.edu:/scratch/MyID/workDir`

Windows user:



Useful Links

- GACRC Web: http://gacrc.uga.edu/
- GACRC Wiki: https://wiki.gacrc.uga.edu/wiki/Main_Page
- GACRC FAQ: https://wiki.gacrc.uga.edu/wiki/Sapelo2_Frequently_Asked_Questions
- GACRC Help: http://gacrc.uga.edu/help/
- GACRC Training: https://wiki.gacrc.uga.edu/wiki/Training
- GACRC User Account: https://wiki.gacrc.uga.edu/wiki/User_Accounts
- GACRC Software: https://wiki.gacrc.uga.edu/wiki/Software

Thank You!