

# Introduction to HPC Using zcluster at GACRC

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Georgia Advanced Computing Resource Center

University of Georgia

Zhuofei Hou, HPC Trainer

[zhuofei@uga.edu](mailto:zhuofei@uga.edu)

# Outline

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

# What is GACRC?

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## Who Are We?

- Georgia **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)
- [https://wiki.gacrc.uga.edu/wiki/Getting\\_Help](https://wiki.gacrc.uga.edu/wiki/Getting_Help) (Support)
- <https://blog.gacrc.uga.edu> (Blog)      <http://forums.gacrc.uga.edu> (Forums)

# GACRC Users September 2015

| <b>Colleges &amp; Schools</b>                    | <b>Depts</b> | <b>PIs</b> | <b>Users</b> |
|--|--------------|------------|--------------|
| Franklin College of Arts and Sciences            | <b>14</b>    | <b>117</b> | <b>661</b>   |
| College of Agricultural & Environmental Sciences | <b>9</b>     | <b>29</b>  | <b>128</b>   |
| College of Engineering                           | <b>1</b>     | <b>12</b>  | <b>33</b>    |
| School of Forestry & Natural Resources           | <b>1</b>     | <b>12</b>  | <b>31</b>    |
| College of Veterinary Medicine                   | <b>4</b>     | <b>12</b>  | <b>29</b>    |
| College of Public Health                         | <b>2</b>     | <b>8</b>   | <b>28</b>    |
| College of Education                             | <b>2</b>     | <b>5</b>   | <b>20</b>    |
| Terry College of Business                        | <b>3</b>     | <b>5</b>   | <b>10</b>    |
| School of Ecology                                | <b>1</b>     | <b>8</b>   | <b>22</b>    |
| School of Public and International Affairs       | <b>1</b>     | <b>3</b>   | <b>3</b>     |
| College of Pharmacy                              | <b>2</b>     | <b>3</b>   | <b>5</b>     |
|  | <b>40</b>    | <b>214</b> | <b>970</b>   |
| <b>Centers &amp; Institutes</b>                  | <b>9</b>     | <b>19</b>  | <b>59</b>    |
| <b>TOTALS:</b>                                   | <b>49</b>    | <b>233</b> | <b>1029</b>  |

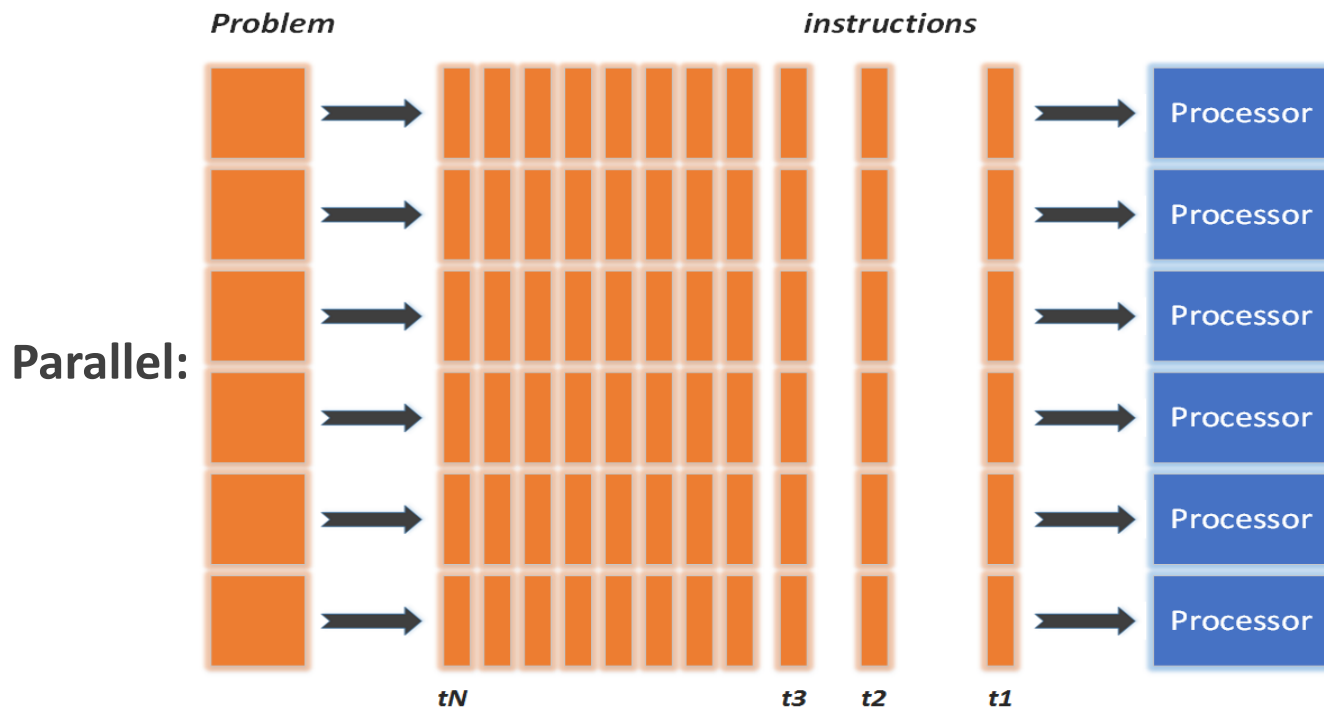
# GACRC Users September 2015

| <b>Centers &amp; Institutes</b>            | <b>PIs</b> | <b>Users</b> |
|--|------------|--------------|
| Center for Applied Isotope Study           | <b>1</b>   | <b>1</b>     |
| Center for Computational Quantum Chemistry | <b>3</b>   | <b>10</b>    |
| Complex Carbohydrate Research Center       | <b>6</b>   | <b>28</b>    |
| Georgia Genomics Facility                  | <b>1</b>   | <b>5</b>     |
| Institute of Bioinformatics                | <b>1</b>   | <b>1</b>     |
| Savannah River Ecology Laboratory          | <b>3</b>   | <b>9</b>     |
| Skidaway Institute of Oceanography         | <b>2</b>   | <b>2</b>     |
| Center for Family Research                 | <b>1</b>   | <b>1</b>     |
| Carl Vinson Institute of Government        | <b>1</b>   | <b>2</b>     |
|  | <b>19</b>  | <b>59</b>    |

# What is HPC Concept



- ✓ Problem broken into **discrete** instructions
- ✓ Instructions executed **sequentially**
- ✓ Only **1** instruction executed at any moment on a **single processor**



- ✓ Problem broken into parts can be solved **concurrently**
- ✓ Further broken into a series of instructions
- ✓ Instructions executed **simultaneously** on multiply processors
- ✓ **Synchronization/communication** mechanism employed

# What is zcluster?

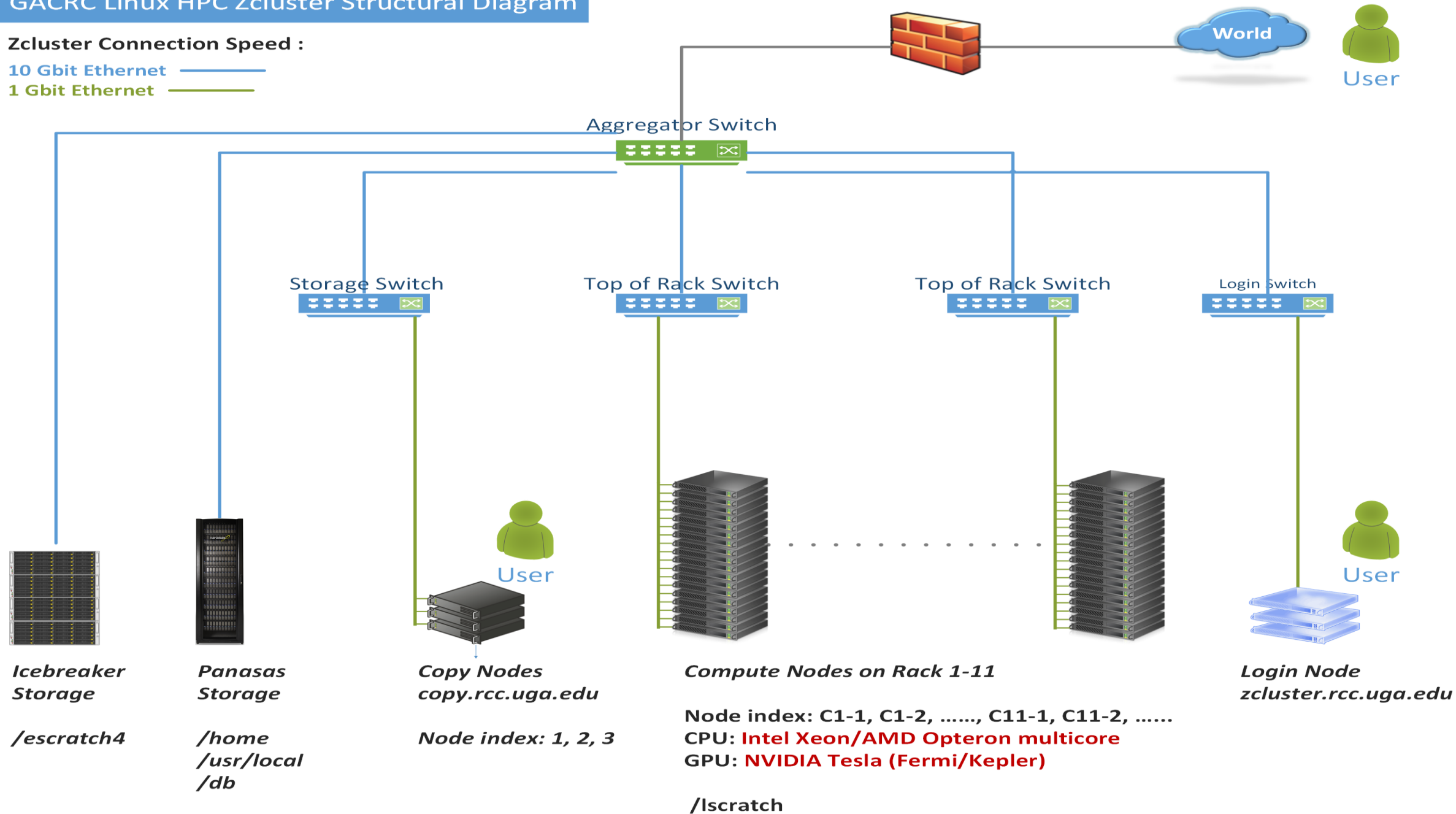
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- Cluster Structural Diagram
- General Information
- Computing Resources
- Disk Storage

# GACRC Linux HPC Zcluster Structural Diagram

Zcluster Connection Speed :

10 Gbit Ethernet   
1 Gbit Ethernet 





# What is zcluster – General Information

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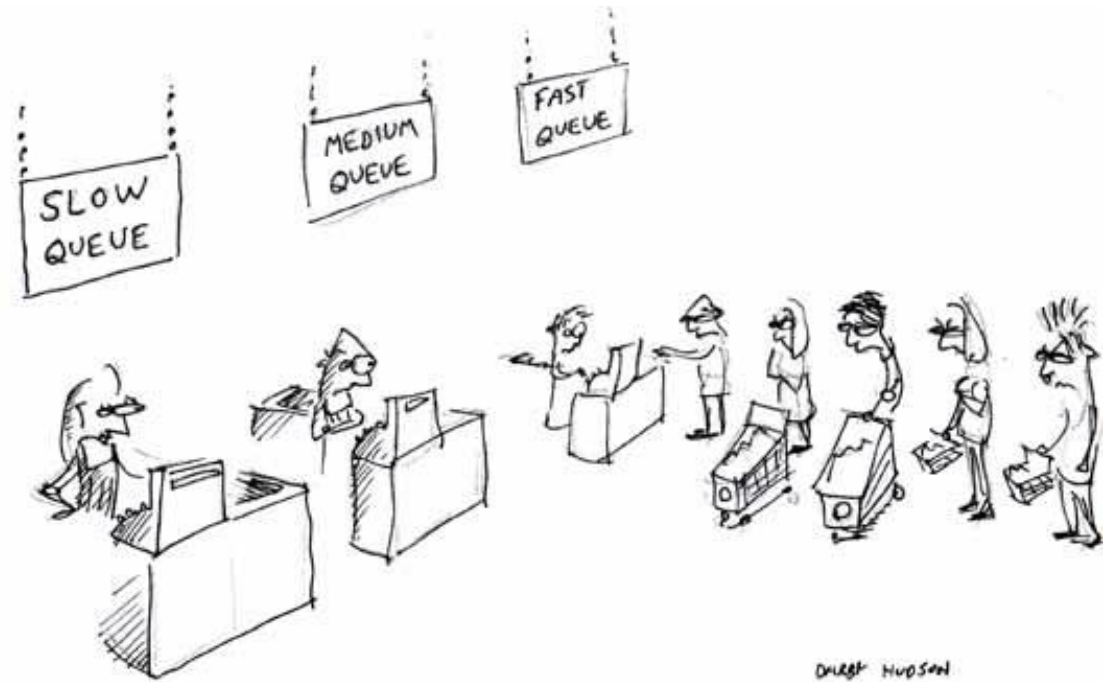
zcluster is a Linux high performance computing (HPC) cluster:

- Operating System: **64-bit Red Hat Enterprise Linux 5 (RHEL 5)**
- Login Node: [zcluster.rcc.uga.edu](http://zcluster.rcc.uga.edu)  
Copy Node: [copy.rcc.uga.edu](http://copy.rcc.uga.edu)
- Internodal Communication: **1Gbit** network
  - compute nodes ↔ compute nodes
  - compute nodes ↔ storage systems

# What is zcluster – General Information

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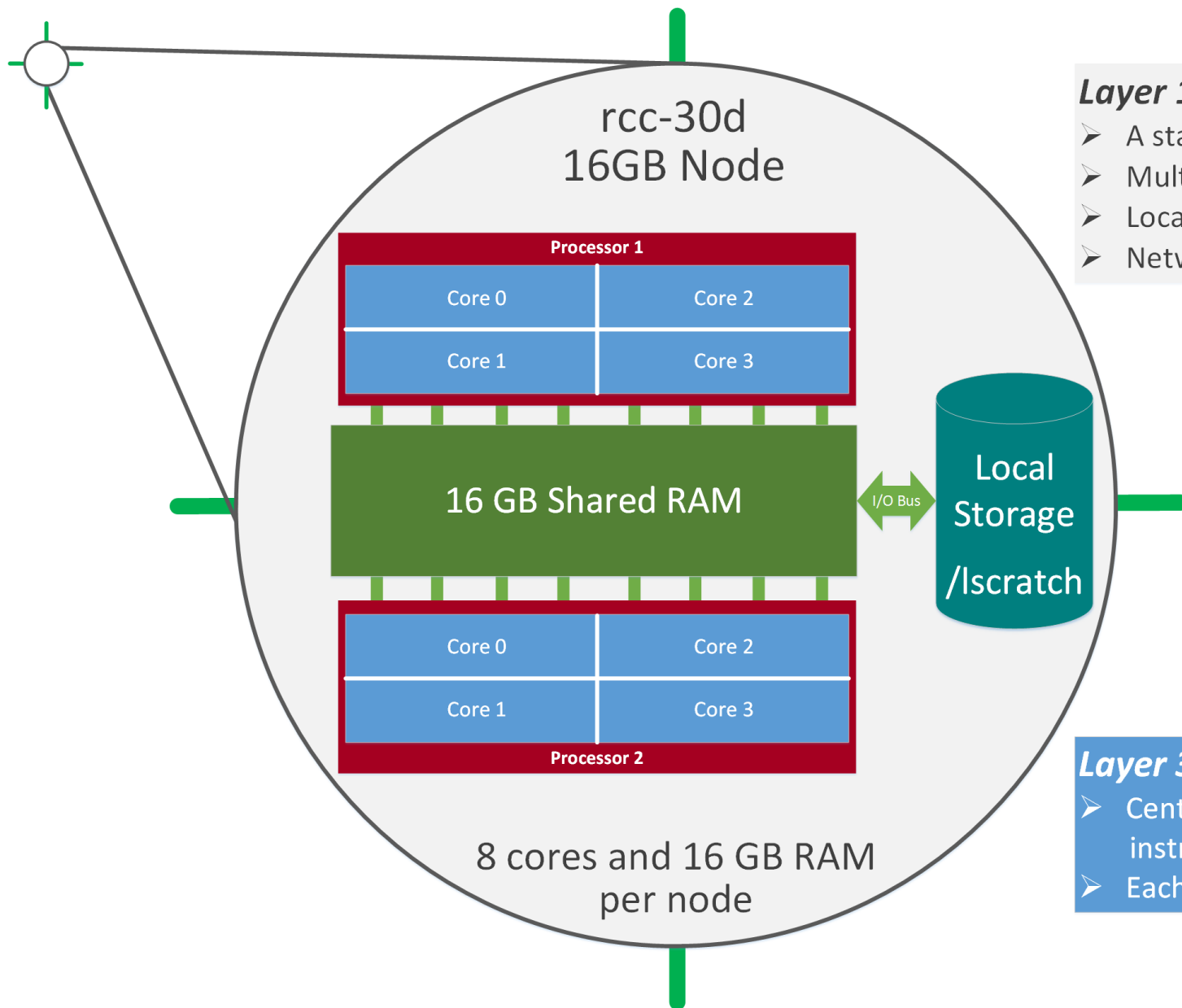
- Batch-queueing System:
  - Jobs can be started (submitted), monitored, and controlled
  - Determine which compute node is the best place to run a job
  - Determine appropriate execution priority for a job to run
- On zcluster: **Sun Grid Engine (SGE)**



# 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 | 4     | Intel Xeon  | 8          | 192          | 32    | N/A                           |
|             |              | 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 – Disk Storage

- **Home directory** → */home/groupname/username*
  - 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     .lessht       .mozilla         Pthreads  .ssh     ← .snapshot is NOT
zhuofei@zcluster:~$ cd .snapshot ← can “cd” into .snapshot      shown here!
zhuofei@zcluster:~/ .snapshot$ ls ← then “ls” to list its contents
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
```

# What is zcluster – Disk Storage

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- **Local scratch** → `/lscratch/username`
  - 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** → `/scratch4/zhuofei_Jun_22`
  - Create with `make_escalch` command
  - Visible to **all nodes** with a quota of **4TB**
  - **No snapshot backup**
  - To be deleted after **37 days**

# How to work with zcluster?

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## *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](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?

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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





# How to work with zcluster?

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

# How to work with zcluster – Start with zcluster

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- You need a **User Account** : [username@zcluster.rcc.uga.edu](mailto:username@zcluster.rcc.uga.edu)
- Procedure: [https://wiki.gacrc.uga.edu/wiki/User\\_Accounts](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

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

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

or

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

<sup>(1)</sup> `-X` is for X windows application running on the cluster to be forwarded to your local machine

<sup>(2)</sup> 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**

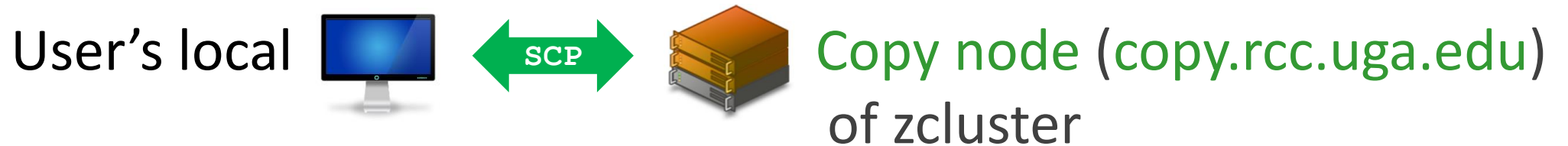
```
zhuofei@zcluster.rcc.uga.edu's password: █
```

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

- Logging out: `exit` to leave the system

```
zhuofei@zcluster:~$ exit
```

# How to work with zcluster – Transfer Files



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

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

```
scp file1 username@copy.rcc.uga.edu:~/subdir
```

```
scp *.dat username@copy.rcc.uga.edu:~/subdir
```

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

```
scp username@copy.rcc.uga.edu:~/subdir/file ./
```

```
scp username@copy.rcc.uga.edu:~/subdir/*.dat ./
```

- On Window: **FileZilla**, **WinSCP**, etc.

# How to work with zcluster – Softwares Installed

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- 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, 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

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

```

zhuofei@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, remember to **exit** the session! 
- Detailed information, like interactive parallel job? Go to: [https://wiki.gacrc.uga.edu/wiki/Running Jobs on zcluster](https://wiki.gacrc.uga.edu/wiki/Running_Jobs_on_zcluster)

# How to work with zcluster – Run Batch Jobs

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- Components you need to run a batch job:
  - **Softwares** 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.

# How to work with zcluster – Run Batch *Serial* Jobs

- **Step 1:** Create a job submission script *sub.sh* running Samtools:

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

cd ${HOME}/testdir   → Specify and enter (cd) the working directory (${HOME}/testdir)

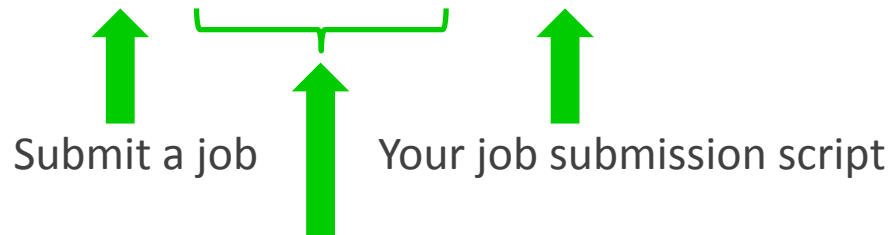
time /usr/local/samtools/latest/samtools <command> [options] → Run samtools with 'time' command to measure amount of time it takes to run the application
```

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

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

OR

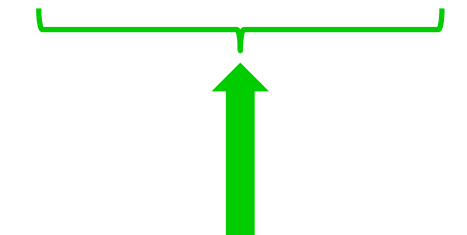
```
$ qsub -q rcc-30d -l mem_total=20g sub.sh
```



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

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



# How to work with zcluster – Run Batch *Threaded* Jobs

- **Step 1:** Create a job submission script *sub.sh* running bowtie2:

```
#!/bin/bash

cd ${HOME}/testdir

/usr/local/bowtie2/latest/bin/bowtie2 -p 4 [options] → Run bowtie2 with 4 threads (-p 4)
```

Number of Threads =  
Number of Cores Requested

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

```
$ qsub -q rcc-30d -l mem_total=20g -pe thread 4 sub.sh
```

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

4 cores requested

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

# How to work with zcluster – Run Batch *MPI* Jobs

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

```
#!/bin/bash
cd ${HOME}/testdir
```

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

→ Define and export environment variable (**MPIRUN**) for convenient usage

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

→ 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

# 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
  
```

Thank You for Your Attention!

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From Yecheng:

- Software support issue:

What kind of software support we are responsible for the users? or definition of our software support

From Shan-Ho:

- rcc-30d : For MPI, max 75 cores total to be requested
- rcc-mc-30d : max 32 threads to be allowed
- rcc-m128-30d: max 5 cores to be requested
- rcc-m512-30d: max 8 cores to be requested