

# Introduction to HPC Using zcluster at GACRC

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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?

- 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 highperformance 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)



## GACRC Users September 2015

Colleges & Schools	Depts	Pls	Users
Franklin College of Arts and Sciences	14	117	661
College of Agricultural & Environmental Sciences	9	<b>29</b>	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
Centers & Institutes	9	19	59
TOTALS	S: 49	233	1029



## GACRC Users September 2015

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



## 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)

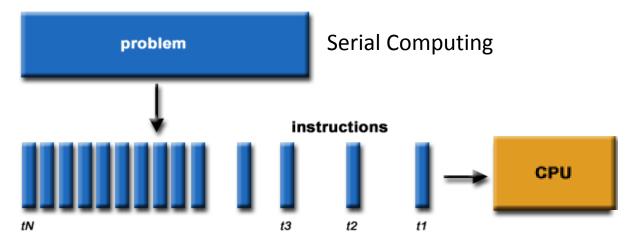
## **High Performance Computing (HPC)**

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 instructions The problem of the

#### **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



#### 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 zcluster.rcc.uga.edu
  Interactive Node: compute-14-7/9
- Copy Node: copy.rcc.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)



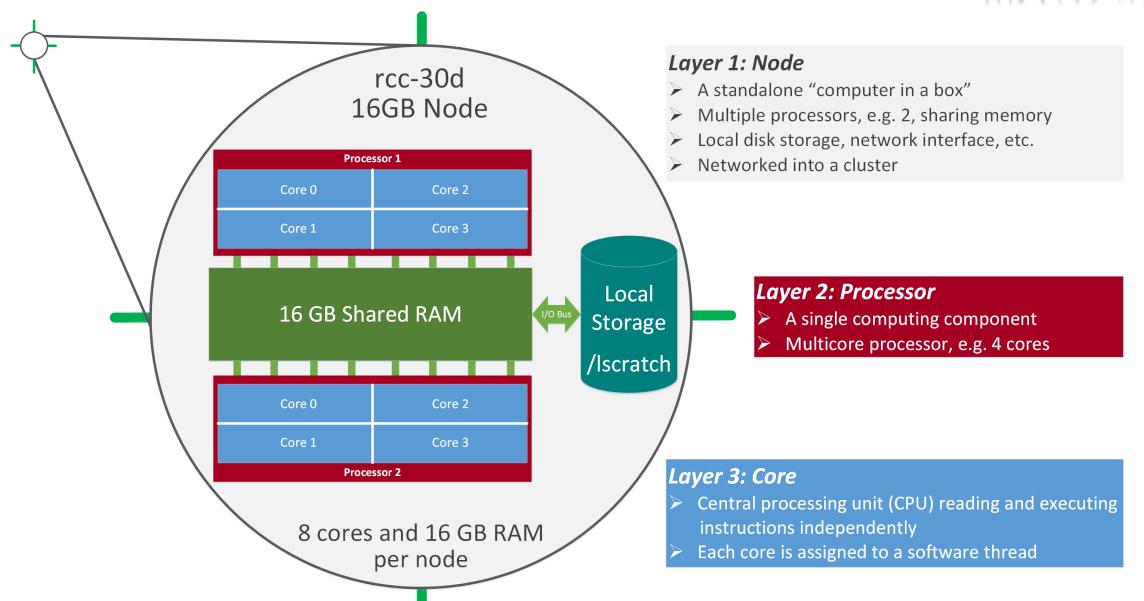


## zcluster – Computing Resources

	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	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** 







- Mainly, there are 4 different storage locations:
  - Home directory where you would land after logging in to the zcluster
  - **Iscratch** 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.



- **♦ 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
                                                                                                   RNA SEQ
                                                                                         .java
               .bash_history.compute-14-9
                                           .bash logout
                                                                batchsub demo
                                                                                         .mozilla
                                                                                                          .snapshot is NOT
.bash_history .bash_history.zcluster
                                           .bash profile
                                                                                                   .viminfo shown here!
                                                                Blast
                                                                                         ncbidb
                                                                               .emacs
pakala@zcluster:~$ cd .snapshot
                                    Can "cd" into ".snapshot
pakala@zcluster:~/.snapshot$ ls
                                    And "Is" 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
```



- ❖ 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 escratch command
  - Visible to all nodes with a quota of 4TB
  - No snapshot backup
  - To be deleted after 37 days



Filesystem	Role	Quota	Accessible from Intended Use		Notes
/home/abclab/username	Home	100GB	zcluster.rcc.uga.edu (Login)	Highly static data being used frequently	Snapshots
/escratch4/username	Scratch	4TB	copy.rcc.uga.edu (Copy) Interactive nodes (Interactive) compute nodes (Compute)	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

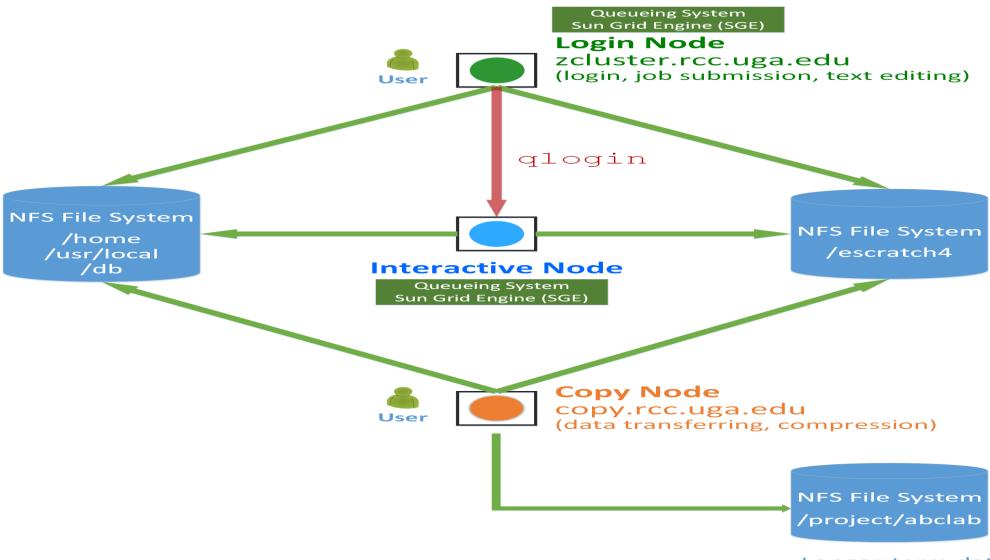
2. To login to Interactive nodes, use qlogin from Login node



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



## How does zcluster operate?



Longer-term data storage:
1. Lifecycle too long for /escratch4

2. Size too big for /home



## Zcluster – Tips, Dos and Don'ts

#### Before we start:

- To get zcluster to be your best HPC buddy, go to GACRC Wiki (<a href="http://wiki.gacrc.uga.edu">http://wiki.gacrc.uga.edu</a>)

  GACRC Web (<a href="http://gacrc.uga.edu">http://gacrc.uga.edu</a>)
- To get the most effective and qualified support from us, go to GACRC Support (<a href="https://wiki.gacrc.uga.edu/wiki/Getting-Help">https://wiki.gacrc.uga.edu/wiki/Getting-Help</a>)
- To work happily and productively, follow the cluster's Community Code of Conduct (CCOC)



## zcluster – Tips, Dos and Don'ts - continued

#### 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

- 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

- You need a User Account : username@zcluster.rcc.uga.edu
- Procedure: <a href="https://wiki.gacrc.uga.edu/wiki/User Accounts">https://wiki.gacrc.uga.edu/wiki/User Accounts</a>
- 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: <a href="http://help.gacrc.uga.edu/userAcct.php">http://help.gacrc.uga.edu/userAcct.php</a>



## 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

 $(^1-X)$  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

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

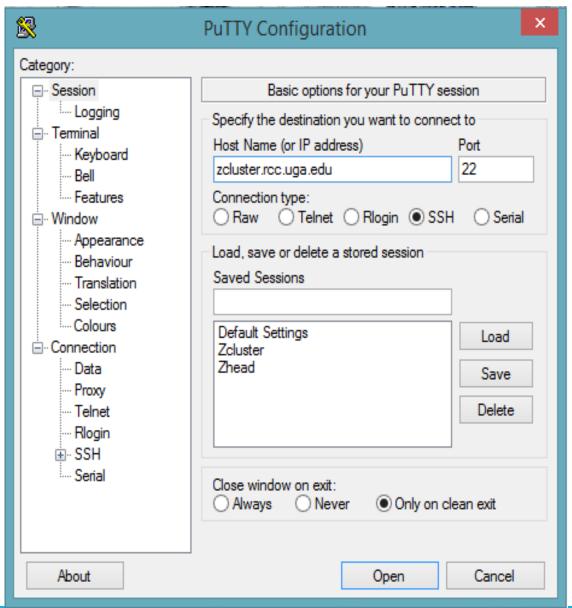
(3 On Linux/Mac, when you type in the password, the prompt blinks and does not move)

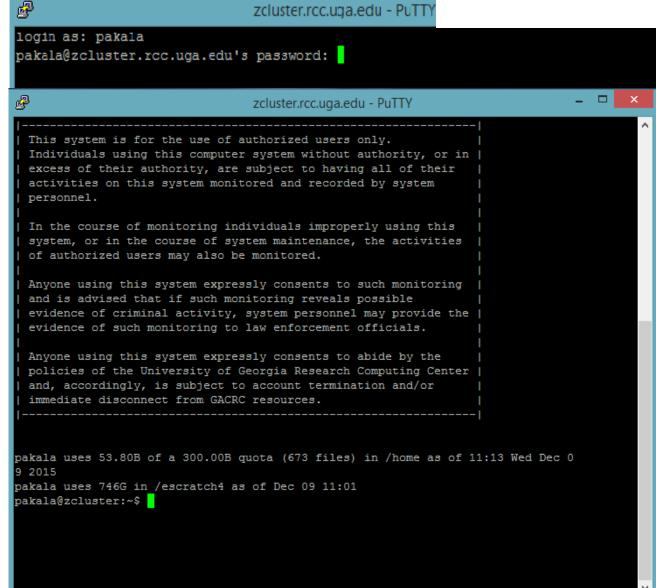
Logging out: exit to leave the system

pakala@zcluster:~\$ exit

#### **PUTTY: LOGIN**









## Transfer Files @ zcluster

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

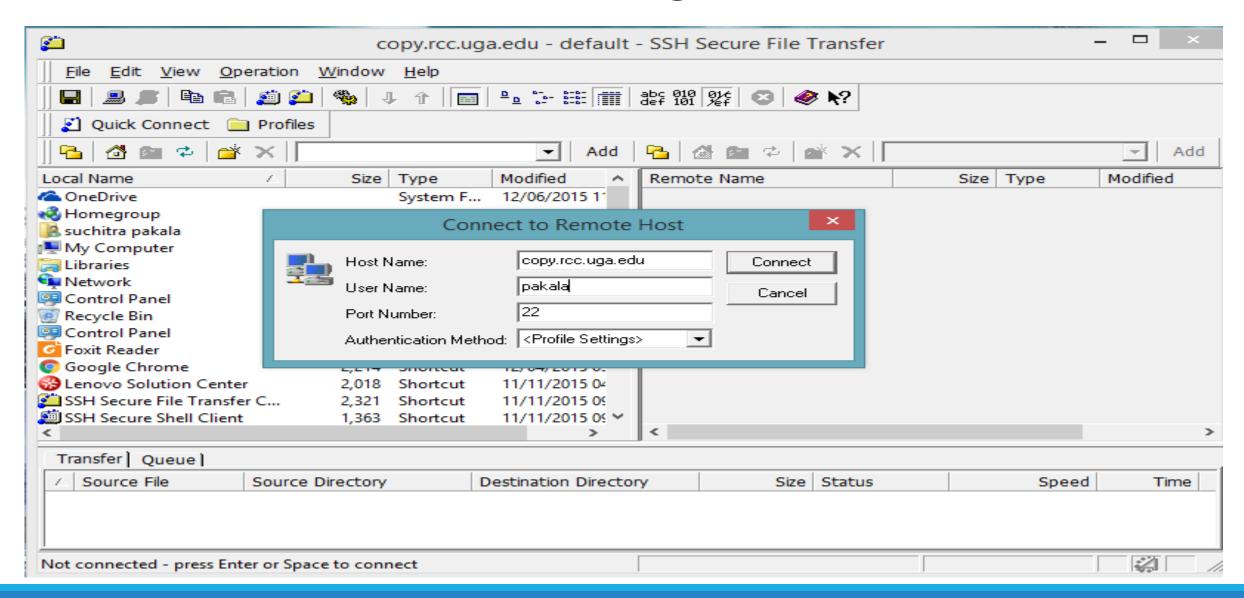
E.g. 2: On local machine, do zcluster → Local

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

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

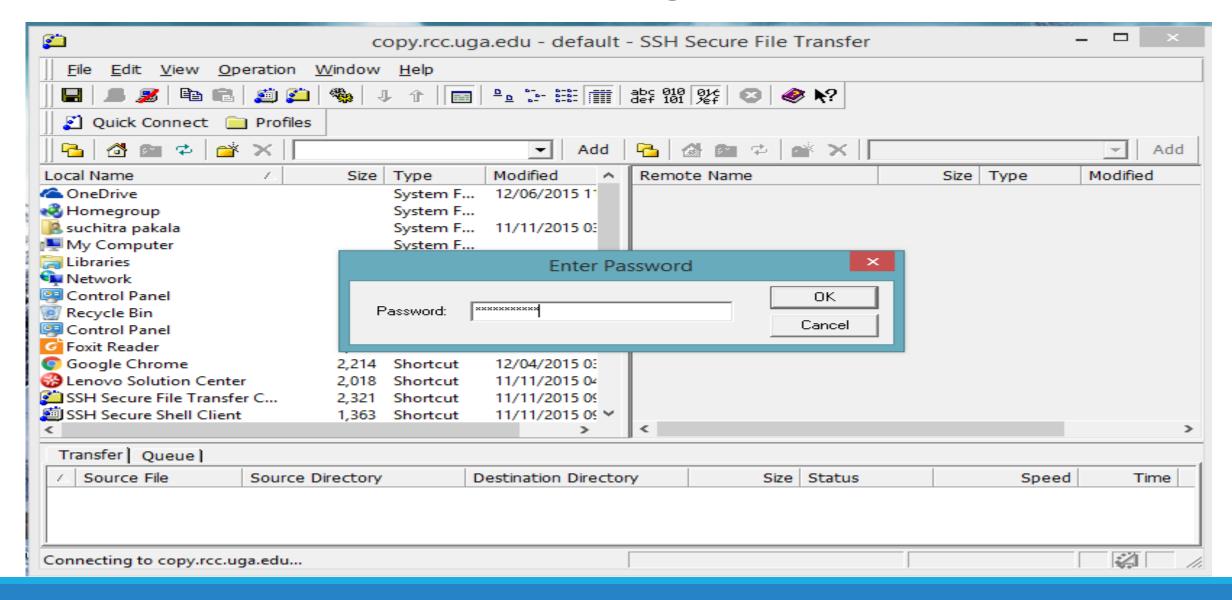
## SSH Secure Client: Connecting to COPY Node





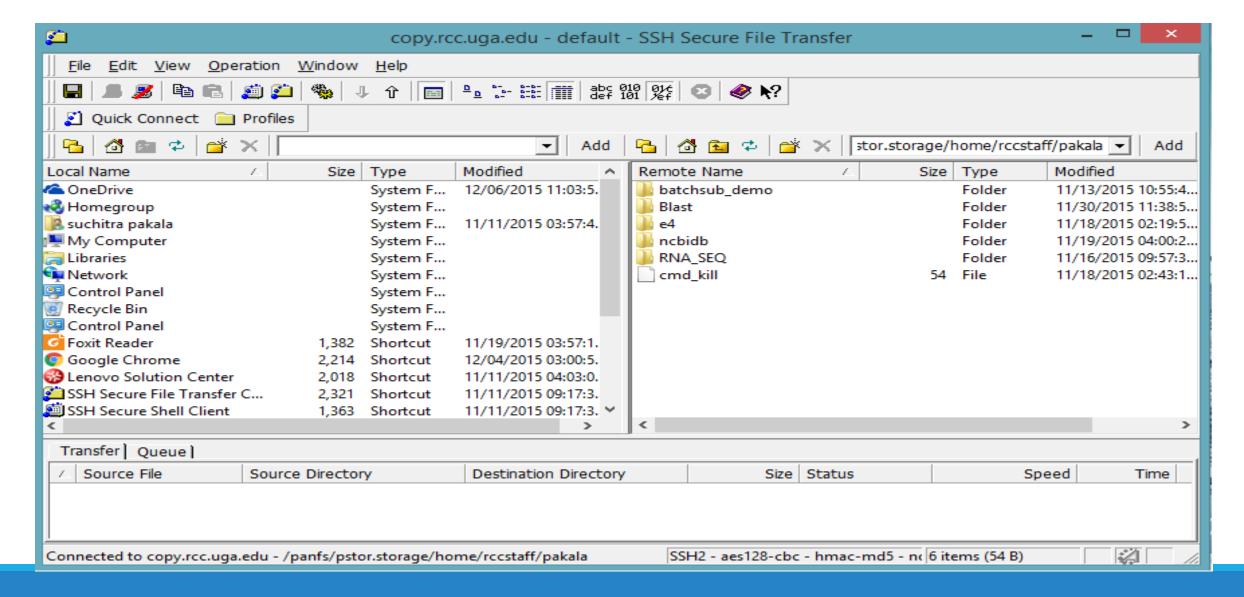


## SSH Secure Client: Connecting to COPY Node



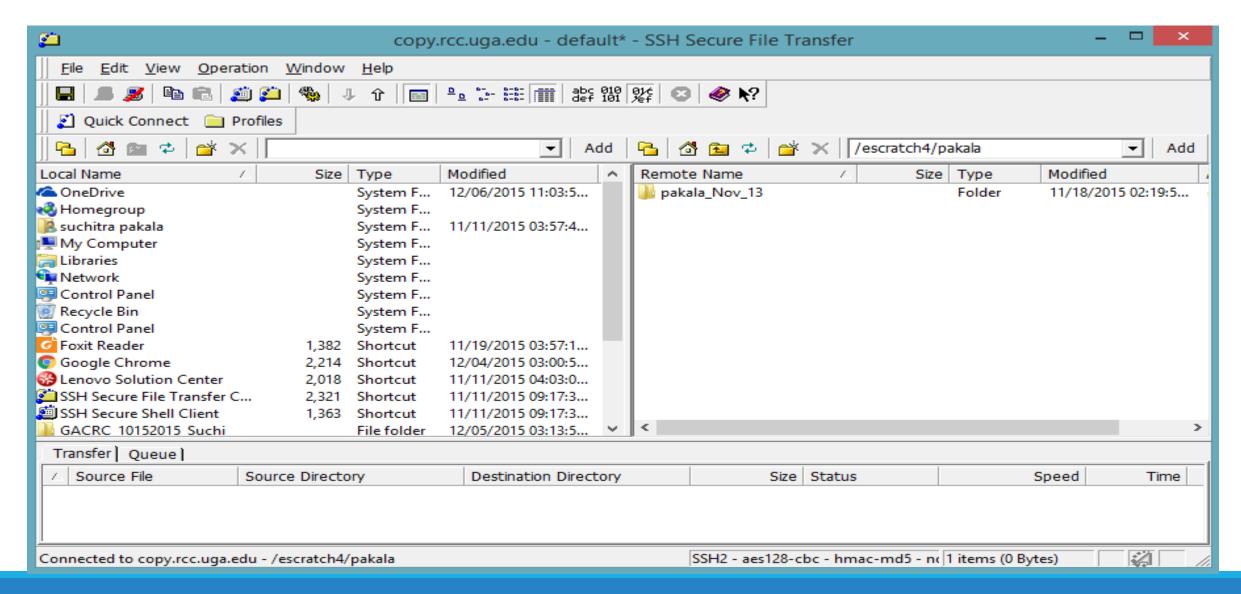


#### SSH Secure: Connected to Home Directory





## SSH Secure: Navigated to /escratch4/pakala





#### Run Interactive Jobs @ zcluster

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

- 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



#### 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.

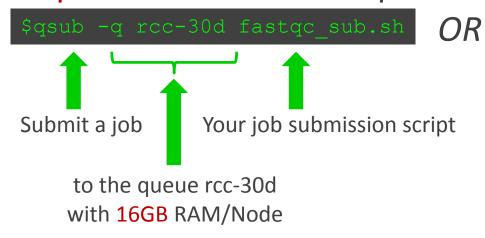


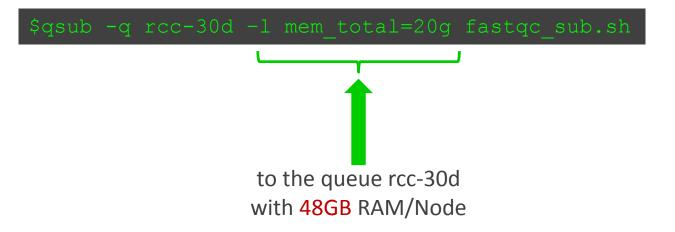
#### Batch Serial Job @ zcluster

#### Step 1: Create a job submission script fastqc\_sub.sh running Fastqc tool:



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







#### Batch *Threaded* Job @ zcluster

2 cores requested

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

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:

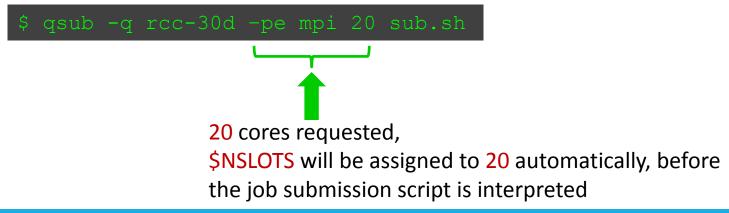
```
#!/bin/bash
cd /escratch4/pakala/pakala_Nov_13

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:





#### Check and Cancel Jobs @ zcluster

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

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

→ shows information, e.g., maxvmem, about the ENDED job with JOBID 12345
```



#### 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, etc.
- RCCBatchBlast (RCCBatchBlastPlus) to distribute NCBI Blast (NCBI Blast+) searches to multiple nodes.
- Many Bioinformatics Databases: NCBI Blast, Pfam, uniprot, etc. <a href="https://wiki.gacrc.uga.edu/wiki/Bioinformatics">https://wiki.gacrc.uga.edu/wiki/Bioinformatics</a> Databases
- For a complete list of applications: <a href="https://wiki.gacrc.uga.edu/wiki/Software">https://wiki.gacrc.uga.edu/wiki/Software</a>

## 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?