

# Introduction to HPC Using zcluster at GACRC

Georgia Advanced Computing Resource Center

University of Georgia

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Slides courtesy: Zhoufei Hou

# OVERVIEW

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

# Georgia Advanced Computing Resource Center

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## Who Are We?

- ❖ Georgia Advanced Computing Resource Center (**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](https://wiki.gacrc.uga.edu/wiki/Getting_Help) (Wiki Help)

# GACRC Users September 2015

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

# Computer Cluster

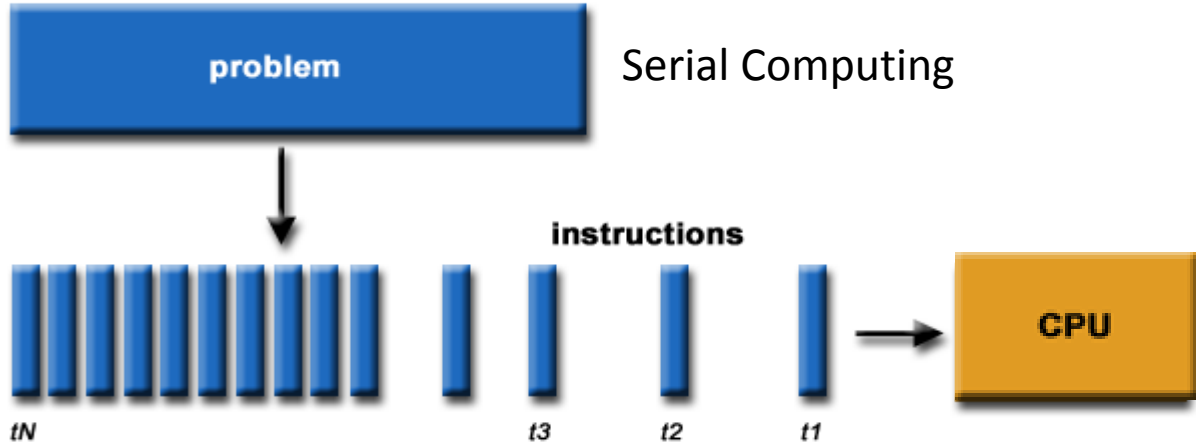
- ❖ Cluster is a widely used term meaning independent computers combined into a unified system through software and high speed dedicated network
  - ❖ It provides greater computational power than a single computer can provide – LARGER problems can be solved
- ❖ Used for:
  - ❖ High Availability (HA)
  - ❖ Greater reliability
  - ❖ High Performance Computing (HPC)

# High Performance Computing (HPC)

Several “definitions” can be found, but, in general:

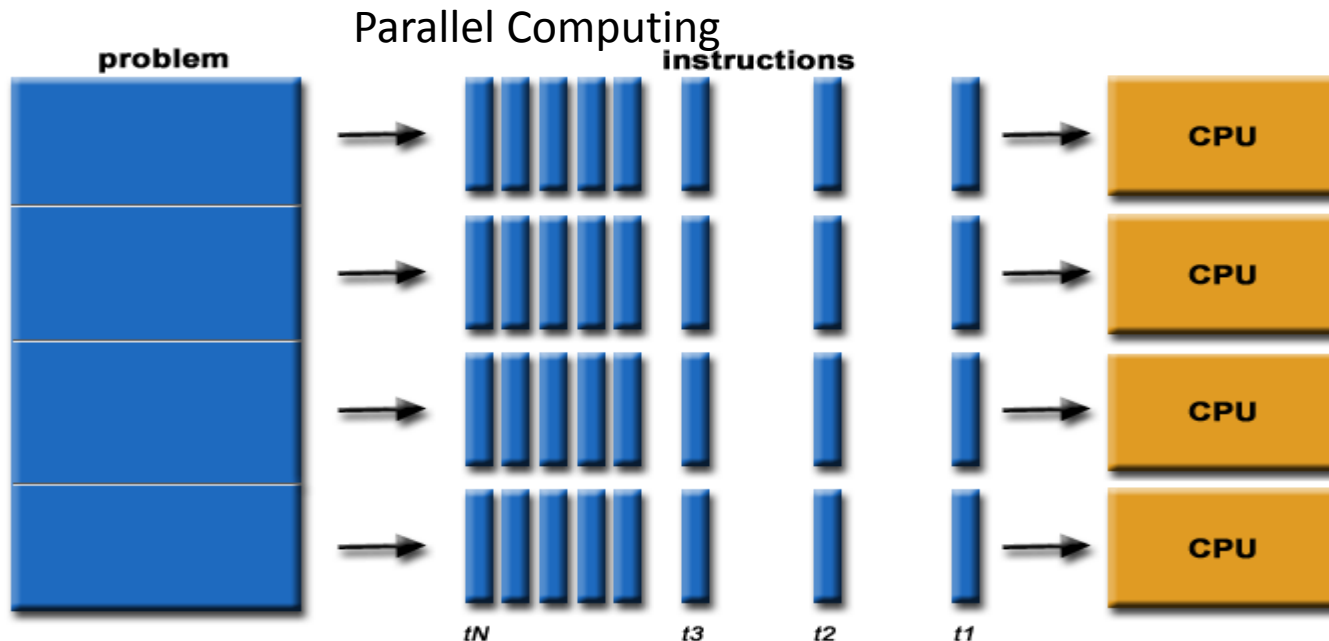
*Use of Parallel processing for solving complex computational problems using advanced application programs efficiently, reliably and quickly*

# High Performance Computing (HPC)



## 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

- ❖ 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

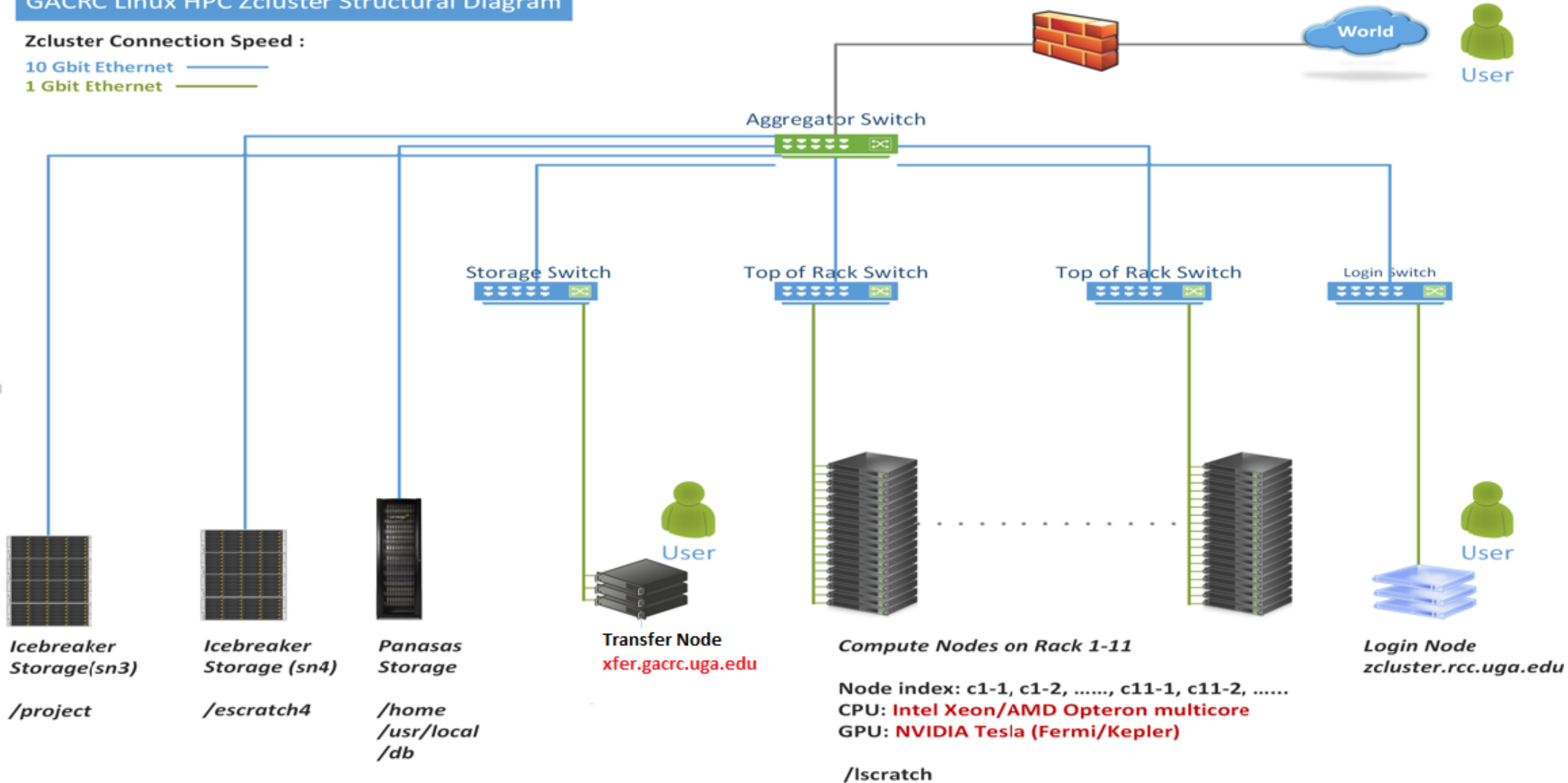
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- ❖ zcluster Structure
- ❖ General Information
- ❖ Computing Resources
- ❖ Storage Environment

# GACRC Linux HPC Zcluster Structural Diagram


Zcluster Connection Speed :

10 Gbit Ethernet ————  
1 Gbit Ethernet ————



# 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](http://zcluster.rcc.uga.edu)  
[zcluster.rcc.uga.edu](http://zcluster.rcc.uga.edu) <sup>qlogin</sup>  Interactive Node: [compute-14-7/9](http://compute-14-7/9)
- ❖ Transfer Node: [xfer.gacrc.uga.edu](http://xfer.gacrc.uga.edu)
- ❖ Internodal Communication: **1Gbit** network
  - compute nodes ↔ compute nodes
  - compute nodes ↔ storage systems

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

# zcluster – General Information

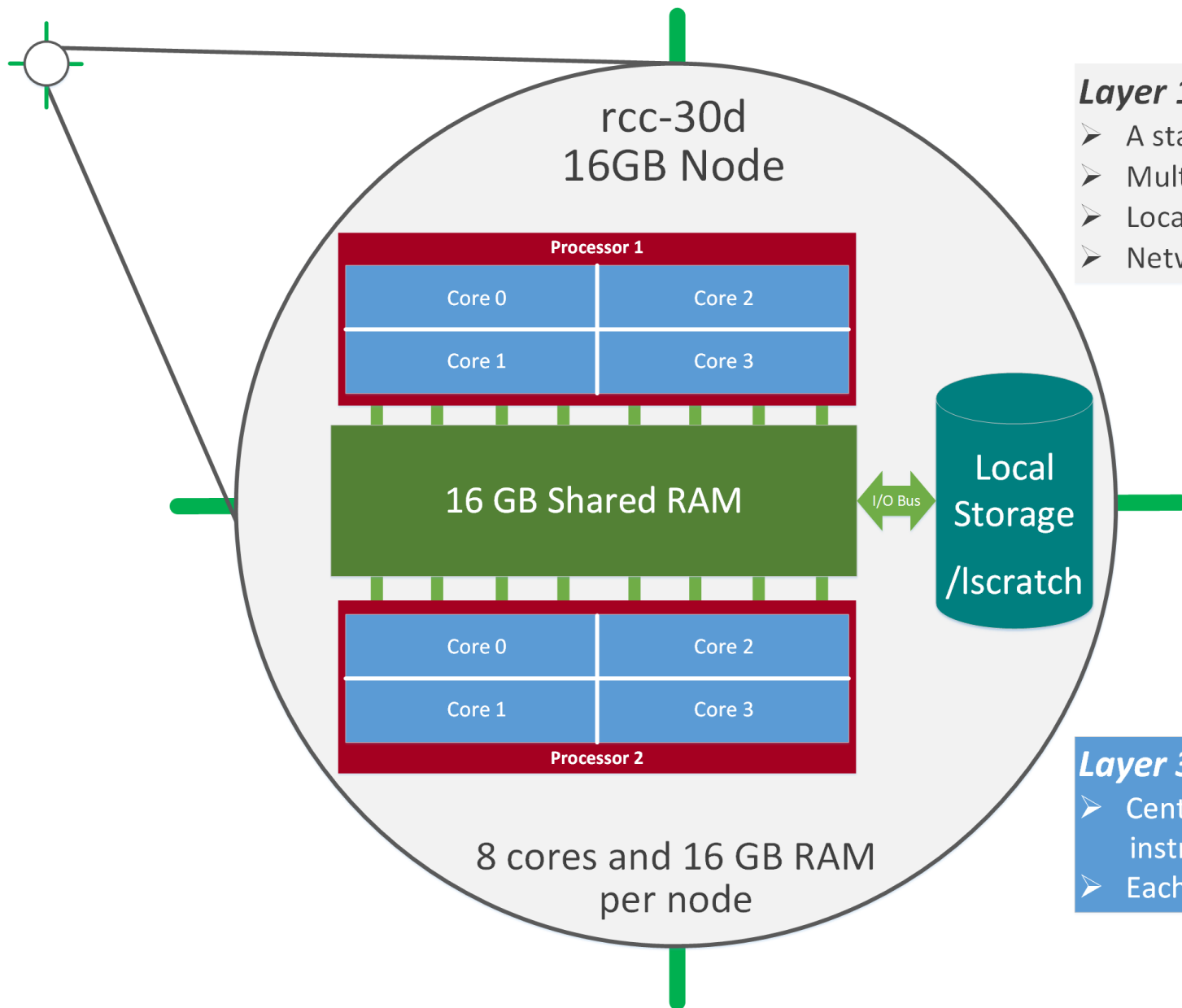
- ❖ Batch-queueing System:
  - ❖ Jobs can be started (submitted), monitored, and controlled
  - ❖ Determine which compute node is the best place to run a job
  - ❖ Determine appropriate execution priority for a job to run
- ❖ On zcluster: **Sun Grid Engine (SGE)**



# 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

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- ❖ Mainly, there are 4 different storage locations:
  - ❖ **Home directory** - where you would land after logging in to the zcluster
  - ❖ **lscratch** - is the storage that is local to the computation nodes
  - ❖ **escratch4** - is temporary scratch which is visible to all nodes
  - ❖ **Project** storage area - is long term, and is created for a lab.

# zcluster – Storage Environment

- ❖ **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”:

```

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  → .snapshot is NOT
.bash_history  .bash_history.zcluster    .bash_profile      Blast           .emacs   ncbidb  .viminfo  shown here!
pakala@zcluster:~$ cd .snapshot  → Can “cd” into “.snapshot”
pakala@zcluster:~/ .snapshot$ ls  → And “ls” to list its contents
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

```



# zcluster – Storage Environment

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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** → `/escratch4/pakala/pakala_Nov_13`
  - ❖ Create with `make_есrаtсh` command
  - ❖ 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	<a href="http://zcluster.rcc.uga.edu">zcluster.rcc.uga.edu</a> (Login)	Highly static data being used frequently	Snapshots
/escratch4/username	Scratch	4TB	<a href="http://xfer.gacrc.uga.edu">xfer.gacrc.uga.edu</a> (Transfer) Interactive nodes (Interactive) compute nodes (Compute)	Temporarily storing large data being used by jobs	Auto-deleted in <b>37</b> days
/lscratch/username	Local Scratch	18 ~ 370GB	Individual compute node	Jobs with heavy disk I/O	User to clean up
/project/abclab	Storage	Variable	<a href="http://xfer.gacrc.uga.edu">xfer.gacrc.uga.edu</a> (Transfer)	Long-term data storage	Group sharing possible

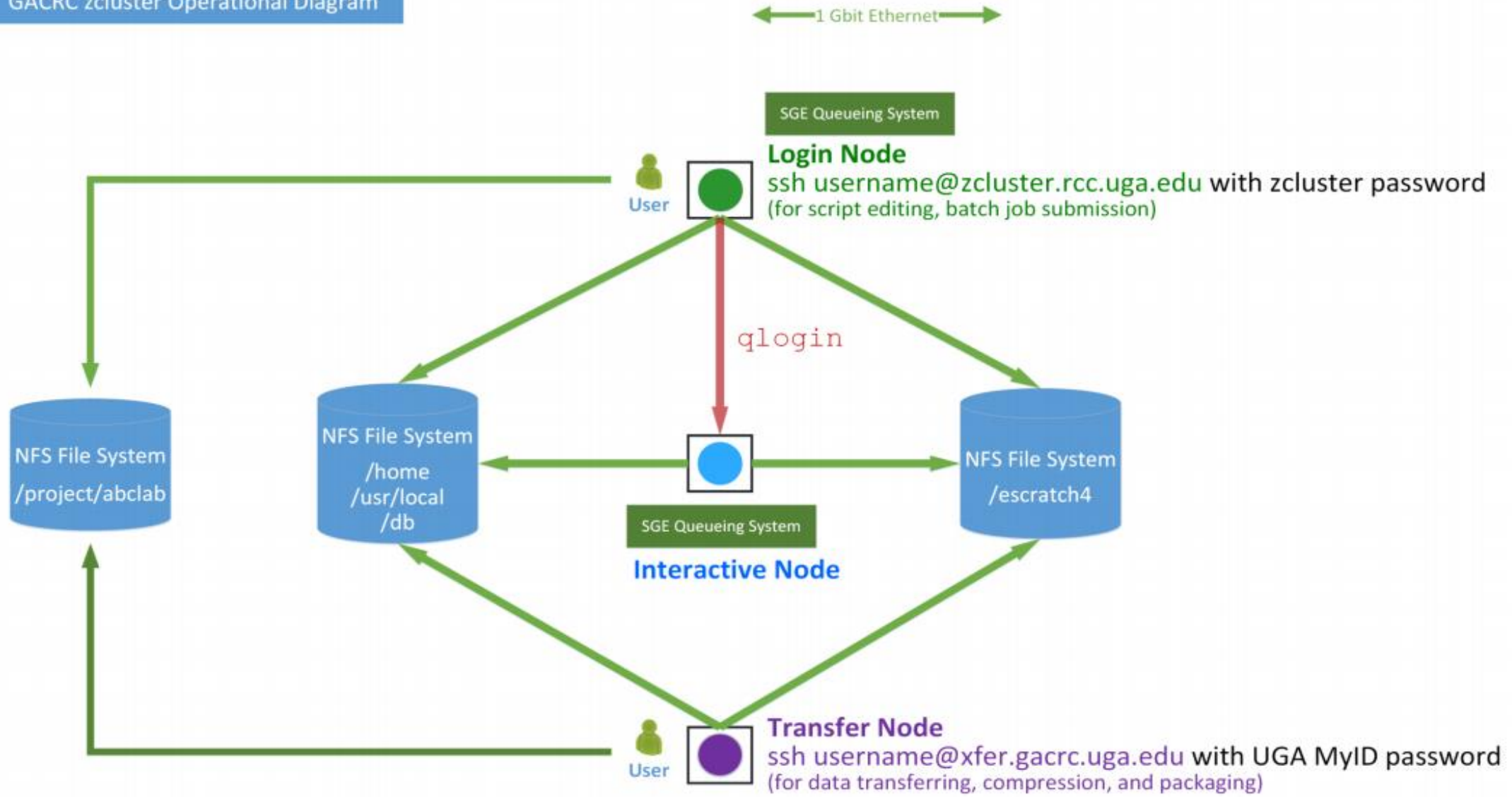
- Note:
1. /usr/local : Software installation directory  
/db : bioinformatics database installation directory
  2. To login to [Interactive](#) nodes, use [qlogin](#) from [Login](#) node

# zcluster – Storage Environment

6 Main Function	On/From-Node	Related Filesystem
Login Landing	Login Transfer	/home/abclab/username (Home) ( <b>Always!</b> ) /home/username (Transfer)
Batch Job Submitting	Login or Interactive	/escratch4/username/username_mth_date (Scratch) ( <b>Suggested!</b> ) /home/abclab/username (Home)
Interactive Job Running	Interactive	/escratch4/username/username_mth_date (Scratch) /home/abclab/username (Home)
Data Archiving , Compressing and Transferring	Transfer	/escratch4/username/username_mth_date (Scratch) /panfs/pstor.storage/home/abclab/username (Home)
Job Data Temporarily Storing	Compute	/lscratch/username (Local Scratch) /escratch4/username/username_mth_date (Scratch)
Long-term Data Storing	Login or Transfer	/project/abclab

How does zcluster operate?

# GACRC zcluster Operational Diagram



# Zcluster – Tips, Dos and Don'ts

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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**)

# 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



# How to work with zcluster? - Overview

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



# Getting Started 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)
- ❖ 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 pakala@zcluster.rcc.uga.edu
```

or

```
ssh -X pakala@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**

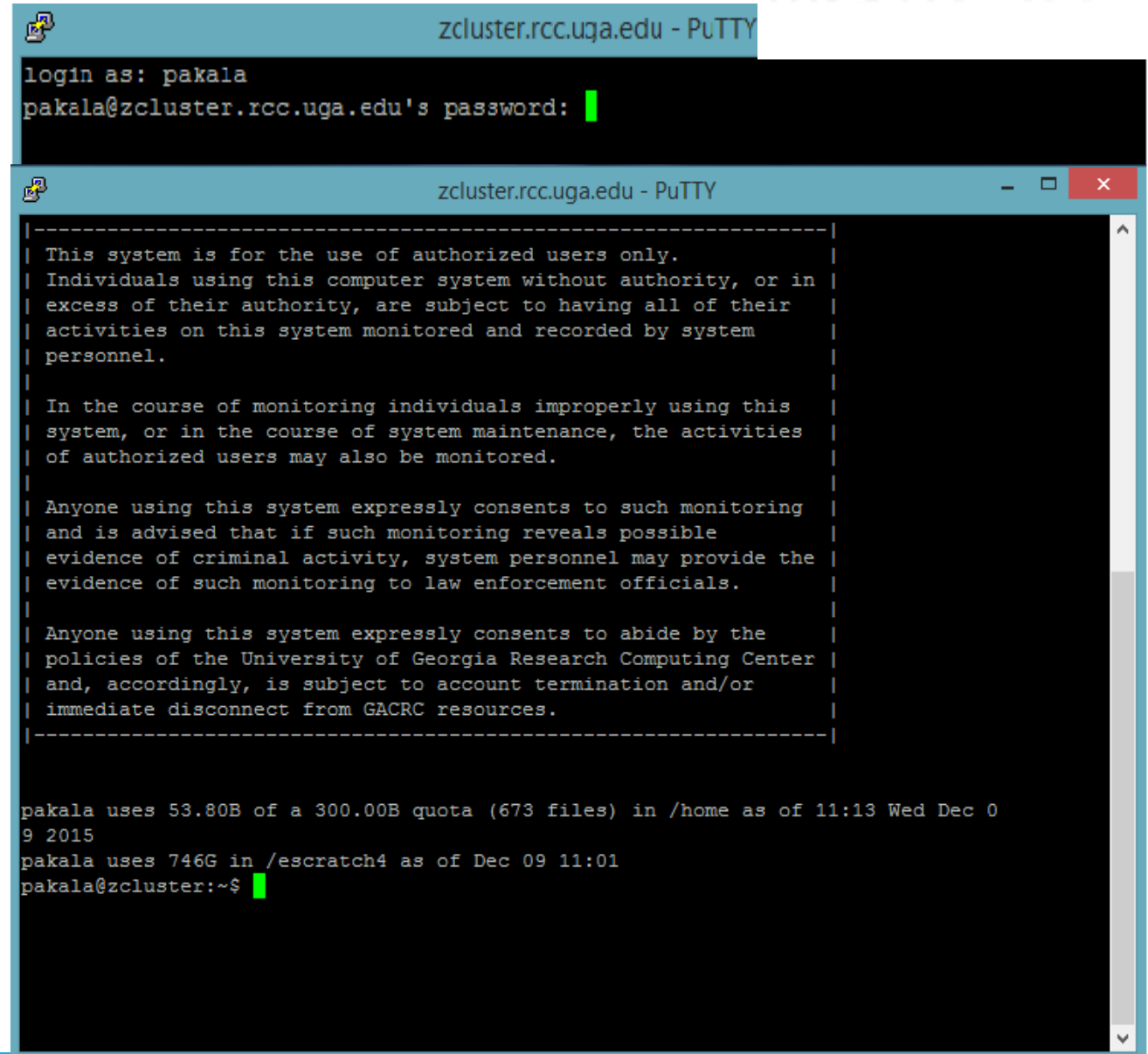
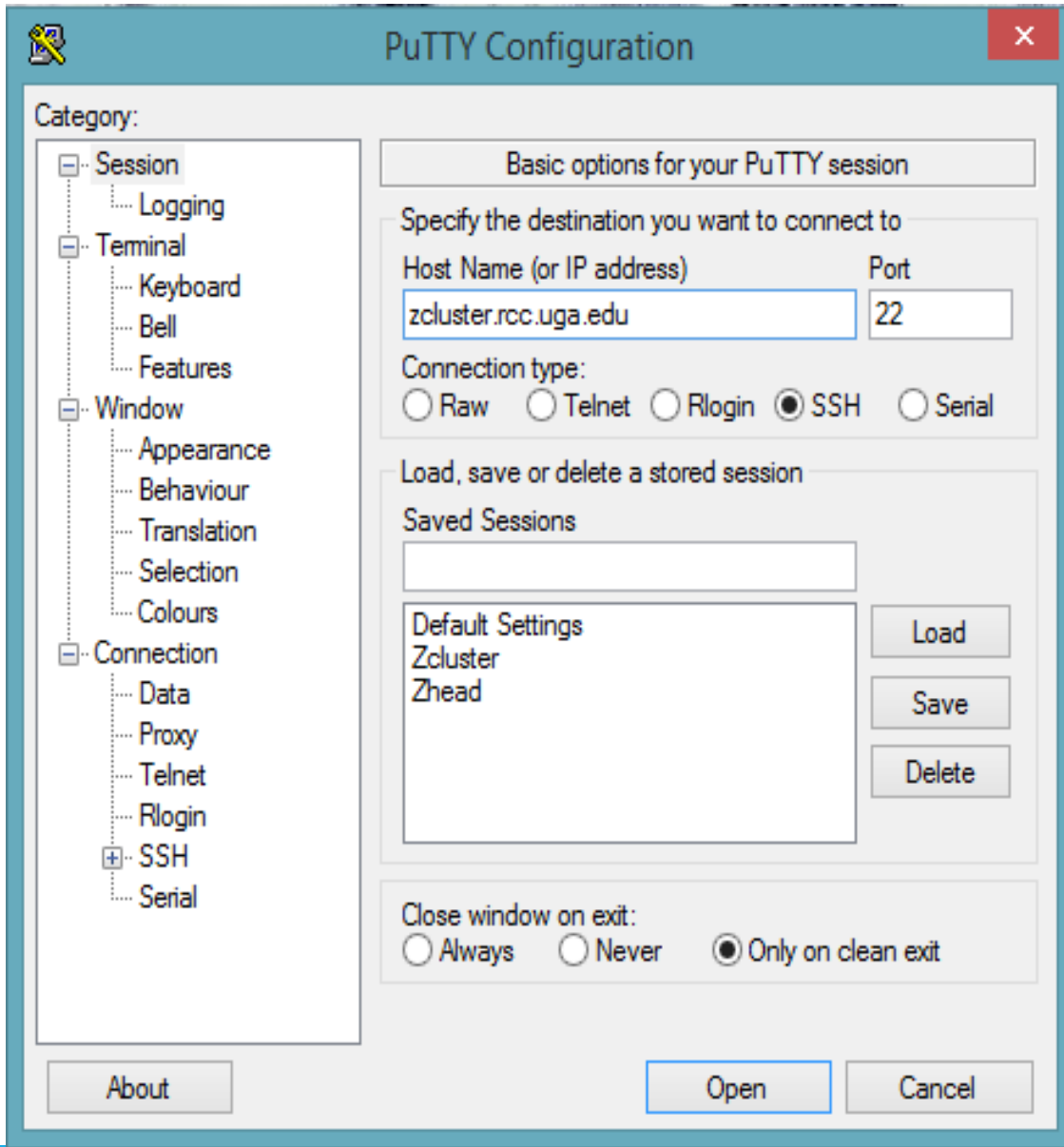
```
pakala@zcluster.rcc.uga.edu's password:
```

<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

```
pakala@zcluster:~$ exit
```

# PUTTY: LOGIN



# Transfer Files Using Transfer Node [xfer.gacrc.uga.edu](https://xfer.gacrc.uga.edu)

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- ✓ Login with **UGA MyID password**; Landing directory: `/home/username`
- ✓ Move data into and out of zcluster (`scp`, `sftp`, `rsync`, **SSH Secure Shell File Transfer**, **FileZilla**, **WinSCP**)
- ✓ Compress or package data on zcluster (`tar`, `gzip`)
- ✓ Transfer data between zcluster and Sapelo (`cp`, `mv`)
- ✓ Filesystems accessible:
  - `/home/username/` : Transfer home (Landing home)
  - `/panfs/pstor.storage/home/abclab/username/` : zcluster home
  - `/escratch4/username/` : zcluster scratch
  - `/project/abclab/` : long-term active data storage
- ✓ Most file systems on Transfer are **auto-mounted** upon **the first time full-path access**, e.g.,  
`cd /project/abclab`

# Transfer Files @ zcluster

User's local    Transfer Node ([xfer.gacrc.uga.edu](http://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 username@xfer.gacrc.uga.edu:~/subdir
```

```
scp *.dat username@xfer.gacrc.uga.edu:~/subdir
```

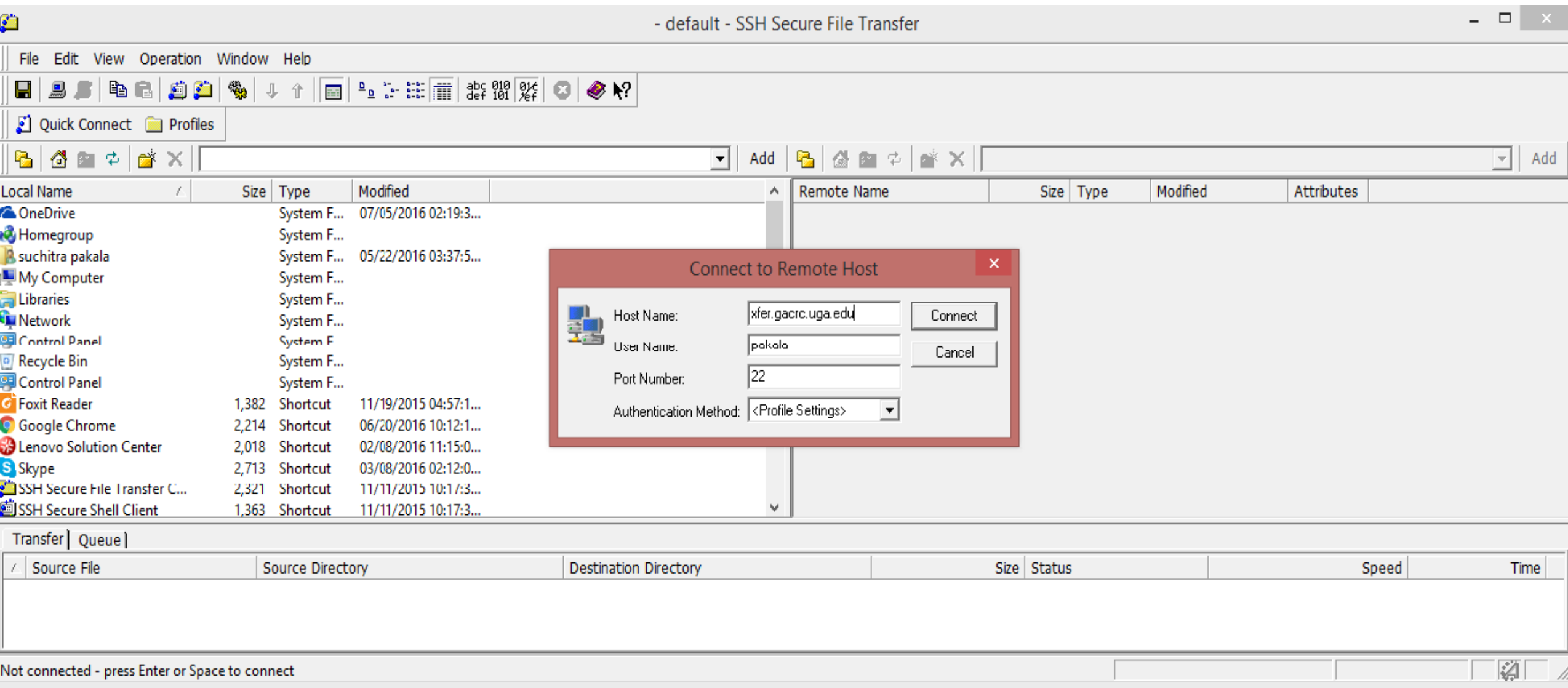
*E.g. 2:* On local machine, do zcluster  Local

```
scp username@xfer.gacrc.uga.edu:~/subdir/file ./
```

```
scp username@xfer.gacrc.uga.edu:~/subdir/*.dat ./
```

❖ On Windows: [FileZilla](#), [WinSCP](#), [SSH Secure Client](#), etc.

# SSH Secure Client: Connecting to Transfer Node



The screenshot displays the SSH Secure File Transfer application window. The main interface is divided into two panes: a local file system on the left and a remote file system on the right. A modal dialog box titled "Connect to Remote Host" is open in the center, prompting for connection details.

**Connect to Remote Host Dialog:**

- Host Name: xfer.gacrc.uga.edu
- User Name: pakala
- Port Number: 22
- Authentication Method: <Profile Settings>

**Local File System Table:**

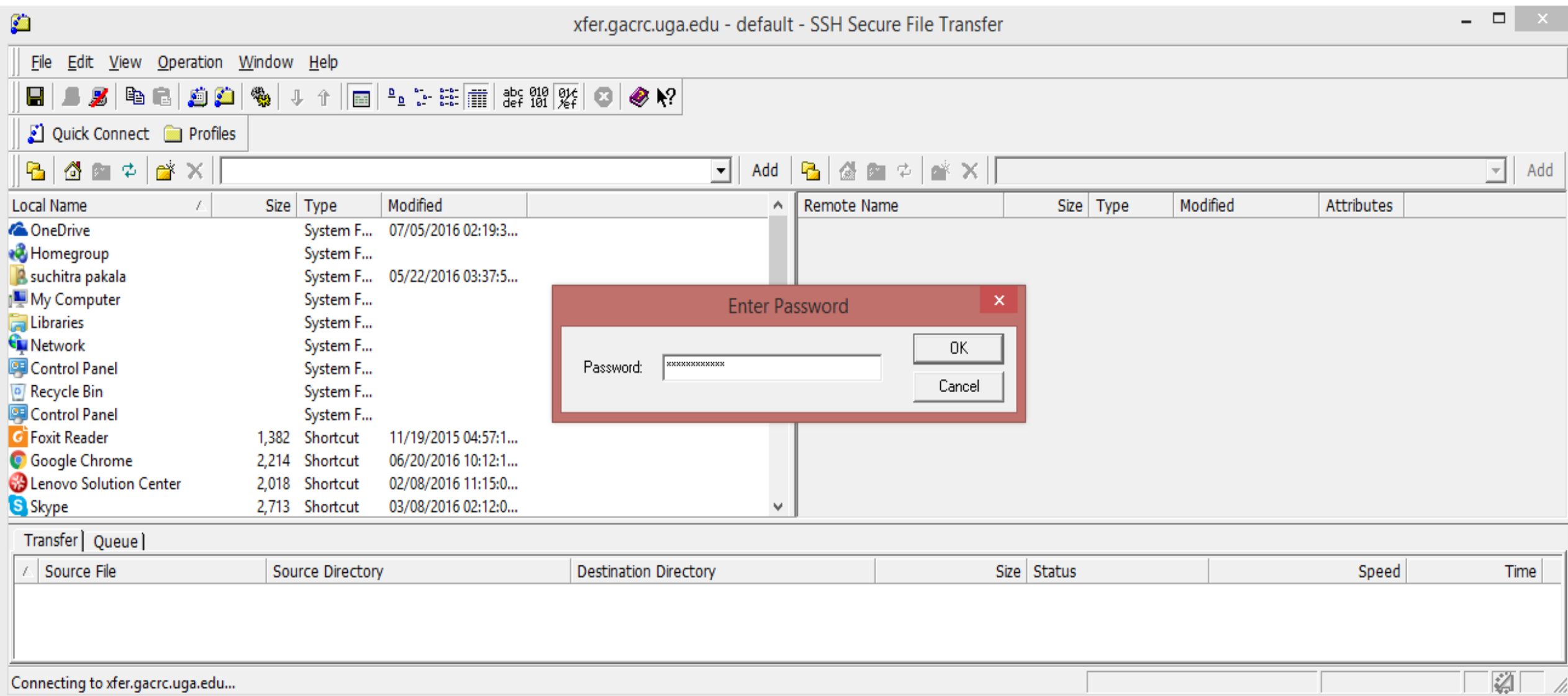
Local Name	Size	Type	Modified
OneDrive		System F...	07/05/2016 02:19:3...
Homegroup		System F...	
suchitra pakala		System F...	05/22/2016 03:37:5...
My Computer		System F...	
Libraries		System F...	
Network		System F...	
Control Panel		System F	
Recycle Bin		System F...	
Control Panel		System F...	
Foxit Reader	1,382	Shortcut	11/19/2015 04:57:1...
Google Chrome	2,214	Shortcut	06/20/2016 10:12:1...
Lenovo Solution Center	2,018	Shortcut	02/08/2016 11:15:0...
Skype	2,713	Shortcut	03/08/2016 02:12:0...
SSH Secure File Transfer C...	2,321	Shortcut	11/11/2015 10:17:3...
SSH Secure Shell Client	1,363	Shortcut	11/11/2015 10:17:3...

**Transfer Queue Table:**

Source File	Source Directory	Destination Directory	Size	Status	Speed	Time
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Not connected - press Enter or Space to connect

# SSH Secure Client: Connecting to Transfer Node



The screenshot shows the SSH Secure File Transfer client interface. The main window title is "xfer.gacrc.uga.edu - default - SSH Secure File Transfer". The interface includes a menu bar (File, Edit, View, Operation, Window, Help), a toolbar with various icons, and a "Quick Connect" section with "Profiles". The main area is split into two panes: "Local Name" on the left and "Remote Name" on the right. The "Local Name" pane shows a list of files and folders, including system folders like OneDrive, Homegroup, and My Computer, as well as application shortcuts like Foxit Reader, Google Chrome, and Skype. The "Remote Name" pane is currently empty. A "Transfer | Queue" section at the bottom shows a table with columns for Source File, Source Directory, Destination Directory, Size, Status, Speed, and Time. A red "Enter Password" dialog box is overlaid on the interface, prompting for a password with a masked input field and "OK" and "Cancel" buttons. The status bar at the bottom indicates "Connecting to xfer.gacrc.uga.edu...".

Local Name	Size	Type	Modified	Remote Name	Size	Type	Modified	Attributes
OneDrive		System F...	07/05/2016 02:19:3...					
Homegroup		System F...						
suchitra pakala		System F...	05/22/2016 03:37:5...					
My Computer		System F...						
Libraries		System F...						
Network		System F...						
Control Panel		System F...						
Recycle Bin		System F...						
Control Panel		System F...						
Foxit Reader	1,382	Shortcut	11/19/2015 04:57:1...					
Google Chrome	2,214	Shortcut	06/20/2016 10:12:1...					
Lenovo Solution Center	2,018	Shortcut	02/08/2016 11:15:0...					
Skype	2,713	Shortcut	03/08/2016 02:12:0...					

Source File	Source Directory	Destination Directory	Size	Status	Speed	Time
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# SSH Secure : Connected to Home Directory

xfer.gacrc.uga.edu - default - SSH Secure File Transfer

File Edit View Operation Window Help

Quick Connect Profiles

/panfs/pstor.storage/home/gacrc-instruction/pakala

Local Name	Size	Type	Modified	Remote Name	Size	Type	Modified	Attributes
OneDrive		System F...	07/05/2016 02:19:3...	.java		Folder	11/17/2015 12:00:5...	drwxr-xr-x
Homegroup		System F...		.mozilla		Folder	10/16/2015 12:55:2...	drwxr-xr-x
suchitra pakala		System F...	05/22/2016 03:37:5...	.ssh		Folder	11/12/2015 12:40:4...	drwx-----
My Computer		System F...		Blast		Folder	02/25/2016 08:10:5...	drwxrwxr...
Libraries		System F...		e6		Folder	07/07/2016 10:38:0...	drwxrwxr...
Network		System F...		iprac		Folder	07/05/2016 02:23:3...	drwxr-xr-x
Control Panel		System F...		ncbidb		Folder	03/03/2016 12:57:0...	drwxr-xr-x
Recycle Bin		System F...		RNA_SEQ		Folder	11/16/2015 09:57:3...	drwxr-xr-x
Control Panel		System F...		.bash_history	614	BASH_HI...	05/18/2016 01:31:5...	-rw-----
Foxit Reader	1,382	Shortcut	11/19/2015 04:57:1...	.bash_history.compute-14-7	7,482	COMPU...	04/11/2016 10:50:0...	-rw-----
Google Chrome	2,214	Shortcut	06/20/2016 10:12:1...	.bash_history.compute-14-9	6,655	COMPU...	04/11/2016 10:34:2...	-rw-----
Lenovo Solution Center	2,018	Shortcut	02/08/2016 11:15:0...	.bash_history.compute-18-8	395	COMPU...	07/05/2016 02:25:4...	-rw-----
Skype	2,713	Shortcut	03/08/2016 02:12:0...	.bash_history.zcluster	5,604	ZCLUSTE...	07/07/2016 10:49:2...	-rw-----
SSH Secure File Transfer C...	2,321	Shortcut	11/11/2015 10:17:3...	.bash_history.zhead	3,035	ZHEAD F...	03/10/2016 10:49:1...	-rw-----
SSH Secure Shell Client	1,363	Shortcut	11/11/2015 10:17:3...	.bash_logout	33	BASH_L...	10/16/2015 12:55:2...	-rw-r--r--
DO_NOT_DELETE		File folder	07/05/2016 02:32:1...	.bash_profile	176	BASH_PR...	10/16/2015 12:55:2...	-rw-r--r--
GACRC_10152015_Suchi		File folder	07/05/2016 11:32:1...	.bashrc	124	BASHRC ...	10/16/2015 12:55:2...	-rw-r--r--
North_Oconee		File folder	05/07/2016 06:50:0...	.emacs	515	EMACS F...	10/16/2015 12:55:2...	-rw-r--r--
North_Oconee_Girls		File folder	05/07/2016 06:37:0...	.viminfo	6,821	VIMINFO...	05/18/2016 01:31:5...	-rw-r--r--
Shivank		File folder	07/05/2016 03:52:4...					
Suchi_Samsung_Pics		File folder	06/27/2016 12:24:2...					

Transfer | Queue |

Source File	Source Directory	Destination Directory	Size	Status	Speed	Time

Connected to xfer.gacrc.uga.edu - /panfs/pstor.storage/home/gacrc-instruction/pakala

SSH2 - aes128-cbc - hmac-md5 - n 19 items (31.5 KB)



# SSH Secure : Navigated to /escratch4/pakala

xfer.gacrc.uga.edu - default - SSH Secure File Transfer

File Edit View Operation Window Help

Quick Connect Profiles

/escratch4/pakala

Local Name	Size	Type	Modified	Remote Name	Size	Type	Modified	Attributes
OneDrive		System F...	07/05/2016 02:19:3...	pakala_Feb_02		Folder	07/07/2016 10:38:0...	drwxrwxr...
Homegroup		System F...		pakala_Jul_07		Folder	07/07/2016 09:54:2...	drwx-----
suchitra pakala		System F...	05/22/2016 03:37:5...	pakala_Mar_03		Folder	03/03/2016 11:24:4...	drwxrwxr...
My Computer		System F...						
Libraries		System F...						
Network		System F...						
Control Panel		System F...						
Recycle Bin		System F...						
Control Panel		System F...						
Foxit Reader	1,382	Shortcut	11/19/2015 04:57:1...					
Google Chrome	2,214	Shortcut	06/20/2016 10:12:1...					
Lenovo Solution Center	2,018	Shortcut	02/08/2016 11:15:0...					
Skype	2,713	Shortcut	03/08/2016 02:12:0...					

Transfer | Queue |

Source File	Source Directory	Destination Directory	Size	Status	Speed	Time
-------------	------------------	-----------------------	------	--------	-------	------

Connected to xfer.gacrc.uga.edu - /escratch4/pakala


SSH2 - aes128-cbc - hmac-md5 - n 3 items (0 Bytes)

## 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](https://wiki.gacrc.uga.edu/wiki/Running_Jobs_on_zcluster)

# Submit Batch Jobs @ zcluster

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- ❖ 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 `fastqc_sub.sh` running Fastqc tool:

```
#!/bin/bash
```

→ Linux shell (`bash`)

```
cd /escratch4/pakala/pakala_Nov_13
```

→ Specify and enter (`cd`) the working directory

```
export PATH=/usr/local/fastqc/latest:${PATH}
```

→ Export command helps to set the Environment variables

```
time fastqc SRR1369670.fastq -o Output_File
```

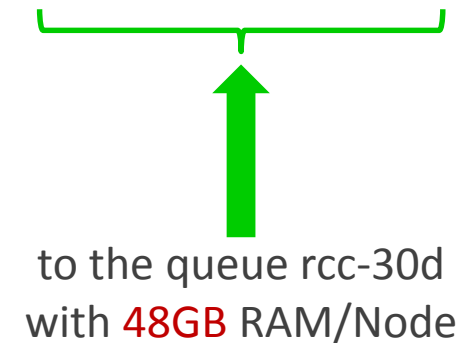
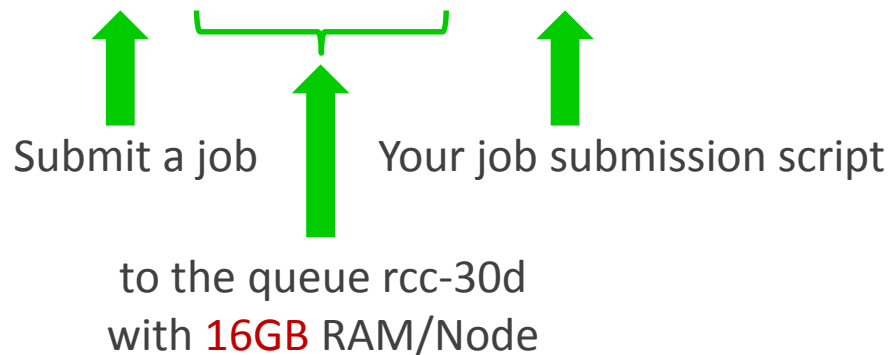
→ Run `Fastqc` with '`time`' command to measure amount of time it takes to run the application

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

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

OR

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



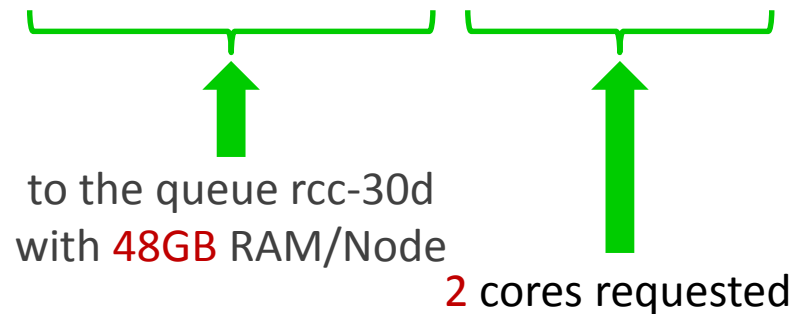
# Batch *Threaded* Job @ zcluster

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

```
#!/bin/bash
cd /escratch4/pakala/pakala_Nov_13
time /usr/local/ncbiblast/latest/bin/blastall -p 2 [options] → Run Blastall with 2 threads
```

- ❖ **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

Number of Threads =  
Number of 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
```

→ 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

# 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
  
```

# Software Installed @ zcluster

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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.  
[https://wiki.gacrc.uga.edu/wiki/Bioinformatics\\_Databases](https://wiki.gacrc.uga.edu/wiki/Bioinformatics_Databases)
- ❖ For a complete list of applications: <https://wiki.gacrc.uga.edu/wiki/Software>



# 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

THANK YOU for your  
patience



# Questions?