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Introduction to HPC Using zcluster at GACRC

On-class PBIO/BINF8350

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Outline

- What is GACRC?
- What is HPC Concept?
- What is zcluster?
- How does zcluster operate?
- How to work with zcluster?

What is GACRC?

Who Are We?

- **G**eorgia **A**dvanced **C**omputing **R**esource **C**enter
- 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?

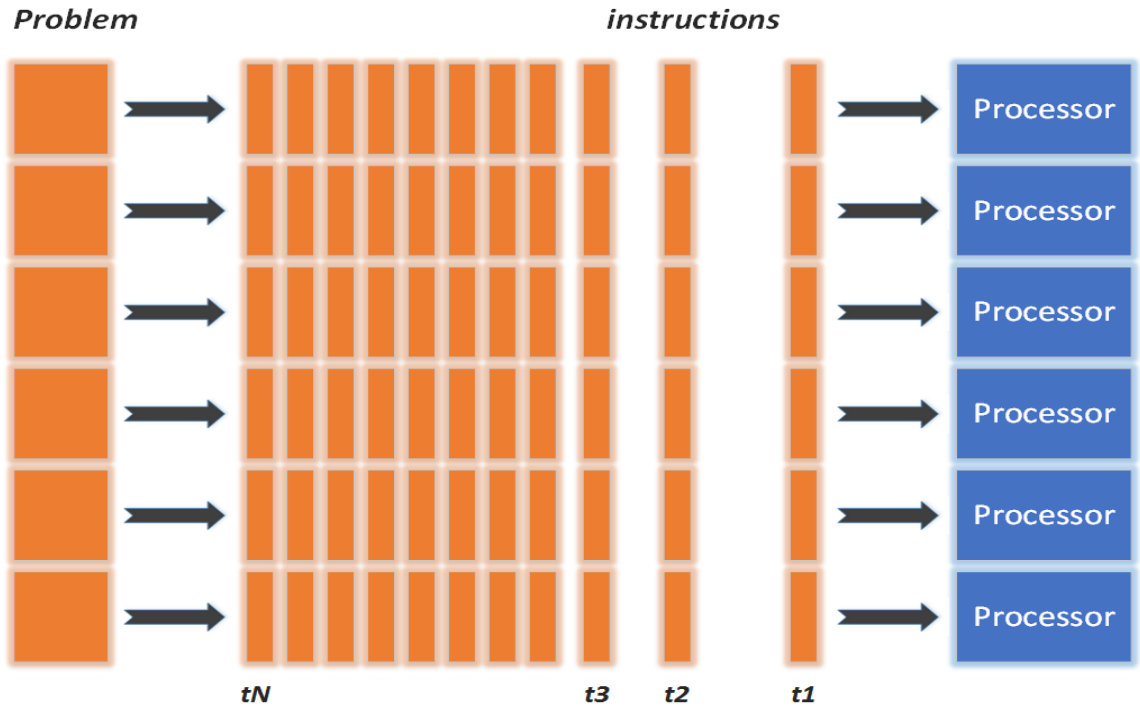
- http://gacrc.uga.edu (Web)
- http://wiki.gacrc.uga.edu (Wiki)
- http://gacrc.uga.edu/help/ (Web Help)
- https://wiki.gacrc.uga.edu/wiki/Getting_Help (Wiki Help)

Concept of High Performance Computing (HPC)

Serial:

- ✓ Serial problem can not be broken
- ✓ *Discrete* instructions executed *sequentially*
- ✓ Only *1* instruction executed at any moment on a *single* processor

Parallel:



- ✓ Problem broken into *parallel* parts can be solved *concurrently*
- ✓ Instructions executed *simultaneously* on *multiply* processors
- ✓ Synchronization/communication employed
- ✓ Shared-memory multithreaded job or MPI job (Message Passing Interface)

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What is zcluster?

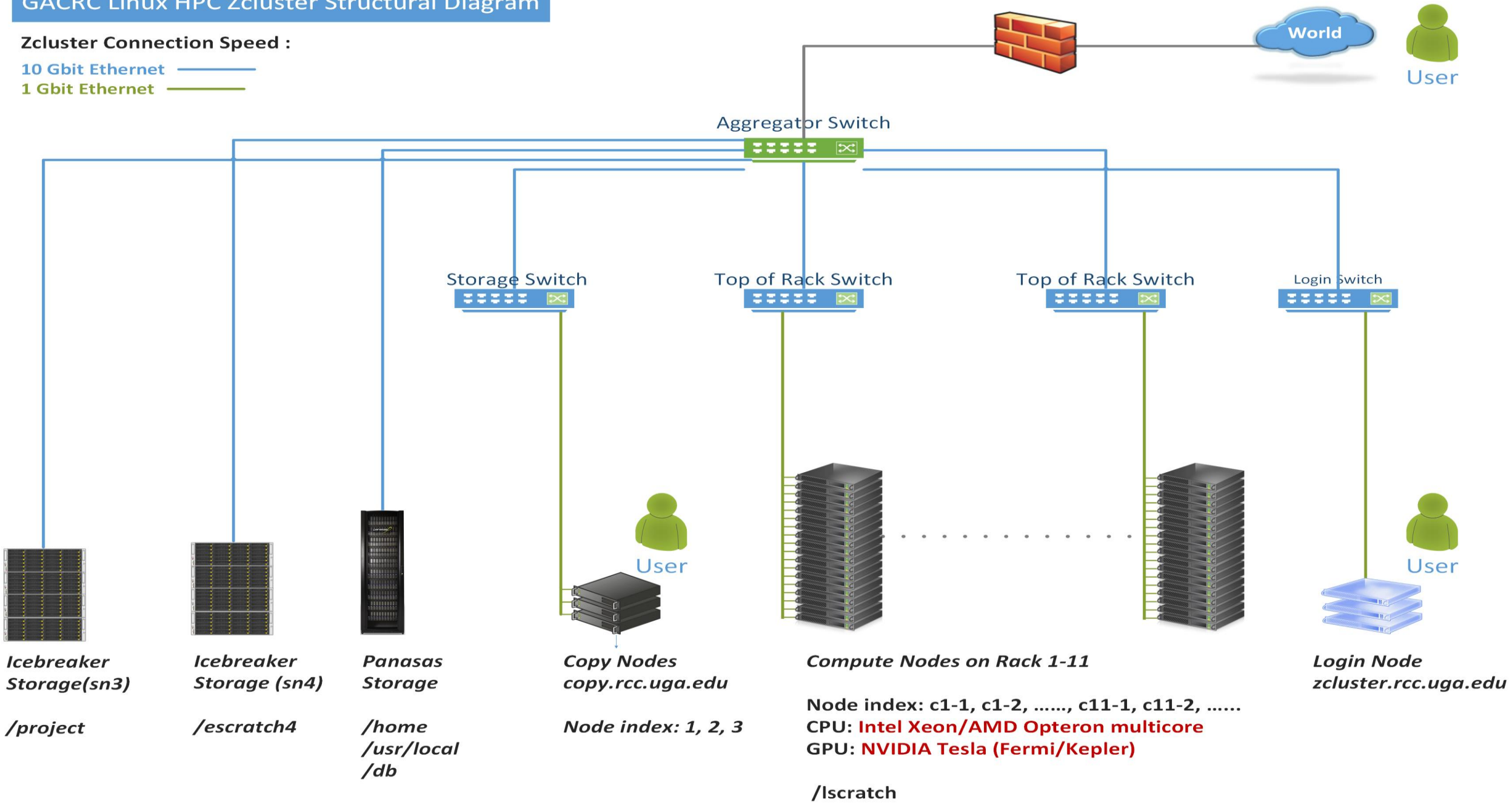
- Cluster Structural Diagram
- General Information
- Computing Resources
- Storage Environment

GACRC Linux HPC Zcluster Structural Diagram

Zcluster Connection Speed :

10 Gbit Ethernet

1 Gbit Ethernet



Icebreaker Storage(sn3)

/project

Icebreaker Storage (sn4)

/escratch4

Panasas Storage

/home
/usr/local
/db

Copy Nodes
copy.rcc.uga.edu

Node index: 1, 2, 3

Compute Nodes on Rack 1-11

Node index: c1-1, c1-2, ……, c11-1, c11-2, ……
CPU: Intel Xeon/AMD Opteron multicore
GPU: NVIDIA Tesla (Fermi/Kepler)

/lscratch

Login Node
zcluster.rcc.uga.edu

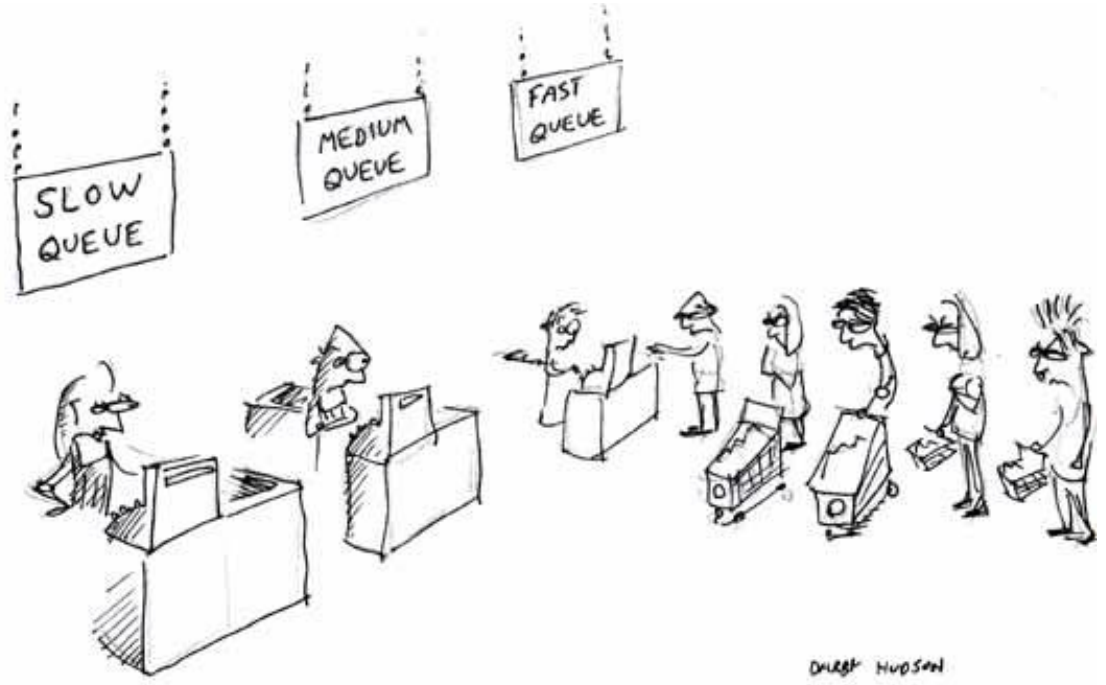
What is zcluster – General Information

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 `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

What is zcluster – General Information

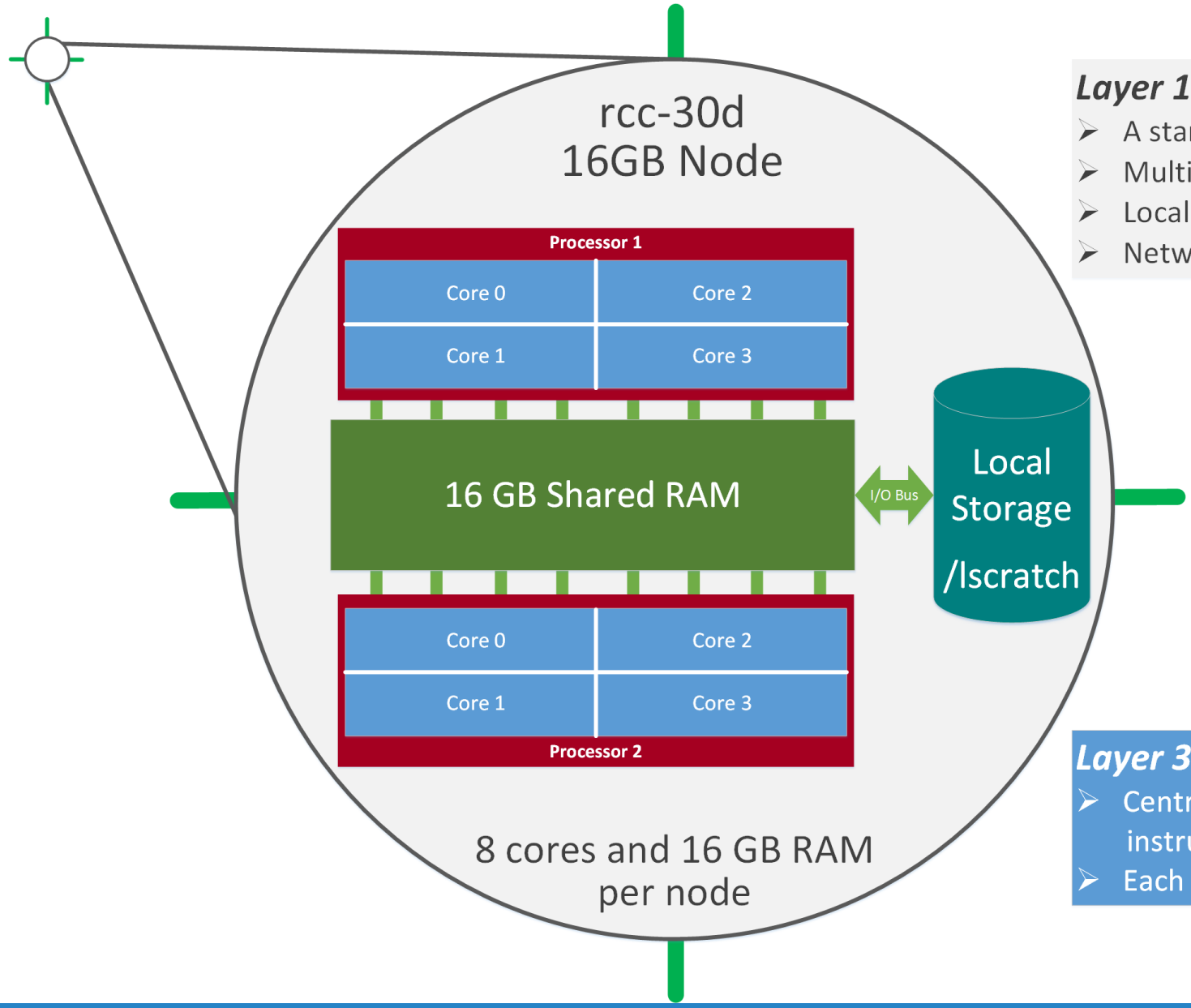
- Batch-queueing System:
  - Jobs can be started (submitted), monitored, and controlled
  - Determine which compute node is the best place to run a job
  - Determine appropriate execution priority for a job to run
- On zcluster: Sun Grid Engine (SGE)



What is 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

What is zcluster – Storage Environment

- **Home directory** ➔ /home/student/pbio8350/s_20
- 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":

```
zhuofei@zcluster:~$ ls -a
.               .bash_profile  .emacs.d    .fontconfig       .maple_history  MPIs      scripts  test.sh
..              .bashrc        .ENV_file   .gnuplot_history  .Mathematica    openMPs   serials  .viminfo
.bash_history   downloads      exe         .history          .mc             .profile  sht      .Xauthority
.bash_logout    .emacs         .flexlmrc   .lesshst          .mozilla        Pthreads  .ssh
zhuofei@zcluster:~$ cd .snapshot
zhuofei@zcluster:~/.snapshot$ ls
2015.06.21.00.00.01.weekly  2015.06.27.01.00.01.daily  2015.06.28.01.00.01.daily  2015.06.30.01.00.01.daily
2015.06.26.01.00.01.daily   2015.06.28.00.00.01.weekly 2015.06.29.01.00.01.daily
```

← .snapshot is NOT shown here!

← can "cd" into .snapshot

← then "ls" to list its contents

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What is zcluster – Storage Environment

- **Local scratch** ➔ /lscratch/s_20
  - 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_20/s_20_Jan_15
  - Create with `make_escratch` command
  - Visible to all nodes with a quota of 4TB
  - No snapshot backup
  - To be deleted after 37 days

What is zcluster – Storage Environment

Filesystem	Role	Quota	Accessible from	Intended Use	Notes
/home/student/pbio8350/s_20	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/s_20	Scratch	4TB		Temporarily storing large data being used by jobs	Auto-deleted in 37 days
/lscratch/s_20	Local Scratch	18 ~ 370GB	Individual compute node	Jobs with heavy disk I/O	User to clean up

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

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What is zcluster – Storage Environment

6 Main Function	On/From-Node	Related Filesystem
Login Landing	Login or Copy	/home/student/pbio8350/s_20 (Home) (Always!)
Batch Job Submitting	Login or Interactive	/escratch4/s_20 (Scratch) (Suggested!) /home/student/pbio8350/s_20 (Home)
Interactive Job Running	Interactive	/escratch4/s_20 (Scratch) /home/student/pbio8350/s_20 (Home)
Data Archiving , Compressing and Transferring	Copy	/escratch4/s_20 (Scratch) /home/student/pbio8350/s_20 (Home)
Job Data Temporarily Storing	Compute	/lscratch/s_20 (Local Scratch) /escratch4/s_146 (Scratch)

How does zcluster operate?

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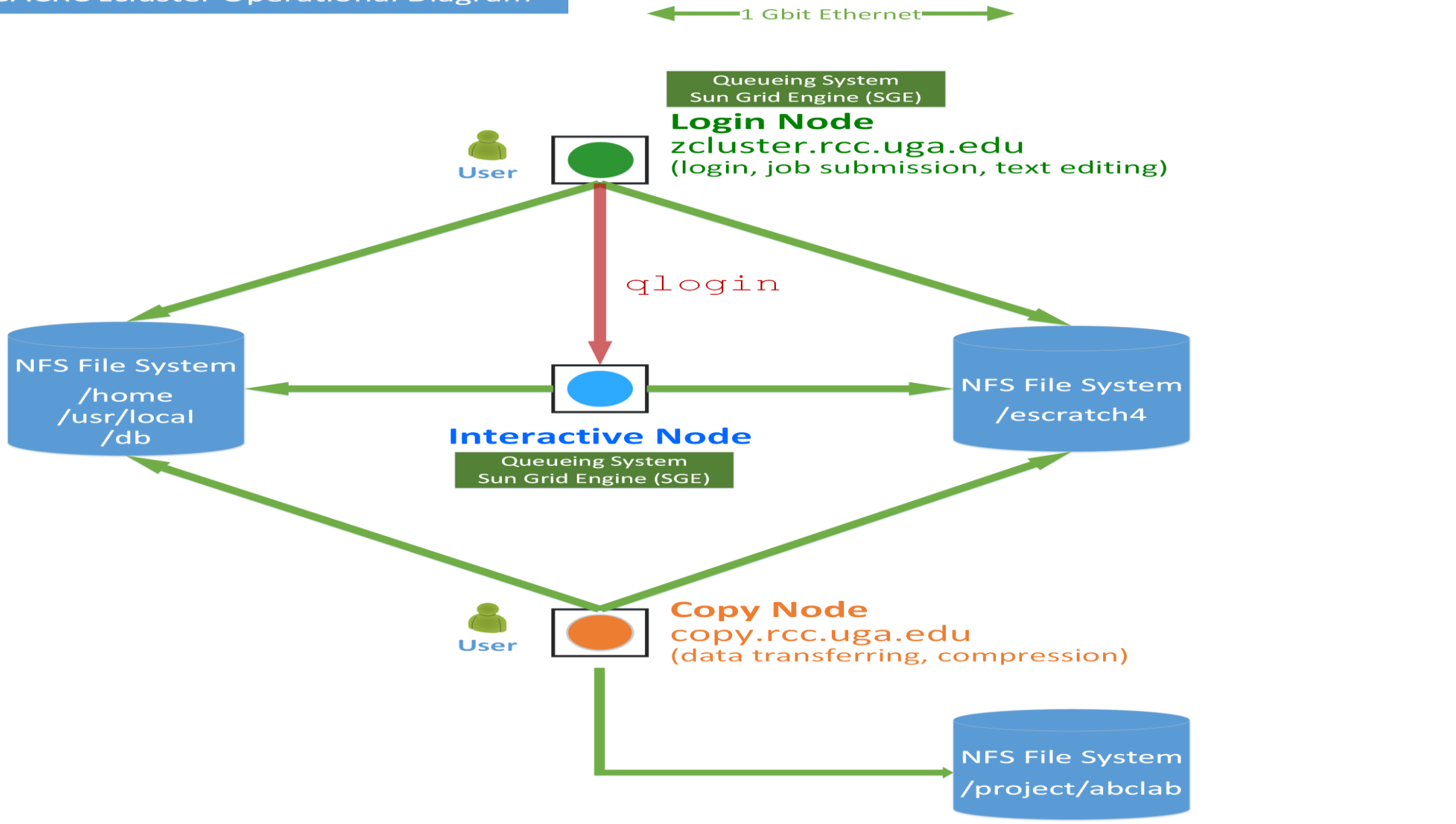
GACRC zcluster Operational Diagram



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

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How to work with zcluster?

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)

How to work with it?

- 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

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How to work with zcluster?

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

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How to work with zcluster – Start with zcluster

- You need a Class User Account : s_20@zcluster.rcc.uga.edu
- Procedure: https://wiki.gacrc.uga.edu/wiki/User_Accounts
- 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
- User receives an email notification once the account is ready
- User can use `passwd` command to change initial temporary password

How to work with zcluster – Connect & Login

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

```
ssh s_20@zcluster.rcc.uga.edu
```

or

```
ssh -X s_20@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_20@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_20@zcluster:~$ exit
```

How to work with zcluster – Transfer Files

User's local 

Copy node (copy.rcc.uga.edu) of zcluster

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

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

```
scp file1 s_20@copy.rcc.uga.edu:/escratch4/s_20/s_20_Jan_15/
```

```
scp *.dat s_20@copy.rcc.uga.edu:/escratch4/s_20/s_20_Jan_15/
```

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

```
scp s_20@copy.rcc.uga.edu:/escratch4/s_20/s_20_Jan_15/file1 ./
```

```
scp s_20@copy.rcc.uga.edu:/escratch4/s_20/s_20_Jan_15/*.dat ./
```

- On Window: FileZilla, SSH Secure Client File Transfer, WinSCP, etc.

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How to work with zcluster – Softwares Installed

- Perl, Python, Java, awk, sed, C/C++ and Fortran compilers
- Matlab, Maple, R
- Many Bioinformatics applications: NCBI Blast+, Velvet, Trinity, TopHat, MrBayes, SoapDeNovo, SAMtools, 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.
- For a complete list of applications installed: https://wiki.gacrc.uga.edu/wiki/Software

How to work with zcluster – Run Interactive Jobs

- From login node, qlogin command to open an interactive session:

Login Node: zcluster.rcc.uga.edu —qlogin→ Interactive Node: compute-14-7/9

```
s_20@zcluster:~$ qlogin
Your job 1391816 ("QLOGIN") has been submitted
waiting for interactive job to be scheduled ...
Your interactive job 1391816 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, `exit` to log out!
- Detailed information, like interactive parallel job? Go to: https://wiki.gacrc.uga.edu/wiki/Running Jobs on zcluster

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How to work with zcluster – Submit Batch Jobs

- Components you need to submit a batch job:
  - Software already installed on zcluster (Mafft, RAxML, PASTA etc.)
  - 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.

How to work with zcluster – Batch *Serial* Job

- **Step 1**: Create a job submission script *pt.sh* running PASTA:

```
#!/bin/bash
cd /escratch4/s_20/s_20_Jan_15
unset MAFFT_BINARIES
export PATH=/usr/local/python/2.7.2/bin/:${PATH}
time python2.7 /usr/local/pasta/1.6.4/run_pasta.py [options]
```

➔ Linux default shell (bash)

➔ Specify and enter (cd) working directory (/escratch4/s_20/s_20_Jan_15)

➔ Run pasta with 'time' command to measure amount of time it takes to run the application

- **Step 2**: Submit *pt.sh* to the queue:

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

Submit a job

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

job submission script

OR

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

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

How to work with zcluster – Batch *Threaded* Job

- **Step 1**: Create a job submission script *mf.sh* running Mafft:

```
#!/bin/bash

cd / escratch4/s_20/s_20_Jan_15

export PATH=/usr/local/mafft/7.215-e/bin/:${PATH}

time /usr/local/mafft/latest/bin/mafft --thread 4 in.fasta > out
```

➔ Run mafft with 4 threads

Number of Threads =
Number of Cores Requested

- **Step 2**: Submit *mf.sh* to the queue:

```
$ qsub -q rcc-30d -pe thread 4 mf.sh
```

4 cores requested

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

How to work with zcluster – Batch *MPI* Job

- **Step 1**: Create a job submission script *raxml.sh* running RAxML:

```
#!/bin/bash

cd / escratch4/s_20/s_20_Jan_15

export MPIRUN=/usr/local/mpich2/1.4.1p1/gcc 4.5.3/bin/mpirun  ➔ Define and export environment variable (MPIRUN)

$MPIRUN -np $NSLOTS /usr/local/raxml/latest/raxmlHPC-MPI-SSE3 [options]  ➔ Run RAxML with 20 MPI processes (-np $NSLOTS )
```

- **Step 2**: Submit *raxml.sh* to the queue:

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

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

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How to work with zcluster – Check and Cancel Jobs

- 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 zhuofei	➔ 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

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Thank You!