GACRC

Introduction to HPC Using zcluster at GACRC

On-Class PBIO/BINF 4550/6550

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Slides courtesy: Zhoufei Hou

OVERVIEW

- GACRC
- High Performance Computing (HPC)
- zcluster – Architecture, Operation
- Access and Working with zcluster

Georgia Advanced Computing Resource Center

Who Are We?

- **G**eorgia **A**dvanced **C**omputing **R**esource **C**enter (**GACRC**)
- Collaboration between the Office of Vice President for Research (**OVPR**) and
- the Office of the Vice President for Information Technology (**OVPIT**)
- Guided by a faculty advisory committee (GACRC-AC)

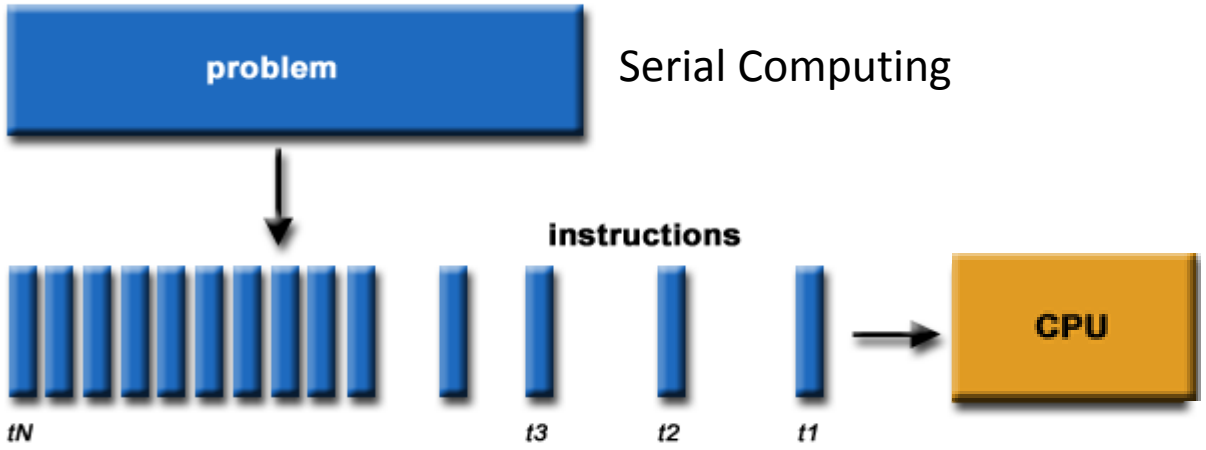
Why Are We Here?

- To provide computing hardware and network infrastructure in support of high-performance computing (**HPC**) at UGA

Where Are We?

- http://gacrc.uga.edu (Web) http://wiki.gacrc.uga.edu (Wiki)
- http://gacrc.uga.edu/help/ (Web Help)
- https://wiki.gacrc.uga.edu/wiki/Getting_Help (Wiki Help)

High Performance Computing (HPC)

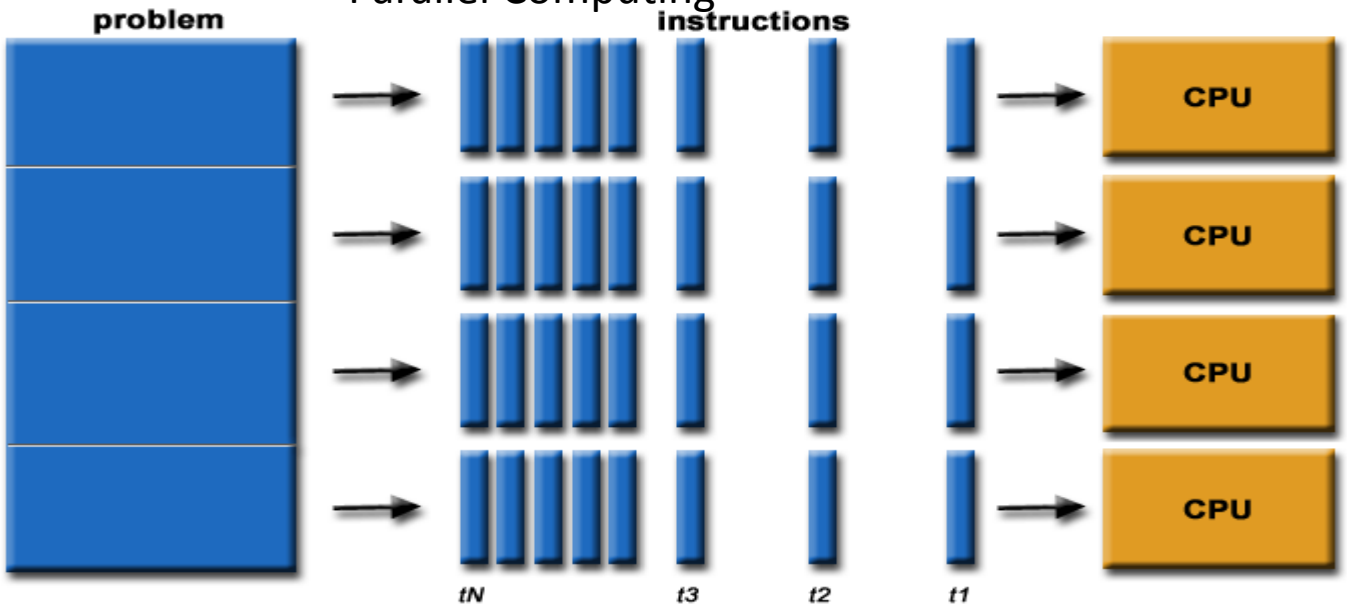


Serial Computing

Serial Computing

- A problem is broken into a discrete series of instructions
- Instructions are executed sequentially
- Executed on a single processor
- Only one instruction may execute at any moment in time

Parallel Computing



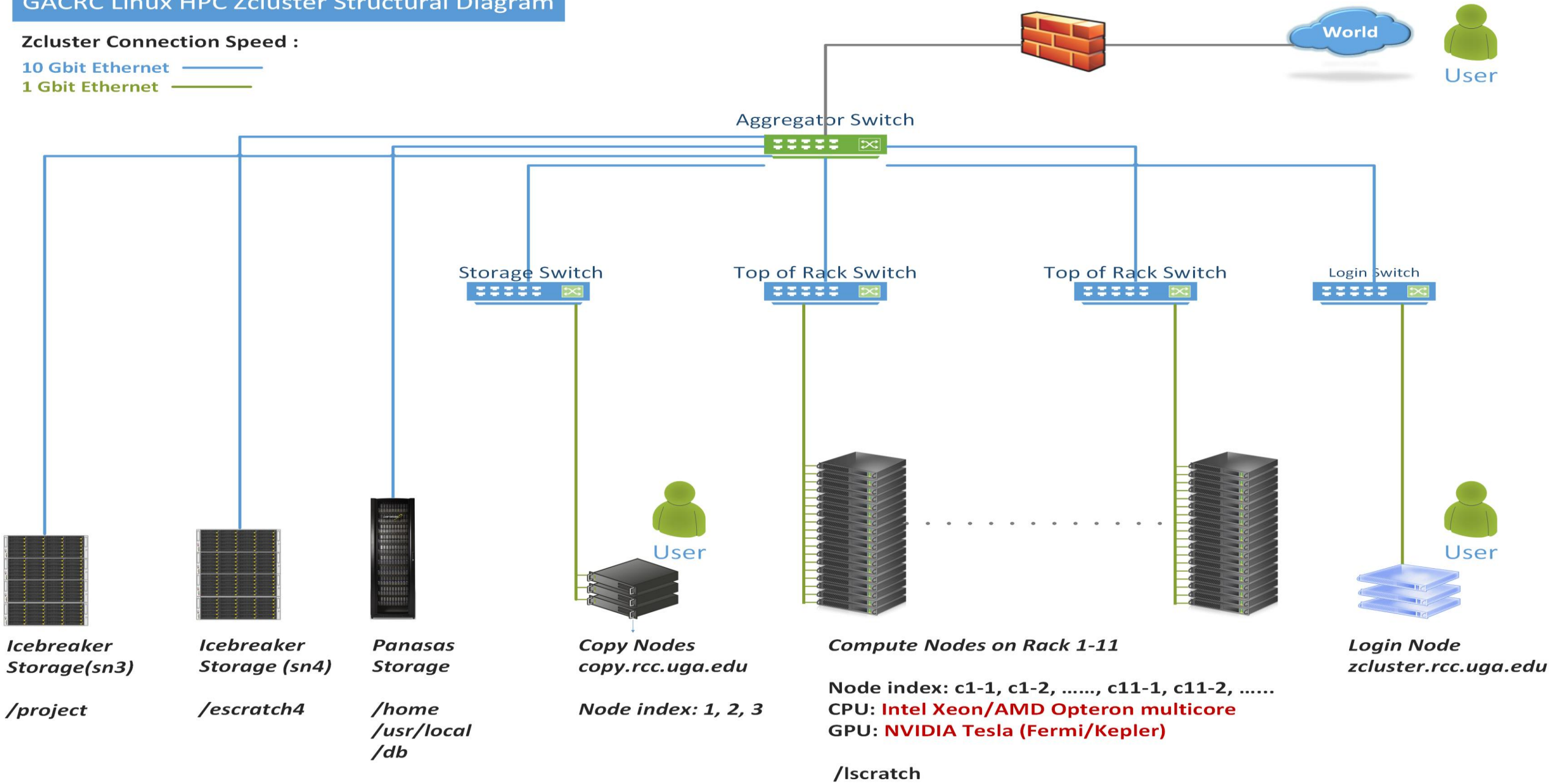
Parallel Computing

- A problem is broken into discrete parts that can be solved concurrently
- Each part is further broken down to a series of instructions
- Instructions from each part execute simultaneously on different processors
- An overall control/coordination mechanism is employed

Zcluster Overview

- zcluster Structure
- General Information
- Computing Resources
- Storage Environment

GACRC Linux HPC Zcluster Structural Diagram



zcluster – General Information

GACRC zcluster is a Linux high performance computing (HPC) cluster:

- Operating System: 64-bit Red Hat Enterprise Linux 5 (RHEL 5)

- Login Node: zcluster.rcc.uga.edu
  zcluster.rcc.uga.edu —`qlogin`→ Interactive Node: compute-14-7/9
- Copy Node: copy.rcc.uga.edu
- Internodal Communication: 1Gbit network
  - compute nodes ⇔ compute nodes
  - compute nodes ⇔ storage systems

<u>NOTE:</u> Please Do Not run jobs on the zcluster login node - use the Queues or the Interactive Nodes.

zcluster – General Information

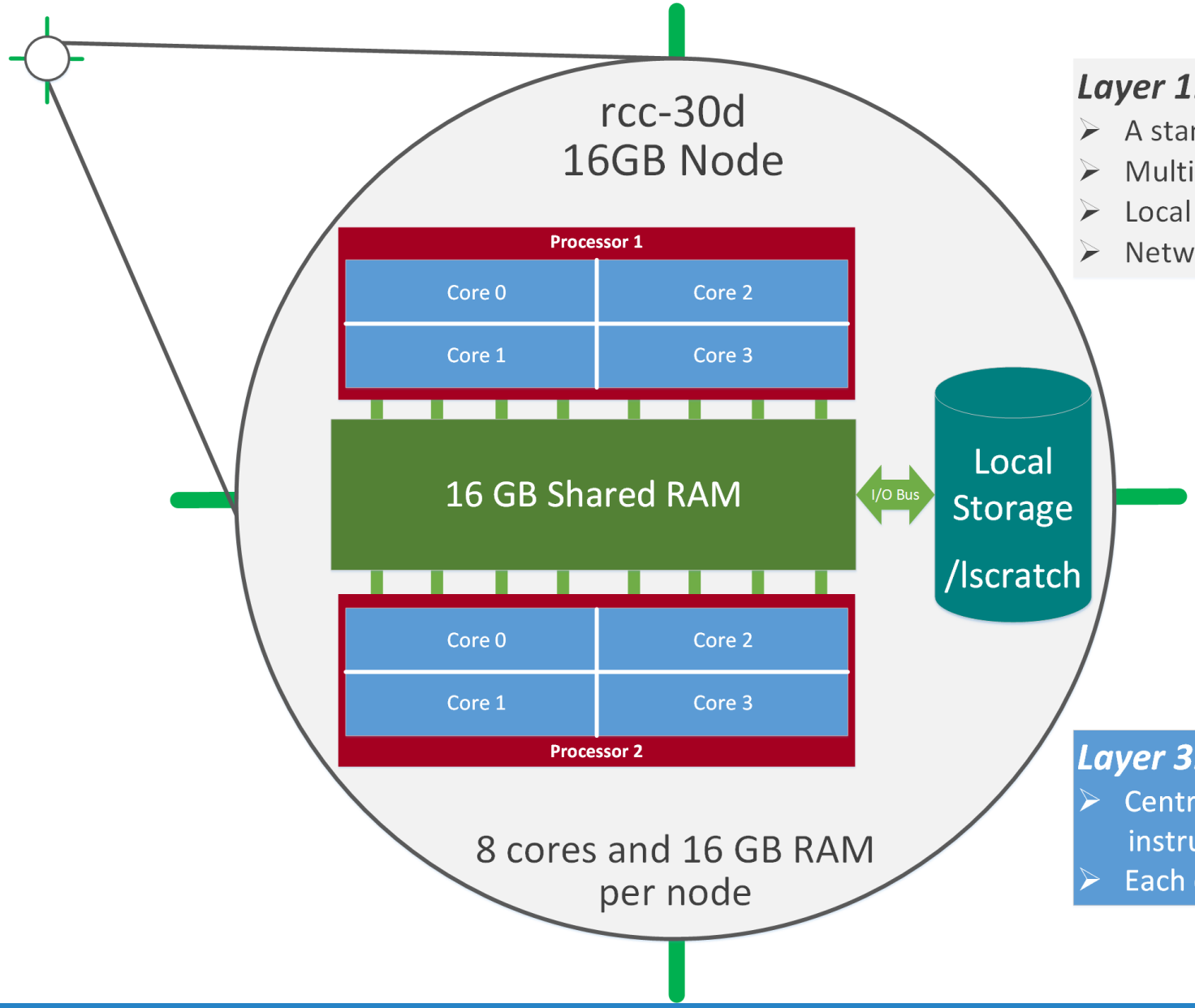
- Batch-queueing System:
  - Jobs can be started (submitted), monitored, and controlled
  - Determine which compute node is the best place to run a job
  - Determine appropriate execution priority for a job to run

- On zcluster: Sun Grid Engine (SGE)

zcluster – Computing Resources

Queue Type	Queue Name	Nodes	Processor	Cores/Node	RAM(GB)/Node	Cores	NVIDIA GPU
Regular	rcc-30d	45	Intel Xeon	12	48	540	N/A
		150		8	16	1200	
High Memory	rcc-m128-30d	1	Intel Xeon	8	128	8	N/A
		4		8	192	32	
		10		12	256	120	
	rcc-m512-30d	2		32	512	64	
Multi Core	rcc-mc-30d	6	AMD Opteron	32	64	192	N/A
Interactive	interq	2	AMD Opteron	48	132	96	N/A
GPU	rcc-sgpu-30d	2	Intel Xeon	8	48	16	4 Tesla S1070 cards
	rcc-mgpu-30d	2		12	48	24	9 Tesla (Fermi) M2070 cards
	rcc-kgpu-30d	4		12	96	24	32 Tesla (Kepler) K20Xm cards

***Total peak performance:* 23 Tflops**



Layer 1: Node

- A standalone "computer in a box"
- Multiple processors, e.g. 2, sharing memory
- Local disk storage, network interface, etc.
- Networked into a cluster

Layer 2: Processor

- A single computing component
- Multicore processor, e.g. 4 cores

Layer 3: Core

- Central processing unit (CPU) reading and executing instructions independently
- Each core is assigned to a software thread

zcluster – Storage Environment

- **Home directory** ➔ */home/student/pbio4550/s_45*
  - Mounted and visible on all nodes, with a quota of ~100GB
  - Any directory on /home has snapshot backups
    - Taken once a day, and maintained 4 daily ones and 1 weekly one
    - Name: .snapshot, e.g., /home/abclab/jsmith/.snapshot
    - Completely invisible, however, user can "cd" into it and then "ls":

```
pakala@zcluster:~$ pwd
/home/rccstaff/pakala
pakala@zcluster:~$ ls -a
.                .bash_history.compute-14-7  .bash_history.zhead  .bashrc        cmd_kill  .java     RNA_SEQ
..               .bash_history.compute-14-9  .bash_logout         batchsub_demo  e4        .mozilla  .ssh
.bash_history    .bash_history.zcluster      .bash_profile        Blast          .emacs    ncbidb    .viminfo
pakala@zcluster:~$ cd .snapshot
pakala@zcluster:~/.snapshot$ ls
2015.11.29.00.00.01.weekly  2015.12.06.00.00.01.weekly  2015.12.07.01.00.01.daily  2015.12.09.01.00.01.daily
2015.12.05.01.00.01.daily   2015.12.06.01.00.01.daily   2015.12.08.01.00.01.daily
```

➔ .snapshot is NOT shown here!

➔ Can "cd" into " .snapshot

➔ And "ls" to list its contents

zcluster – Storage Environment

- **Local scratch** ➔ /lscratch/s_45
- On **local disk** of each **compute** node ➔ node-local storage
  - rcc-30d 8-core nodes: ~18GB, rcc-30d 12-core nodes: ~370GB
  - No snapshot backup
  - Usage Suggestion: *If your job writes results to /lscratch, job submission script should move the data to your home or escratch before exit*
- **Ephemeral Scratch** ➔ /escratch4/s_45/s_20_Aug_18
  - Create with `make_escratch` command at Login Node
  - Visible to all nodes with a quota of 4TB
  - No snapshot backup
  - To be deleted after 37 days

zcluster – Storage Environment

Filesystem	Role	Quota	Accessible from	Intended Use	Notes
/home/abclab/username	Home	100GB	zcluster.rcc.uga.edu (Login) copy.rcc.uga.edu (Copy) Interactive nodes (Interactive) compute nodes (Compute)	Highly static data being used frequently	Snapshots
/escratch4/username	Scratch	4TB		Temporarily storing large data being used by jobs	Auto-deleted in 37 days
/lscratch/username	Local Scratch	18 ~ 370GB	Individual compute node	Jobs with heavy disk I/O	User to clean up
/project/abclab	Storage	Variable	copy.rcc.uga.edu (Copy)	Long-term data storage	Group sharing possible

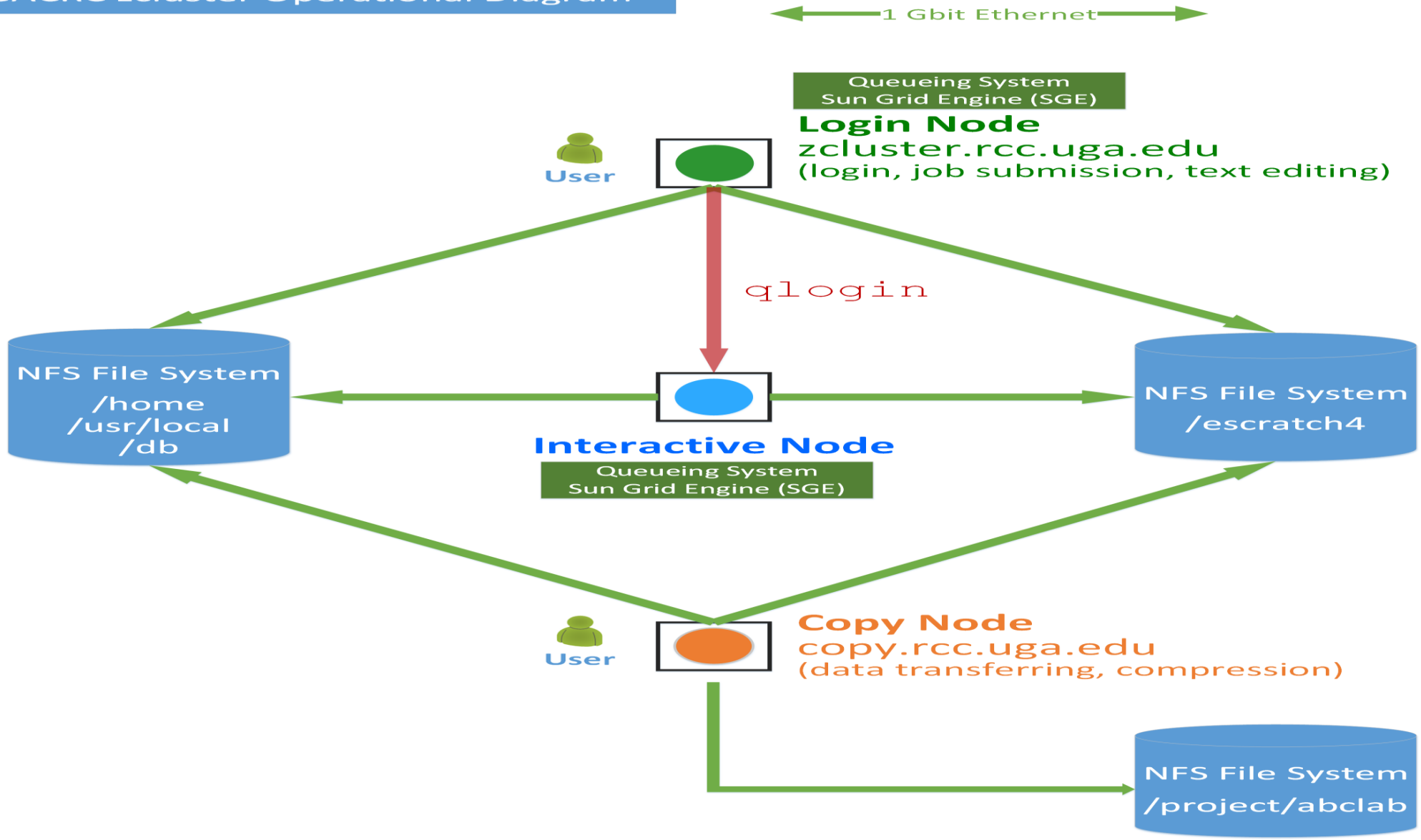
Note: 1. /usr/local : Software installation directory
/db : bioinformatics database installation directory
2. To login to Interactive nodes, use `qlogin` from Login node

zcluster – Storage Environment

6 Main Function	On/From-Node	Related Filesystem
Login Landing	Login or Copy	/home/student/pbio4550/s_45(Home) (Always!)
Batch Job Submitting	Login or Interactive	/escratch4/s_45(Scratch) (Suggested!) /home/student/pbio4550/s_45(Home)
Interactive Job Running	Interactive	/escratch4/s_45 (Scratch) /home/student/pbio4550/s_45 (Home)
Data Archiving , Compressing and Transferring	Copy	/escratch4/s_45 (Scratch) /home/student/pbio4550/s_45(Home)
Job Data Temporarily Storing	Compute	/lscratch/s_45 (Local Scratch) /escratch4/s_45 (Scratch)
Long-term Data Storing	Copy	/project/abclab

How does zcluster operate?

GACRC zcluster Operational Diagram



Longer-term data storage:
1. Lifecycle too long for /escratch4
2. Size too big for /home

How to work with zcluster? - Overview

- Start with zcluster
- Connect & Login
- Transfer Files
- Run Interactive Jobs
- Software Installed
- Submit Batch Jobs
  - How to submit ***serial***, ***threaded***, and ***MPI*** batch jobs
  - How to check job status, cancel a job, etc.

Getting Started with zcluster

- You need a User Account, e.g., s_45@zcluster.rcc.uga.edu
- Procedure: https://wiki.gacrc.uga.edu/wiki/User_Accounts
- User receives an email notification once the account is ready
- User can use `passwd` command to change initial temporary password
- A UGA faculty member (PI) may register a computing lab: http://help.gacrc.uga.edu/labAcct.php
- The PI of a computing lab may request user accounts for members of his/her computing lab: http://help.gacrc.uga.edu/userAcct.php

Connection & Login @ zcluster

- Open a connection: Open a terminal and `ssh` to your account

```
ssh s_45@zcluster.rcc.uga.edu
```

or

```
ssh -X s_45@zcluster.rcc.uga.edu
```

([1] `-X` is for X windows application running on the cluster to be forwarded to your local machine

[2] If using Windows, use SSH client to open connection, get from UGA download software page)

- Logging in: You will be prompted for your zcluster password

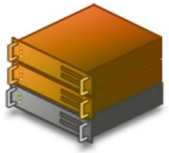
```
s_45@zcluster.rcc.uga.edu's password:
```

([3] On Linux/Mac, when you type in the password, the prompt blinks and does not move)

- Logging out: `exit` to leave the system

```
s_45@zcluster:~$ exit
```

Transfer Files @ zcluster

User's local  SCP  Transfer Node (xfer.gacrc.uga.edu)

- On Linux, Mac or cygwin on Windows : `scp [Source] [Target]`

  E.g. 1: On local machine, do Local → zcluster

```
scp file1 s_45@xfer.gacrc.uga.edu:/escratch4/s_20/s_20_Aug_18/
```

```
scp *.dat s_45@xfer.gacrc.uga.edu:/escratch4/s_20/s_20_Aug_18/
```

  E.g. 2: On local machine, do zcluster → Local

```
scp s_45@xfer.gacrc.uga.edu:/escratch4/s_20/s_20_Aug_18/file ./
```

```
scp s_45@xfer.gacrc.uga.edu:/escratch4/s_20/s_20_Aug_18/*.dat ./
```

- On Windows: FileZilla, WinSCP, SSH Secure Client, etc.

Zcluster – Tips, Dos and Don’ts

Before we start:

- To get zcluster to be your best HPC buddy, go to
  GACRC Wiki (http://wiki.gacrc.uga.edu)
  GACRC Web (http://gacrc.uga.edu)
- To get the most effective and qualified support from us, go to
  GACRC Support (https://wiki.gacrc.uga.edu/wiki/Getting_Help)
- To work happily and productively, follow the cluster’s Community Code of Conduct (CCOC)

zcluster – Tips, Dos and Don’ts - continued

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- Cluster’s CCOC:

On cluster, you are not alone... Each user is sharing finite resources, e.g., CPU cycles, RAM, disk storage, network bandwidth, with other researchers. *What you do may affect other researchers on the cluster*.

6 rules of thumb to remember:

- NO jobs running on login node
- NO multi-threaded job running with only 1 core requested
- NO large memory job running on regular nodes
- NO long job running on interactive node
- NO small memory job running on large memory nodes
- Use the copy node for file transfer and compression

Run Interactive Jobs @ zcluster

- To run an interactive job, you need to open a session on an interactive node using qlogin command:

```
pakala@zcluster:~$ qlogin
Your job 9559204 ("QLOGIN") has been submitted
waiting for interactive job to be scheduled ...
Your interactive job 9559204 has been successfully scheduled.
...
compute-14-7.local$
```

← Now I am on compute-14-7, which is an interactive node

- Current maximum runtime is 12 hours
- When you are done, remember to `exit` the session! ⚠
- Detailed information, about interactive parallel jobs. https://wiki.gacrc.uga.edu/wiki/Running_Jobs_on_zcluster

Software Installed @ zcluster

- Perl, Python, Java, awk, sed, C/C++ and Fortran compilers
- Matlab, Maple, R
- Many Bioinformatics applications: NCBI Blast+, Velvet, Trinity, TopHat, MrBayes, SoapDeNovo, Samtools, RaxML, Mafft, RAxML, PASTA, MrBayes and MP-EST etc
- RCCBatchBlast (RCCBatchBlastPlus) to distribute NCBI Blast (NCBI Blast+) searches to multiple nodes.
- Many Bioinformatics Databases: NCBI Blast, Pfam, uniprot, etc. https://wiki.gacrc.uga.edu/wiki/Bioinformatics_Databases
- For a complete list of applications: https://wiki.gacrc.uga.edu/wiki/Software

Submit Batch Jobs @ zcluster

- Components you need to submit a batch job:
  - Software already installed on zcluster
  - Job submission script to run the software,
    - ✓ Specifying working directory
    - ✓ Exporting environment variables, e.g.,
      OMP_NUM_THREADS (OpenMP threads number)
      LD_LIBRARY_PATH (searching paths for shared libraries)
- Common commands you need:
  - qsub with specifying queue name, threads or MPI rank number
  - qstat, qdel
  - qacct, qsj, etc.

Batch *Serial* Job @ zcluster

Step 1: Create a job submission script *ms.sh* running Muscle:

```
#!/bin/bash                                                  → Linux shell (bash)

cd /escratch4/s_45/s_20_Aug_18                               → Specify and enter (cd) the working directory (s_20_Aug_18)

time /usr/local/muscle/latest/bin/muscle –in seqs.fa –out seqs.afa  → 'time' command to measure amt of time it takes to run the application
```

Step 2: Submit it to the queue:

```
$qsub -q rcc-30d   ms.sh
```

OR

```
$qsub -q rcc-30d -l mem_total=20g ms.sh
```

Submit a job

Your job submission script

to the queue rcc-30d
with 16GB RAM/Node

to the queue rcc-30d
with 48GB RAM/Node

Batch *Threaded* Job @ zcluster

- **Step 1**: Create a job submission script blast.*sh* running Blast:

```
#!/bin/bash

cd /escratch4/s_45/s_20_Aug_18

time /usr/local/ncbiblast/latest/bin/blastall -p 2 [options]
```

➔ Run Blastall with 2 threads

Number of Threads = Number of Cores Requested

- **Step 2**: Submit it to the queue:

```
$ qsub -q rcc-30d -l mem_total=20g -pe thread 2 ./blast.sh
```

to the queue rcc-30d with 48GB RAM/Node

2 cores requested

Note:
Please use the rcc-mc-30d queue,
If using threads more than 8!

Batch *MPI* Job @ zcluster

❖ Step 1: Create a job submission script *sub.sh* running RAxML:

```
#!/bin/bash
cd /escratch4/pakala/pakala_Nov_13

export MPIRUN=/usr/local/mpich2/1.4.1p1/gcc 4.5.3/bin/mpirun

$MPIRUN -np $NSLOTS /usr/local/raxml/latest/raxmlHPC-MPI-SSE3 [options]
```

➔ Define and export environment variable (MPIRUN) for convenient usage

➔ Run RAxML with 20 MPI processes (-np $NSLOTS)

❖ Step 2: Submit it to the queue:

```
$ qsub -q rcc-30d -pe mpi 20 sub.sh
```

20 cores requested,
$NSLOTS will be assigned to 20 automatically, before the job submission script is interpreted

Check and Cancel Jobs @ zcluster

- To check the status of all queued and running jobs: qstat

qstat	➔ shows your job in the pool
qstat –u "*"	➔ shows all the jobs in the pool
qstat –j 12345	➔ shows detailed information, e.g., maxvmem, about the job with JOBID 12345
qstat –g t	➔ list all nodes used by your jobs

- To cancel a queued or running job: qdel

qdel –u pakala	➔ deleted all your jobs
qdel 12345	➔ deletes your job with JOBID 12345

- To list detailed information about a job: qsj, qacct

qsj 12345	➔ shows information, e.g., maxvmem, about the RUNNING job with JOBID 12345
qacct –j 12345	➔ shows information, e.g., maxvmem, about the ENDED job with JOBID 12345

How to Submit Tickets to GACRC

- For Installation/Downloading Software:
  - User needs to provide the name, version (or latest), and website
  - Applications need to be compatible with Linux
  - Note – only FREE software will be installed
- For Troubleshooting:
  - List the path of the working directory, path of the script that is producing errors, Job ID, and the command sent to the queue or interactive node
  - No need to attach the script or huge error messages
- For Testing:
  - Please have a sample dataset at your working directory, so that it can be used for debugging
- These steps will help us in responding quickly and efficiently

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THANK YOU for your patience

Questions?