Running Batch Jobs at CAC

Drew Dolgert

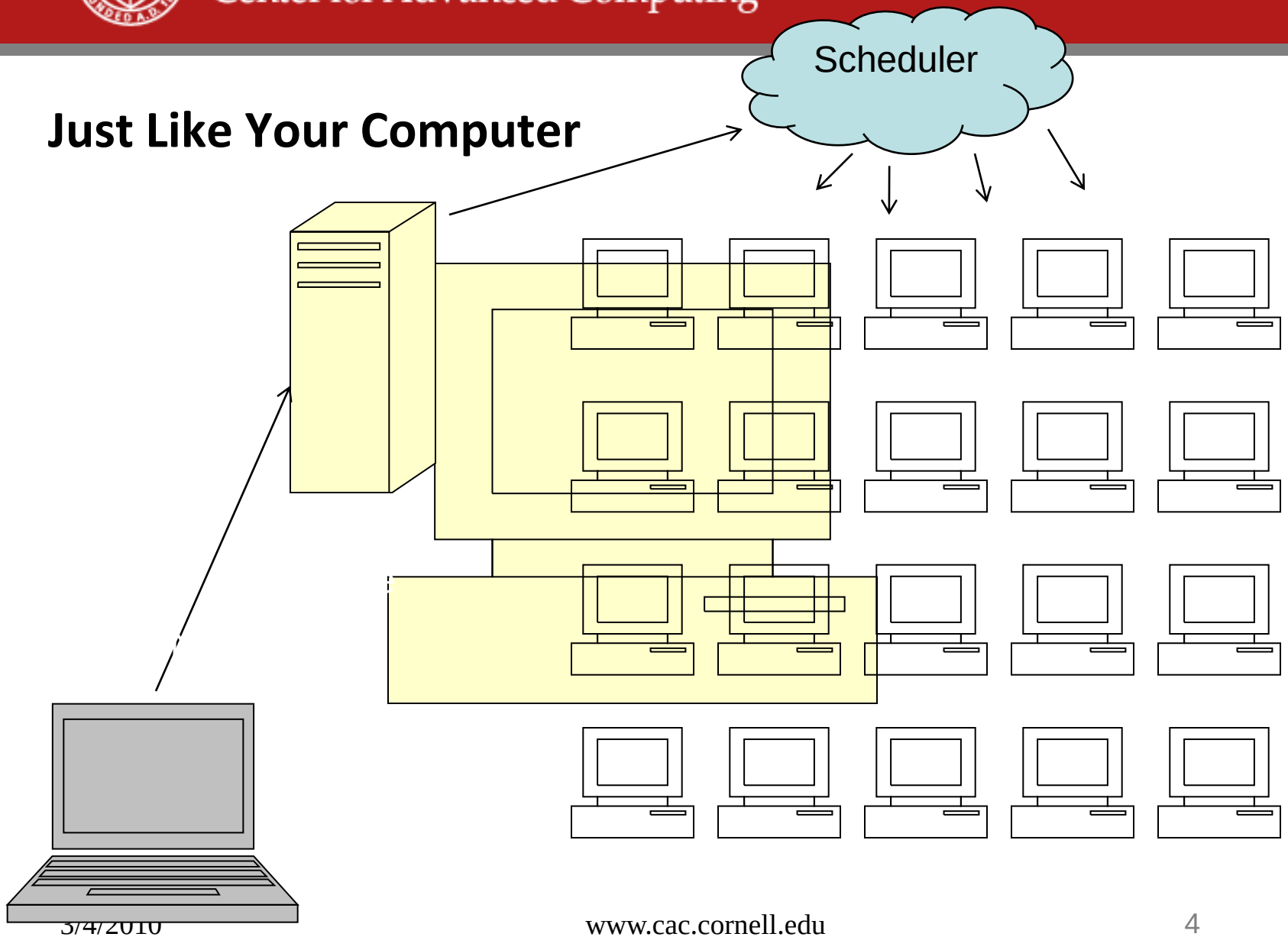
Step-by-step is Separate from Talk

- Homework
  - http://www.cac.cornell.edu/wiki/index.php?title=FirstLinuxClusterJob
  - Look at the gsAssembler link at the end.
- HELP!
  - http://www.cac.cornell.edu/help
  - help@cac.cornell.edu
  - http://www.cac.cornell.edu/wiki

Gear

- A cluster and login nodes
- SSH and X11
- Shell-fu
- Scheduler wrangling

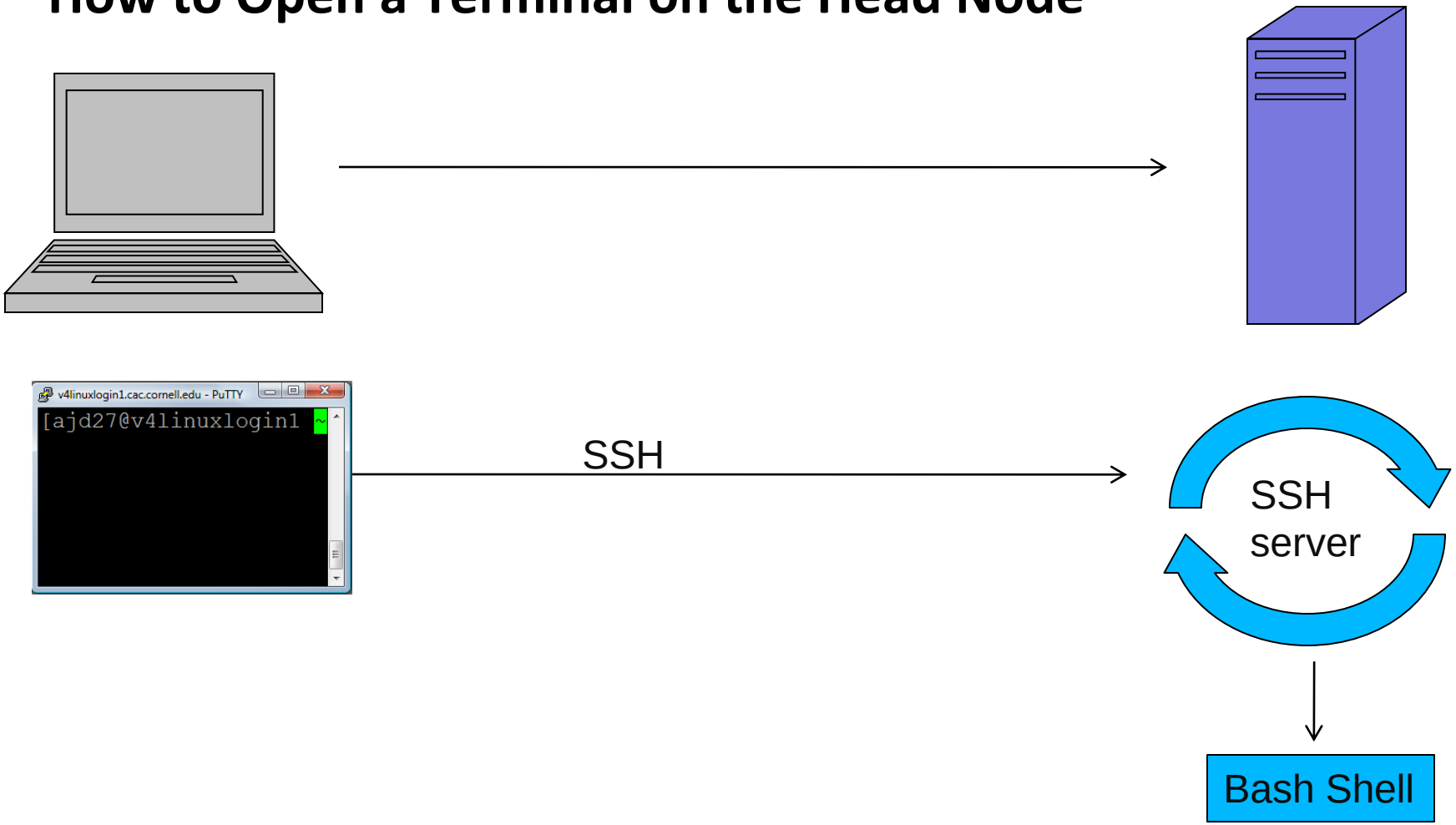
Just Like Your Computer



Definitions

- *Head node* – linuxlogin1.cac.cornell.edu, linuxlogin2.cac.cornell.edu
- *Compute nodes* – similar to compute-3-17.v4linux
- *Job* – A request to the scheduler to perform a task
- *Scheduler* – Decides when and on which nodes your job will run
- *Cores* – Individual processors on each node. A single compute node can often run 8 jobs simultaneously with little loss in speed for any of them.

How to Open a Terminal on the Head Node

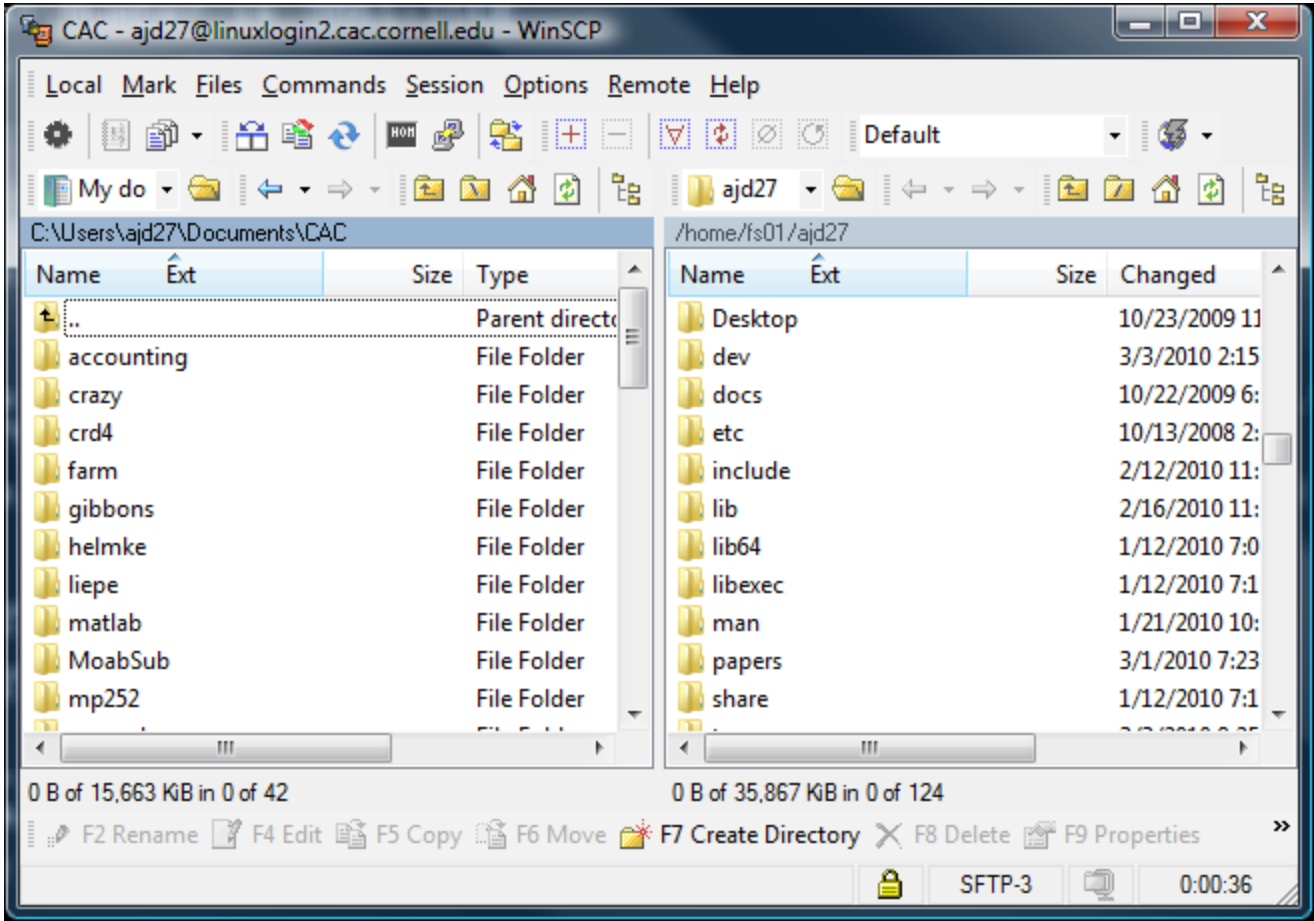


Definitions

- *Secure Shell Protocol* – A definition for how two computers can securely connect with each other.
- *SSH Client* – Software you install on your machine to connect with a server over the SSH protocol. By default, it lets you type and see lines of text sent back and forth.
- *SSH Server* – Always listening on the server for your connection.
- *Bash Shell* – The program the SSH server runs for you on the other end so that you can navigate directories and execute programs.

Copy Files with Same Protocol, Different Tools

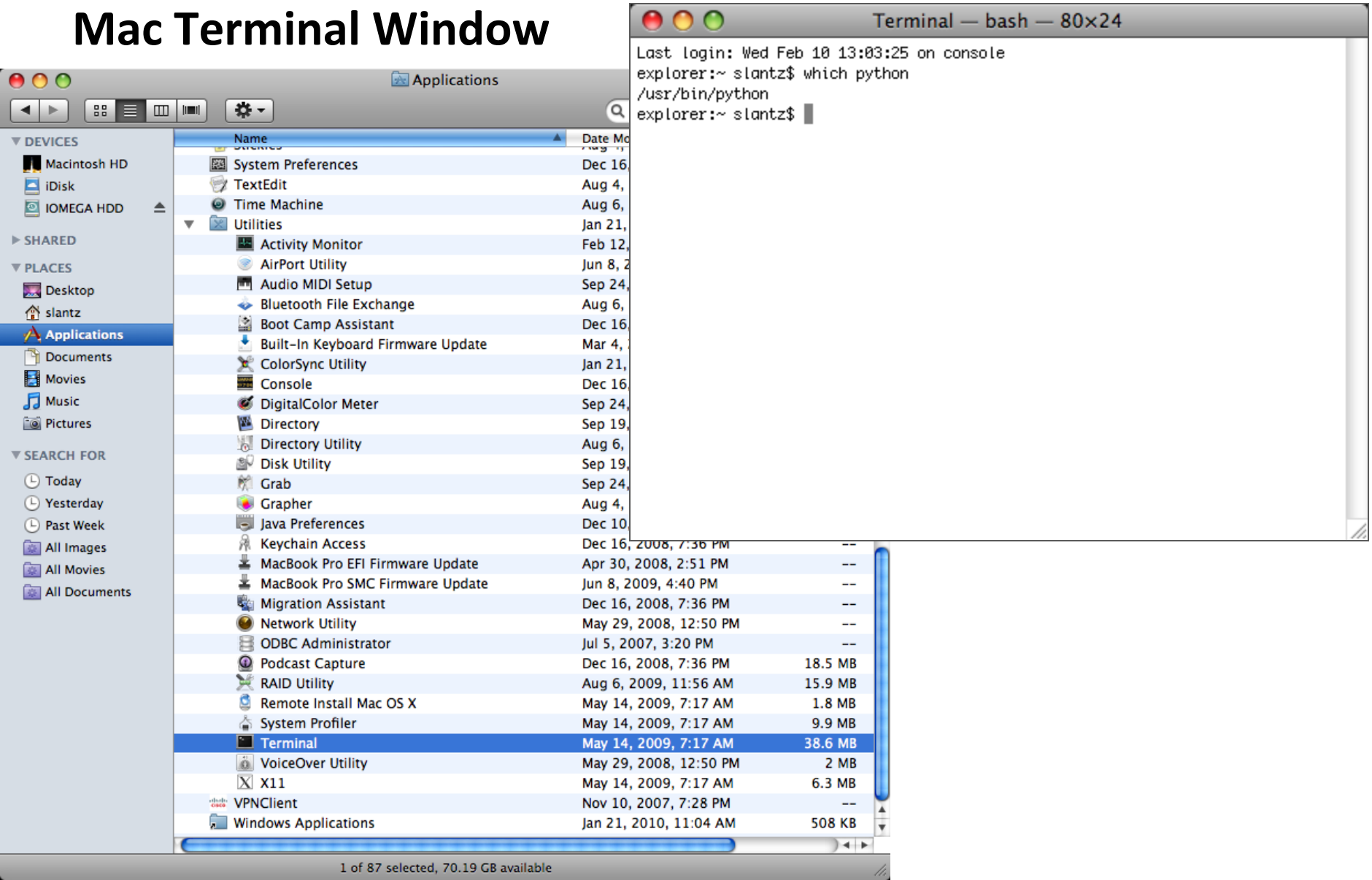
- sftp = sftp ajd27@linuxlogin1.cac.cornell.edu
- scp
  - secure copy



SSH Clients

- Windows
  - Download Putty tools: `putty.exe, psftp.exe`
  - `WinSCP`
- Mac – Open a terminal and type
  - `ssh -X ajd27@linuxlogin1.cac.cornell.edu`
  - `Fetch or sftp ajd27@linuxlogin2.cac.cornell.edu`
  - `scp`
- Linux – Open a terminal and type
  - `ssh -X ajd27@linuxlogin2.cac.cornell.edu`
  - `sftp ajd27@linuxlogin1.cac.cornell.edu`
  - `scp`

Mac Terminal Window



Invoking SSH

- Username
- Password
- Name of remote machine
- Whether to do X11 Forwarding

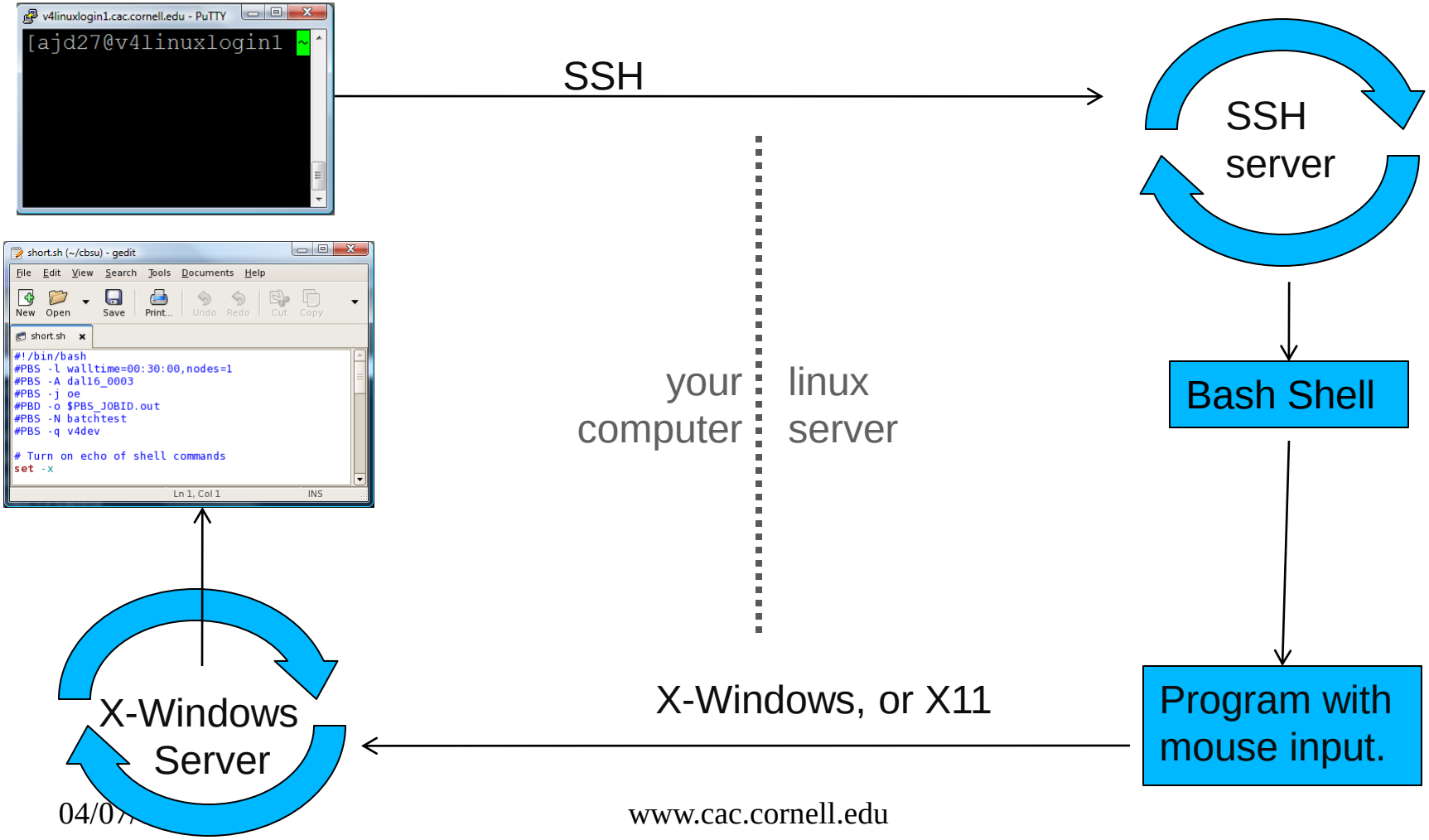
- Type at the terminal window:
- ssh -X ajd27@linuxlogin2.cac.cornell.edu

- Or fill out the form for Putty (see online directions).

v4linuxlogin1.cac.cornell.edu - PuTTY

```
[ajd27@v4linuxlogin1 ~]$ pwd
/home/fs01/ajd27
[ajd27@v4linuxlogin1 ~]$ mkdir cbsu
[ajd27@v4linuxlogin1 ~]$ cd cbsu
[ajd27@v4linuxlogin1 ~/cbsu]$ pwd
/home/fs01/ajd27/cbsu
[ajd27@v4linuxlogin1 ~/cbsu]$ ls
[ajd27@v4linuxlogin1 ~/cbsu]$ cp ~/dev/cbsu/* .
[ajd27@v4linuxlogin1 ~/cbsu]$ ls
1020332.scheduler.v4linux.OU  short.sh  short.sh~  xclock  z.txt
[ajd27@v4linuxlogin1 ~/cbsu]$ less short.sh
[ajd27@v4linuxlogin1 ~/cbsu]$
```

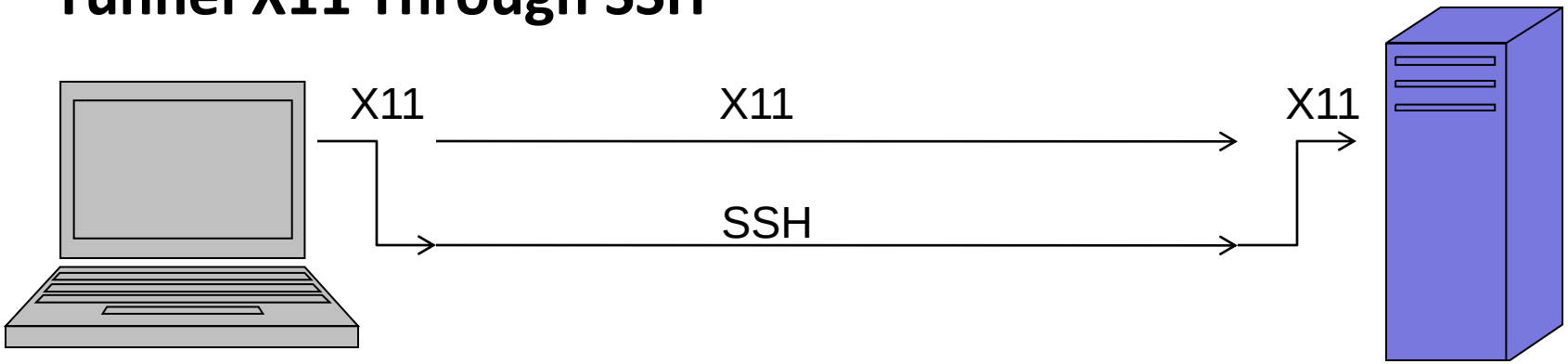
How to Connect to the Head Node



X-Windows Servers

- Windows
  - Download Xming, including its fonts package.
  - Install it.
  - Start Xming before you ssh to the head node.
- Mac – X-Windows is built in.
- Linux – X-Windows is built in.

Tunnel X11 Through SSH



- X11 is insecure
- SSH, as a protocol, can carry anything.
- SSH has automatic switches for X11
  - ssh -X, most of the time
  - ssh -Y, special cases, when -x fails.
  - “Enable X11 Forwarding” on Putty in Windows

Principles of a Shell

- Current working directory – Where you are is where programs run.
- Environment variables
  - PATH – A list of directories the shell searches for programs to run
  - SHELL – The type of the current shell, will be Bash.
  - USER – Username, also found with `whoami` command.
- $HOME – home directory
- Every program has stdin, stdout, stderr
  - ls > contents.txt 2> ls.err

Work with Directories and Files

- pwd
- mkdir nextgen
- cd nextgen
- cd ..
- cd
- rm -rf nextgen

- cat 1010282.out
- grep val 1010282.out
- less 1010282.out
- rm *.out

It's like being a bartender or a soda-jerk. It's easy once you know the basic moves. – The Man Who Wasn't There

Command-line Expansion

```
you: $ ls *.out
prog:$ ls 1020253.out 1020257.out 1020258.out

you: $ ./first_gen –d ${DATA}
prog:$ /home/fs01/ajd27/cbsu/first_gen –d my.dat

you: $ cd ~/dev/jfm17
prog:$ cd /home/fs01/ajd27/dev/jfm17
```

Things That Expand

- Current directory .
- Parent directory ..
- Home directory ~
- Variable $PATH or ${PATH}
- Modified variable: JOB_ID=1020233.v4linux.sched
  ${JOB_ID%%.*}.out -> 1020233.out

Work with Variables

- `env|sort|less`
- `echo $PATH`
- `export MYDIR=$HOME/cbsu`
- `export PATH=/opt/nextgen/bin:${PATH}`

Run in Shell

- `which perl`
- `ctrl-c`
- `./myprogram`
- `emacs&`
- `emacs`
  `ctrl-z`
  `bg`
- `jobs`
- `fg`
- `kill %1`

Surroundings

- `hostname`
- `whoami`
- `ps augx|grep ajd27`

Help in Bash

- `man less`
- `man -k moab`
- `gcc --help`
- `icc -h`

Shell Takeaway

- Environment is working directory and variables, files on disk.
- Those commands form a programming language.
- You will use that programming language to tell the scheduler what to run for you.

v4linuxlogin1.cac.cornell.edu - PuTTY

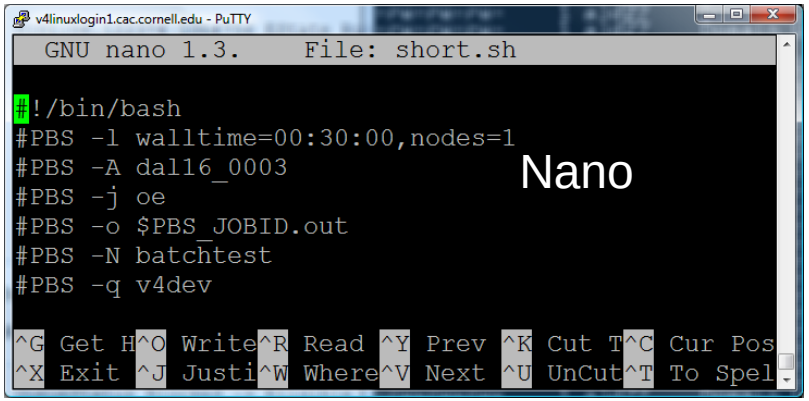
```
  GNU nano 1.3.12            File: short.sh

#!/bin/bash
#PBS -l walltime=00:30:00,nodes=1
#PBS -A dal16_0003
#PBS -j oe
#PBD -o $PBS_JOBID.out
#PBS -N batchtest
#PBS -q v4dev

# Turn on echo of shell commands
set -x


NODECNT=$(wc -l < "$PBS_NODEFILE")
TASKCNT=`expr 8 '*' $NODECNT`
RUNDIR=$PBS_O_WORKDIR
# The job id is something like 613.scheduler.v4linux.
# This deletes everything after the first dot.
                          [ Read 35 lines ]
^G Get Help^O WriteOut^R Read Fil^Y Prev Pag^K Cut Text^C Cur Pos
^X Exit    ^J Justify ^W Where Is^V Next Pag^U UnCut Te^T To Spell
```

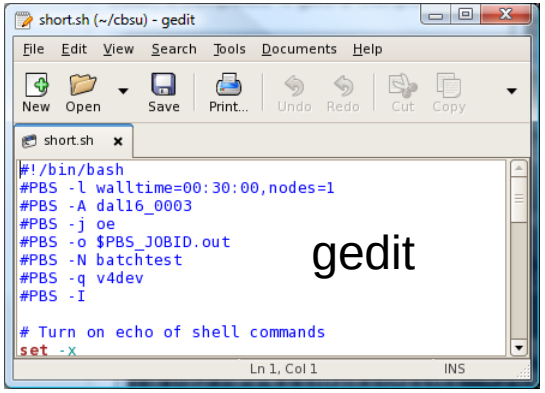
Matrix of Editors on the Login Nodes

in terminal window

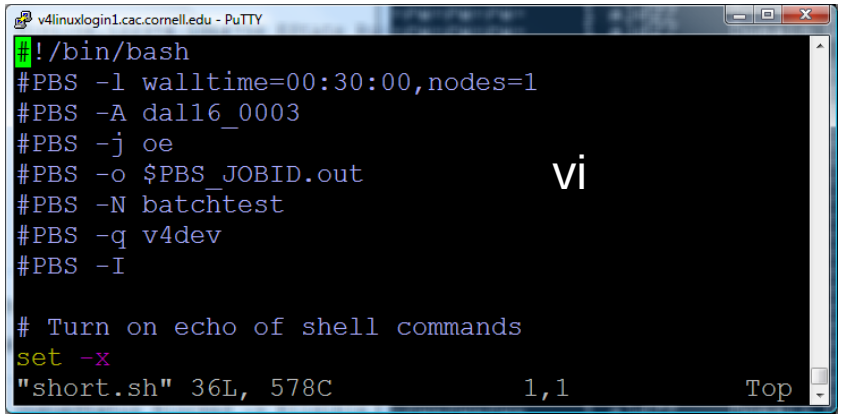
use X-Windows

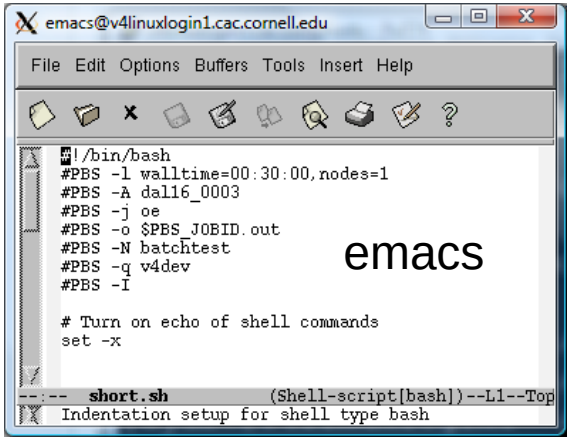
simple





The Unix Way



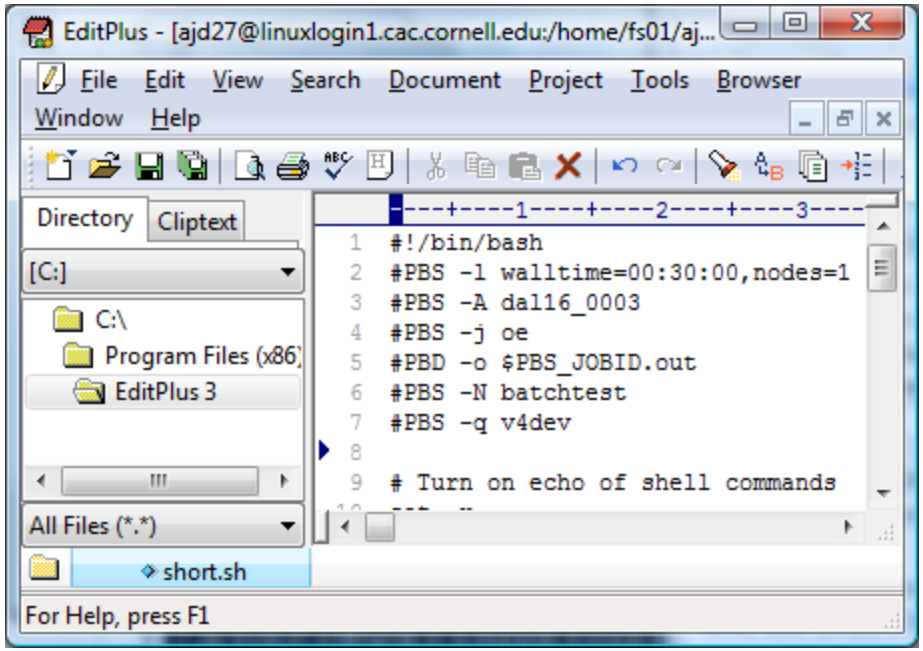


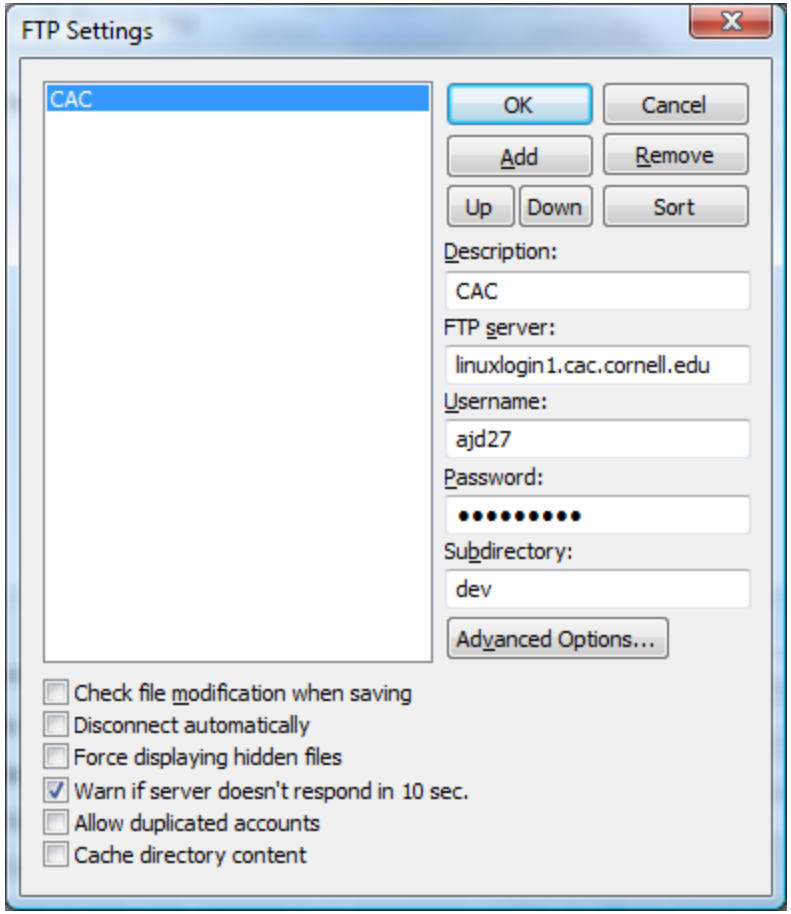
To Edit A File in VI (short for "visual")

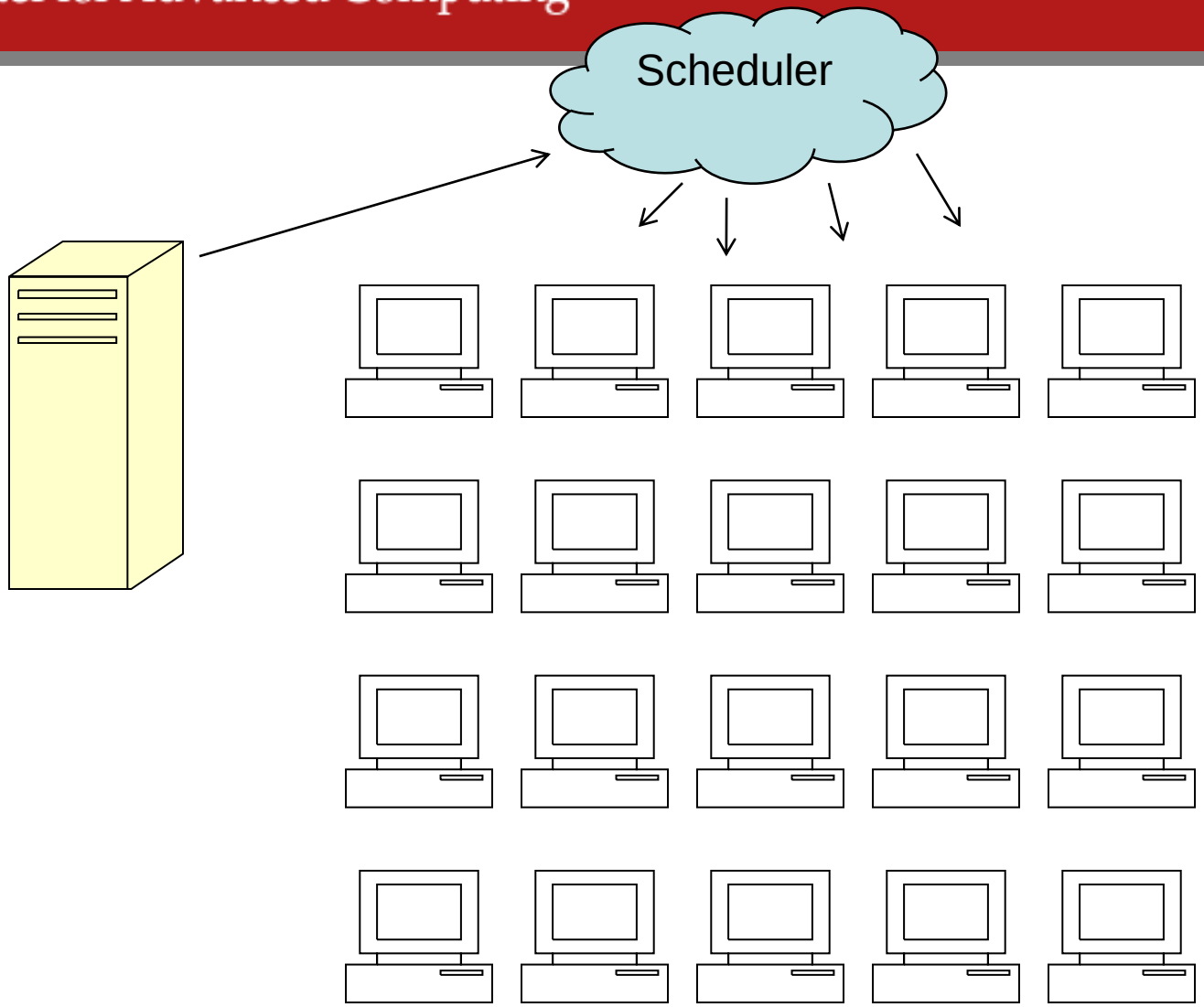
- "`vi filename`" will open it or create it if it doesn't exist.
- Command mode to start, switch to Insert mode.
- Command mode. Cursors work here, too.
  - `:w` Writes a file to disk.
  - `:q` Quits
  - `:q!` Quits even if there are changes to a file
  - `i` Takes you to insert mode
- Insert Mode
  - Cursors, typing characters, and deleting work here.
  - Escape key takes you to command mode.
- Ctrl-c will get you nowhere.

Editor on Your Computer that Saves to Cluster

- EditPlus on Windows
- TextWrangler on Mac






Scheduler

Queues

- v4 – Main queue to get access to compute nodes
  - 19 servers containing 152 cores
  - 16 GB RAM per server
  - Limits: Max 19 nodes, no walltime limit
- v4dev – Development queue for debugging and testing
  - Maximum of 2 nodes (16 cores)
  - Limits: Max 2 nodes, 60 minutes walltime
- v4-64g – Large-memory servers
  - 4 servers, total of 32 cores
  - 64 GB RAM per server
  - Maximum 3 nodes (24 processors), no walltime limit

Leases

- Groups purchase rights to nodes.

```
[ajd27@v4linuxlogin1 ~]$ showqlease
run free wait total queue  lease        nodes
  0   18    0    18 v4     standard     compute-3-[29-46]
  0    8    0     8 v4     acs4_0001    compute-3-[1-8]
  0    1    0     1 v4     ajd27        compute-3-28
  9    0    0     9 v4     asr2004_0001 compute-3-[9-17]
  2    8    0    10 v4     jp86_0005    compute-3-[18-27]
  0    3    0     3 v4-64g standard     lmcompute-4-[1-3]
  0    1    0     1 v4-64g sc167_0001   lmcompute-4-4
  0    2    0     2 v4dev  standard     compute-3-[47-48]
Administrative downtime:
   Wed Mar 10 08:00:00 for 9:00:00 compute-3-[1-48],lmcompute-4-[1-4]
```

Life of a Job

1. You create a job script.
2. You submit job script to scheduler using nsub.
3. Scheduler checks the job and either returns an error or sets its state to Idle / Eligible.
4. When scheduler finds available resources, it
   a) sets job state to Running
   b) asks job manager on selected nodes to run the job in a shell.
5. Job completes because
   a) The script finished executing.
   b) It exceeded its time limit.
6. Scheduler sets job state to Completed.

Batch Script is a File with Directives

```
#!/bin/bash
#PBS -l walltime=00:30:00,nodes=1
#PBS -A dal16_0003
#PBS -j oe
#PBS -o $PBS_O_WORKDIR/$PBS_JOBID.out
#PBS -N batchtest
#PBS -q v4dev
#PBS -V
# Turn on echo of shell commands
set –x
DATADIR=/home/gfs08/jp86/ngw2010/\
session1/lecture2/
DATA=s_8_1_sequence.txt
cp ${DATADIR}/${DATA} ${TMPDIR}
cd ${TMPDIR}
fastx_quality_stats -i $DATA -o stat.xls
cp stat.xls ${PBS_O_WORKDIR}/
```

`-l` requests nodes for a time

`-A` is your account number

`-j` joins output and error from programs for the output file

`-o` is the name of the output file

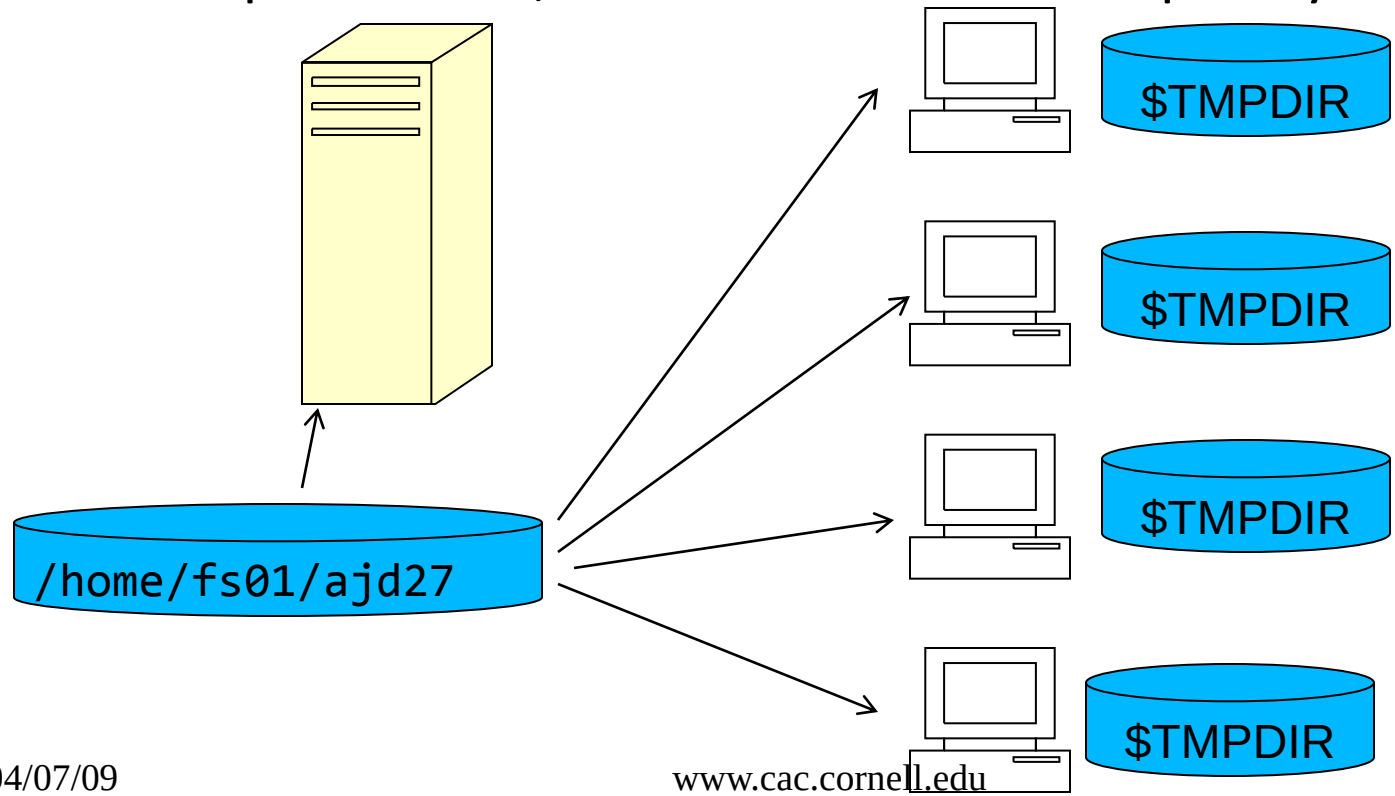
`-N` is the job name

`-q` specifies which queue runs the job

`-V` tells it to use whatever variables were set when you submitted the job

Drives

- Your home drive is available everywhere.
- On compute nodes, $TMPDIR is a local temporary directory.



Using Local Directories in a Batch Script

```
#!/bin/bash
#PBS -l walltime=00:30:00,nodes=1
#PBS -A dal16_0003
#PBS -j oe
#PBS -o $PBS_O_WORKDIR/$PBS_JOBID.out
#PBS -N batchtest
#PBS -q v4dev
#PBS -V
# Turn on echo of shell commands
set –x
DATADIR=/home/gfs08/jp86/ngw2010/session1/lecture2/
DATA=s_8_1_sequence.txt
cp ${DATADIR}/${DATA} ${TMPDIR}
cd ${TMPDIR}
fastx_quality_stats -i ${DATA} -o stat.xls
cp stat.xls ${PBS_O_WORKDIR}/
```

- Copy to TMPDIR.
- Go to TMPDIR.
- Run program.
- Copy to WORKDIR.

Moab Commands

- nsub – Submit a job
  - nsub jobscript.sh
- showq – Display queue information
  - showq
  - showq -w user=ajd27
  - showq -w class=v4dev
- checkjob – How is this one job doing?
  - checkjob -v 1020282
- mjobctl - modify job
  - mjobctl -c 1020282, cancel a job
- showqlease – get a sense of how busy the queues are

Submit a Job

```
[ajd27@v4linuxlogin1 ~/cbsu]$ nsub short.sh
Looking for directives in short.sh

1020333

[ajd27@v4linuxlogin1 ~/cbsu]$ showq
active jobs------------------------
JOBID       USERNAME STATE   PROCS   REMAINING STARTTIME

1020334     lmv47    Running     8    14:10:53  Mon Mar  1 13:22:58
1020335     lmv47    Running     8    14:13:59  Mon Mar  1 13:26:04
1020287     kab2003  Running    64  3:09:47:13  Sun Feb 28 20:59:18

3 active jobs    80 of 416 processors in use by local jobs (19.23%)
                          10 of 52 nodes active      (19.23%)
```

Checkjob

```
[ajd27@v4linuxlogin1 ~]$ checkjob 1020287
job 1020287

AName: mpiTest
State: Running
Creds: user:kab2003 group:Domain Users account:asr2004_0001 class:v4
WallTime:   1:15:41:03 of 4:04:00:00
SubmitTime: Sun Feb 28 20:59:02
  (Time Queued  Total: 00:00:16  Eligible: 00:00:00)
StartTime: Sun Feb 28 20:59:18
NodeMatchPolicy: EXACTNODE
Total Requested Tasks: 8
Req[0]  TaskCount: 8  Partition: scheduler
Allocated Nodes:
[compute-3-17.v4linux:1][compute-3-16.v4linux:1][compute-3-15.v4linux:1
[compute-3-14.v4linux:1][compute-3-13.v4linux:1][compute-3-12.v4linux:1
[compute-3-11.v4linux:1][compute-3-10.v4linux:1]
```

Cornell University
Center for Advanced Computing

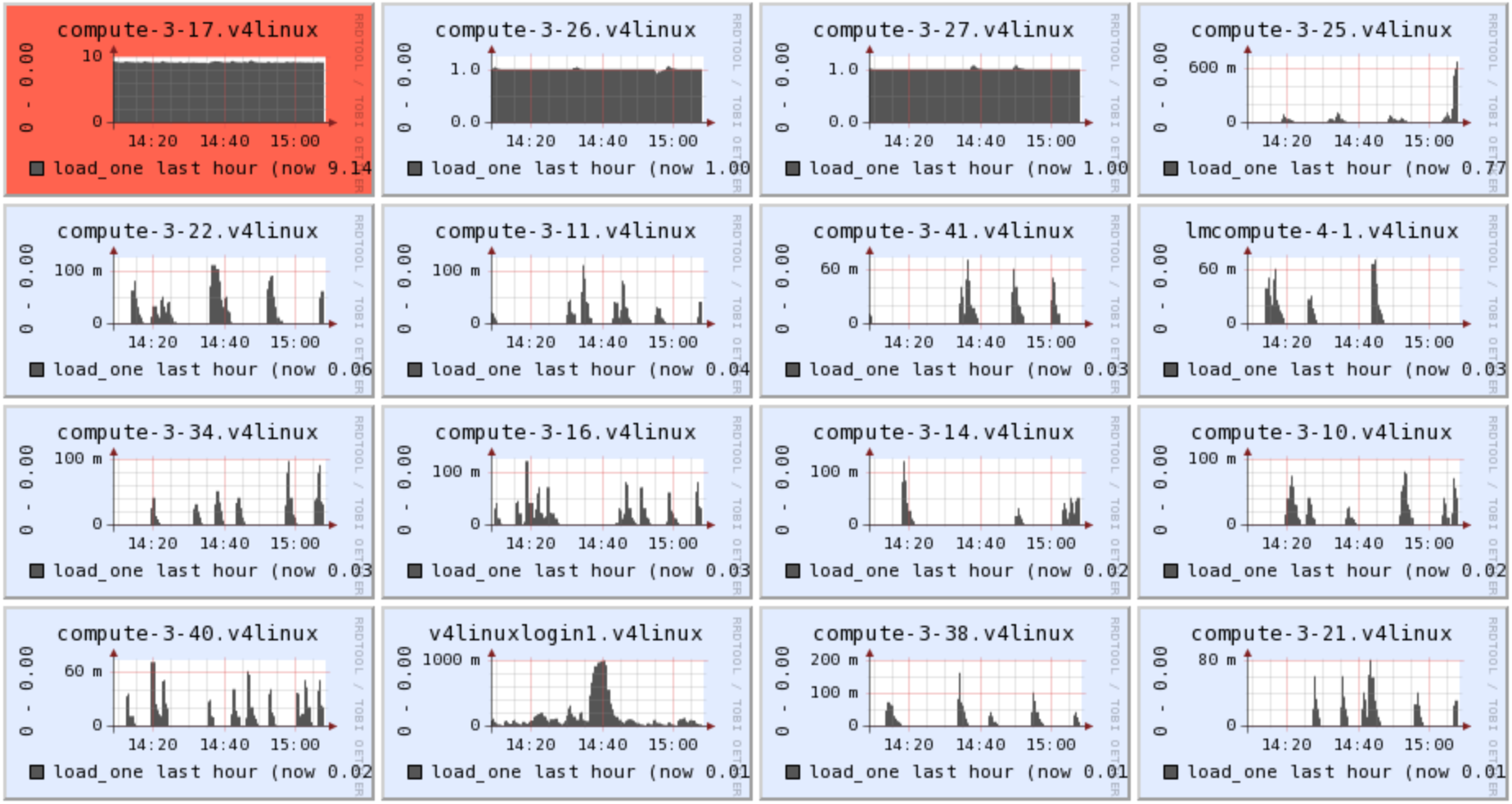
Ganglia Cluster Toolkit:: Cluster Report - Mozilla Firefox

File Edit View History Bookmarks GMarks Tools Help

http://v4.cac.cornell.edu/ganglia/

windows print screen

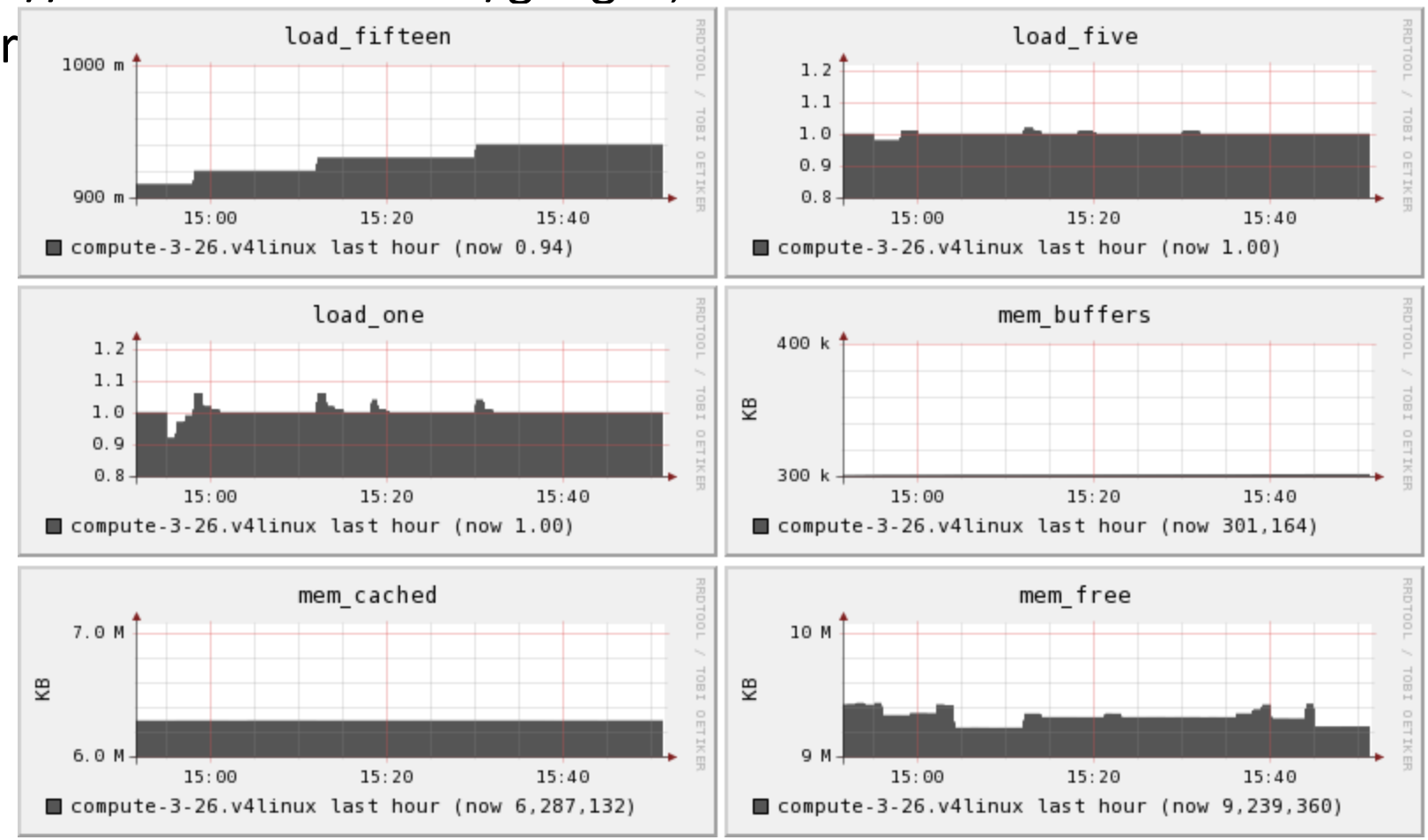
#1627: reserve one node for cb... | MoabCommands - Cornell CA... | windows print screen - Google ... | Ganglia Cluster Toolkit:: Clust...



http://v4.cac.cornell.edu/ganglia/?c=v4Linux Cluster&h=compute-3-10.v4linux&m=&r=hour&s=descending&hc=4

See a Profile of Running Job

- http://v4.cac.cornell.edu/ganglia, then click on the nodes for your



What Can Go Wrong

- Fail immediately
  - Script does not exist
  - Wrong account number
- Make you wait, but eventually work
  - People ahead of you in the queue make it busy
  - You submit one job that says it may use all of your minutes (but doesn't) and another job after it.
- Fail after the job starts
  - Errors in the batch file so it does something wrong
- Stop the job in the queue – Job state Blocked
  - Requested more nodes than the limit of the queue

How to Debug Problems

- Look at log files
- Make an interactive job.

```
#!/bin/bash
#PBS -l walltime=00:30:00,nodes=1
#PBS -A dal16_0003
#PBS -j oe
#PBS -o $PBS_JOBID.out
#PBS -N batchtest
#PBS -q v4dev
#PBS –V
#PBS -I
```

```
[ajd27@v4linuxlogin1 ~/cbsu]$ nsub short.sh
Looking for directives in short.sh
Executing interactive
qsub: waiting for job 1020349.scheduler.v4linux to start
qsub: job 1020349.scheduler.v4linux ready

[ajd27@compute-3-48 ~/cbsu]$ logout
qsub: job 1020349.scheduler.v4linux completed
```

SSH to a Node While It Runs Your Job

- Only when a node is running your job can you login to it.
- You can only get to a compute node from a login node.

```
[ajd27@v4linuxlogin1 ~/cbsu]$ nsub short.sh
Looking for directives in short.sh
1020353
[ajd27@v4linuxlogin1 ~/cbsu]$ showq|grep ajd27
[ajd27@v4linuxlogin1 ~/cbsu]$ checkjob 1020353|grep v4linux
[compute-3-48.v4linux:1]
[ajd27@v4linuxlogin1 ~/cbsu]$ ssh -Y compute-3-48.v4linux
```

Puzzle: How to Start a Batch Job with a GUI

- gsAssembly is a graphical interface on Newbler.
- I want to run it in batch, but I would like to see the graphical interface on the compute node to kick off the job.

- Would interactive batch jobs work?
- Given a regular batch job, what do you put in the script?
- How would the job know when to quit?

Batch Script that Waits for You

```
#!/bin/bash
#PBS -l
walltime=00:30:00,nodes=1
#PBS -A dal16_0003
#PBS -j oe
#PBS -q v4
#PBS –V
```

```
PROG=newbler

echo Wait until user logs in
while who -q|head -1|grep -v
"\b${USER}\b"
do
  sleep 10
done

echo Wait until the user logs off
while who -q|head -1|grep "\b${USER}\b"
do
  sleep 30
done

echo Wait until the ${PROG} finishes
while ps -u ${USER} -o comm|grep $PROG
do
  sleep 30
done

echo ${PROG} finished `date`
```

How to Kickstart a Long Job from a GUI

- Create a batch script that starts but does nothing.
- Wait for the job to start.
- `ssh -Y` to the node.
- Start your program with the magic nohup.
- Configure it and tell it to run.
- Logout and wait for results.

```
nohup script.sh > z.out 2> z.err < /dev/null &
```

What Does It Take to Be Skilled at This?

- Know the shell.
- Understand processes and threads on a Unix system.

- Study
- Experiment