LONI Programming Environment

Alexander B. Pacheco

User Services Consultant
LSU HPC & LONI
sys-help@loni.org

LONI HPC Workshop
Xavier University of Louisiana
New Orleans
Mar 21, 2012

- Two major architectures.

Linux Clusters

- Vendor: Dell
- OS: Red Hat
- CPU: Intel Xeon

AIX Clusters

- Vendor: IBM
- OS: AIX
- CPU: Power 5

- The LONI AIX clusters are on a path to decommissioning.

Linux Clusters

	Name	Peak TeraFLOPS/s	Location	Status	Login
LONI	QueenBee	50.7	ISB	Production	LONI
	Eric	4.7	LSU	Production	LONI
	Louie	4.7	Tulane	Production	LONI
	Oliver	4.7	ULL	Production	LONI
	Painter	4.7	LaTech	Production	LONI
	Poseidon	4.7	UNO	Production	LONI

AIX Clusters

	Name	Peak TF/s	Location	Status	Login
LONI	Bluedawg	0.85	LaTech	Production	LONI
	Ducky	0.85	UNO	Decommissioned	LONI
	Lacumba	0.85	Southern	Decommissioned	LONI
	Neptune	0.85	Tulane	Decommissioned	LONI
	Zeke	0.85	ULL	Decommissioned	LONI

Getting an Account

- LONI account

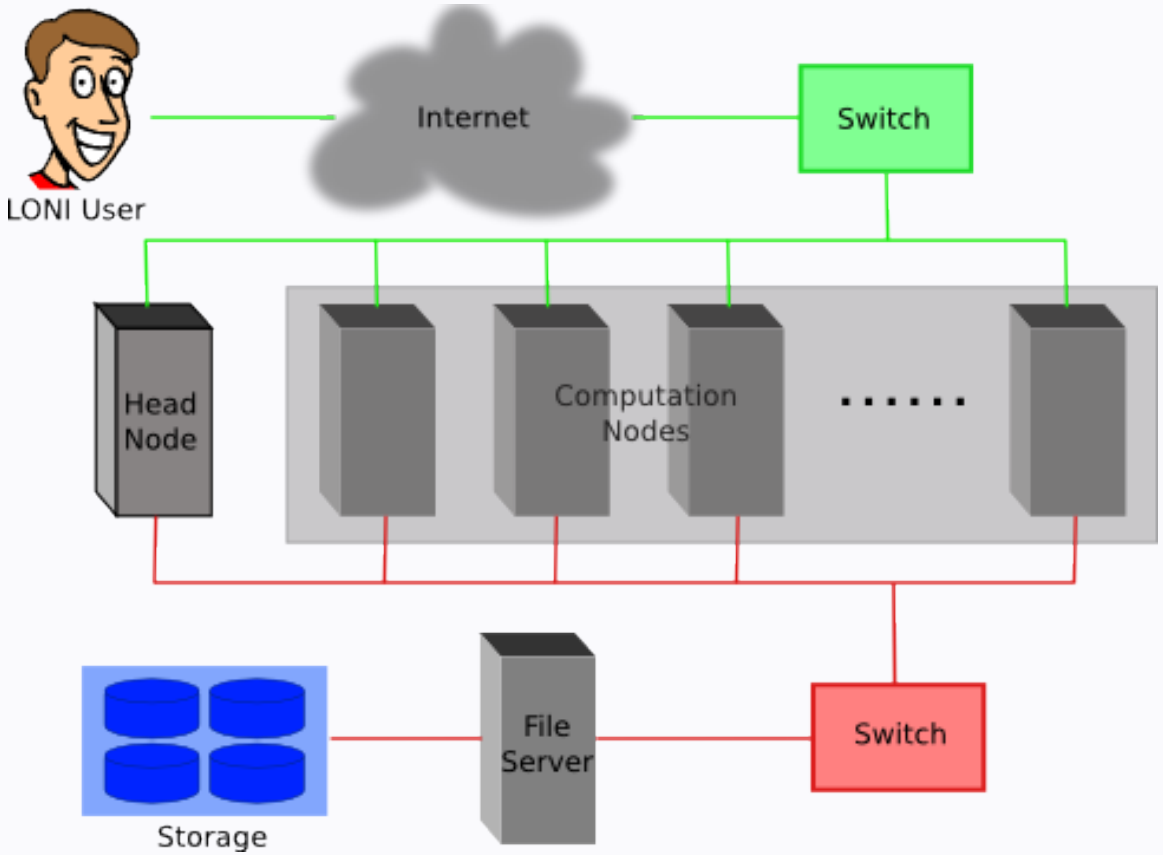
  `https://allocations.loni.org`
- Request Allocations

  `https://allocations.loni.org`
- All LONI AIX clusters are being decommissioned.

Login Shell

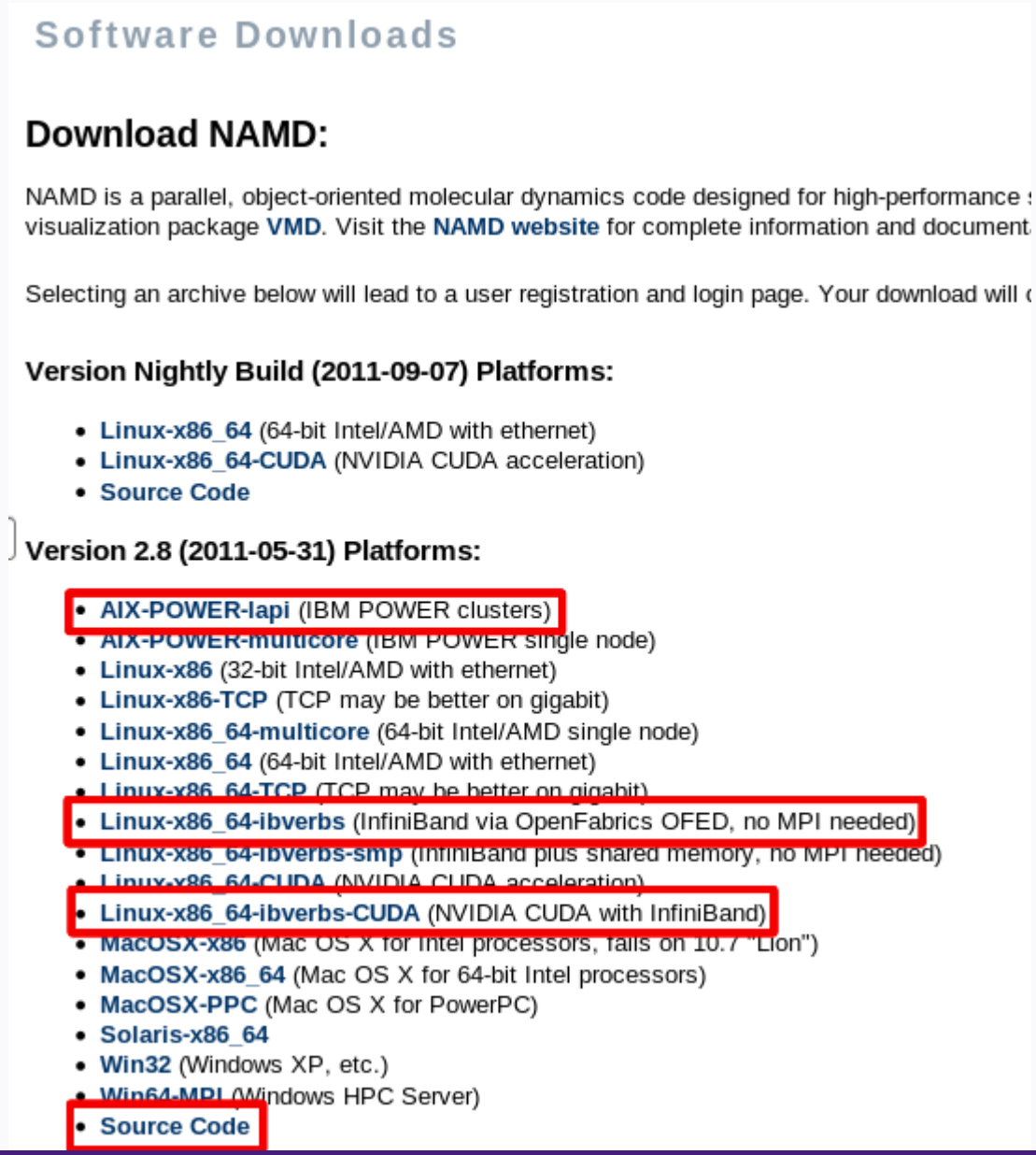
- The default Login shell is bash
- Supported Shells: bash, tcsh, ksh, csh & sh
- Change Login Shell at the profile page

- A cluster is a group of computers (nodes) that works together closely
- Type of nodes
  - Head node
  - Compute node



- Queen Bee
  - 668 nodes: 8 Intel Xeon cores @ 2.33 GHz
  - 8 GB RAM
  - 192 TB storage
- Other LONI Linux clusters
  - 128 nodes: 4 Intel Xeons cores @ 2.33 GHz
  - 4 GB RAM
  - 9 TB storage
- LONI AIX clusters (All except Bluedawg decommissioned)
  - 14 Power5 nodes, 8 IBM Power5 processors @ 1.9 GHz per node
  - 16 GB RAM
  - 280 GB storage

- There are numerous different architectures in the HPC world.
- Choose the software to install or use depending on cluster architecture.
  1. Linux: EM64T, AMD64, X86_64
  2. AIX: Power5, Power7



Software Downloads

Download NAMD:

NAMD is a parallel, object-oriented molecular dynamics code designed for high-performance s
visualization package **VMD**. Visit the **NAMD website** for complete information and document

Selecting an archive below will lead to a user registration and login page. Your download will

Version Nightly Build (2011-09-07) Platforms:

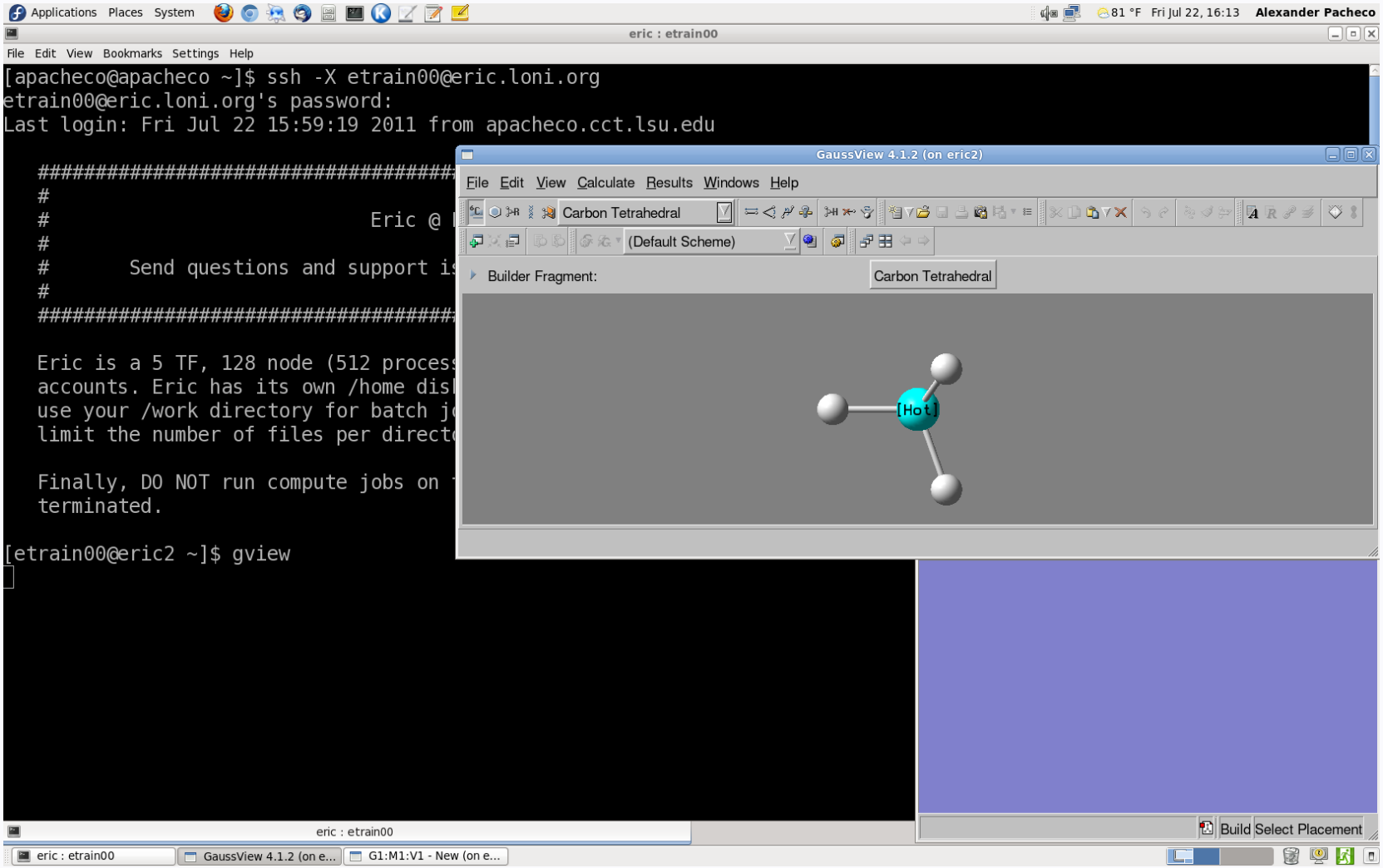
- **Linux-x86_64** (64-bit Intel/AMD with ethernet)
- **Linux-x86_64-CUDA** (NVIDIA CUDA acceleration)
- **Source Code**

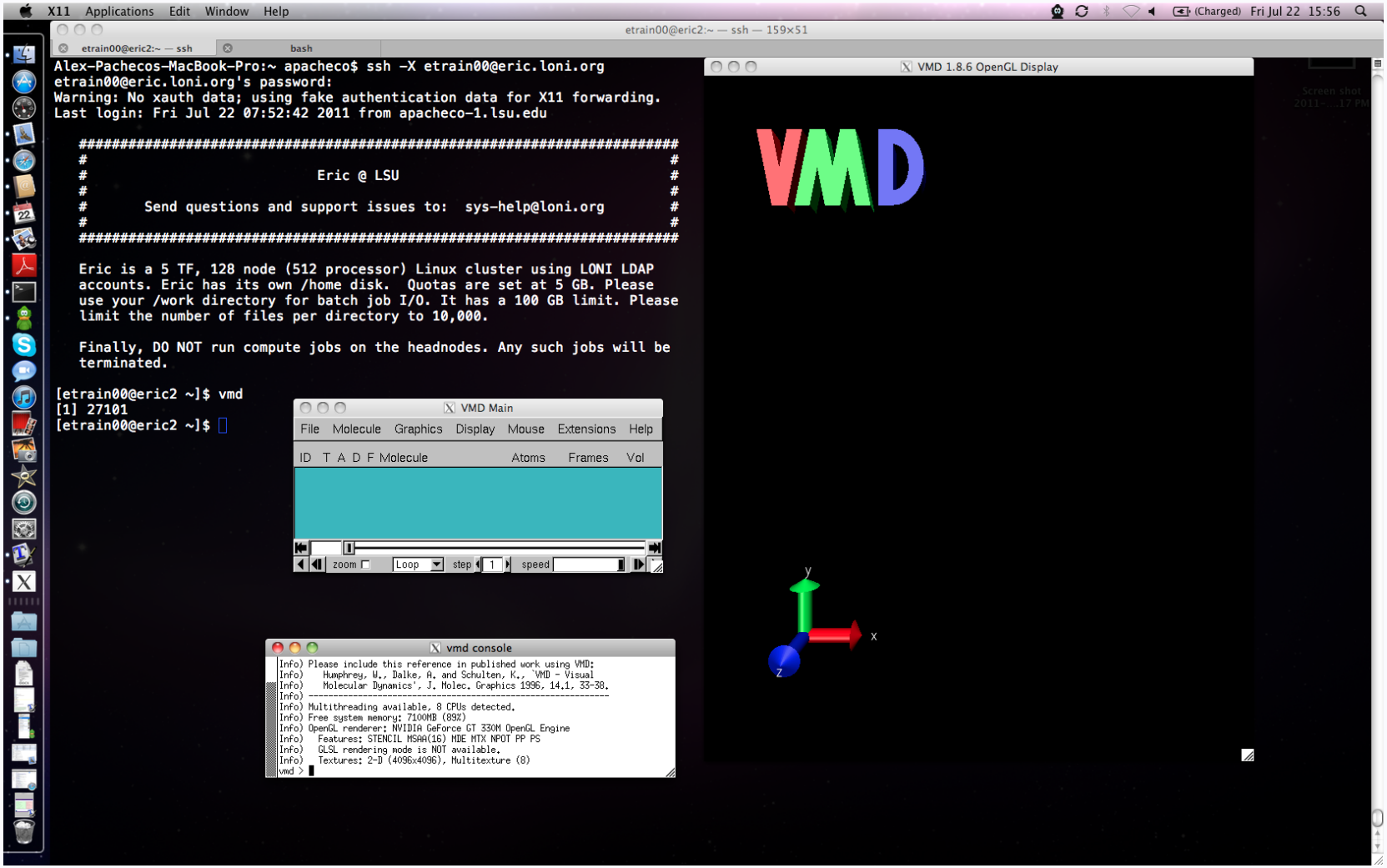
Version 2.8 (2011-05-31) Platforms:

- **AIX-POWER-lapi** (IBM POWER clusters)
- **AIX-POWER-multicore** (IBM POWER single node)
- **Linux-x86** (32-bit Intel/AMD with ethernet)
- **Linux-x86-TCP** (TCP may be better on gigabit)
- **Linux-x86_64-multicore** (64-bit Intel/AMD single node)
- **Linux-x86_64** (64-bit Intel/AMD with ethernet)
- **Linux-x86_64-TCP** (TCP may be better on gigabit)
- **Linux-x86_64-ibverbs** (InfiniBand via OpenFabrics OFED, no MPI needed)
- **Linux-x86_64-ibverbs-smp** (InfiniBand plus shared memory, no MPI needed)
- **Linux-x86_64-CUDA** (NVIDIA CUDA acceleration)
- **Linux-x86_64-ibverbs-CUDA** (NVIDIA CUDA with InfiniBand)
- **MacOSX-x86** (Mac OS X for Intel processors, fails on 10.7 "Lion")
- **MacOSX-x86_64** (Mac OS X for 64-bit Intel processors)
- **MacOSX-PPC** (Mac OS X for PowerPC)
- **Solaris-x86_64**
- **Win32** (Windows XP, etc.)
- **Win64-MPI** (Windows HPC Server)
- **Source Code**

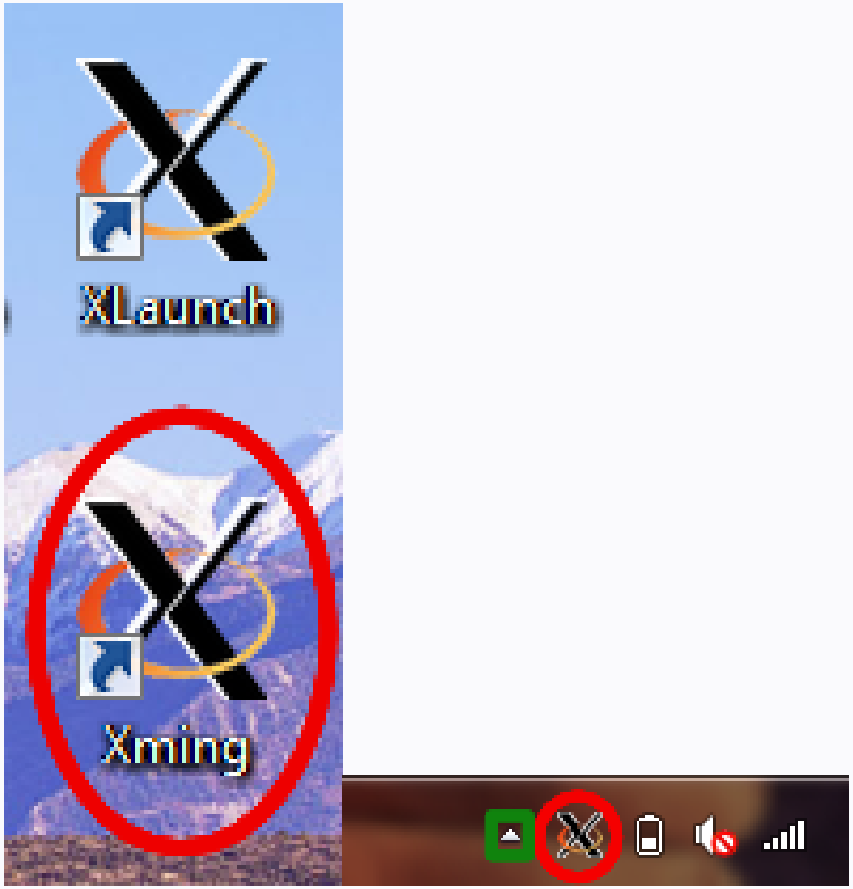
- The amount of installed memory less the amount that is used by the operating system and other utilities
- Max amount per node
  - Linux clusters: ∼6 GB for Queen Bee, ∼3 GB for others
  - AIX clusters: ∼13 GB

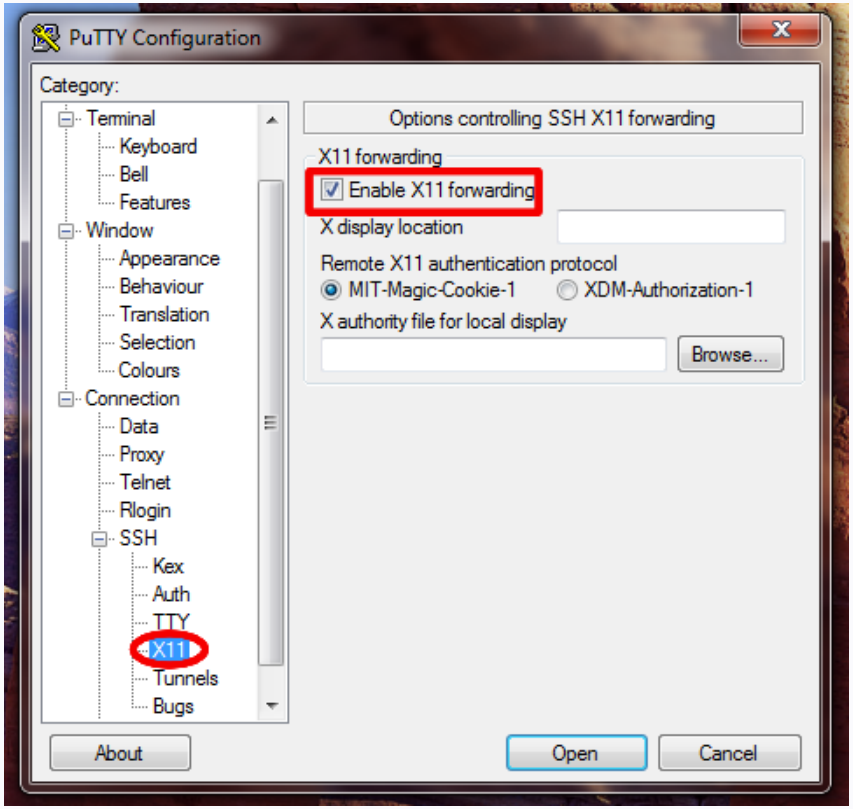
- LONI Host name: `<cluster name>.loni.org`
  - ★ Eric: eric.loni.org
- Use ssh to connect
  - ★ ∗nix and Mac: `ssh <host name>`
  - ★ Windows: use Putty, Secure Shell Client or Bitvise Tunnelier
- The default Login shell is bash
- Supported shells: bash, tcsh, ksh, csh & sh
- Change the login shell at the profile page
  - ♦ LONI: `https://allocations.loni.org`
- Reset your password
  - ♦ LONI: `https://allocations.loni.org/user_reset.php`

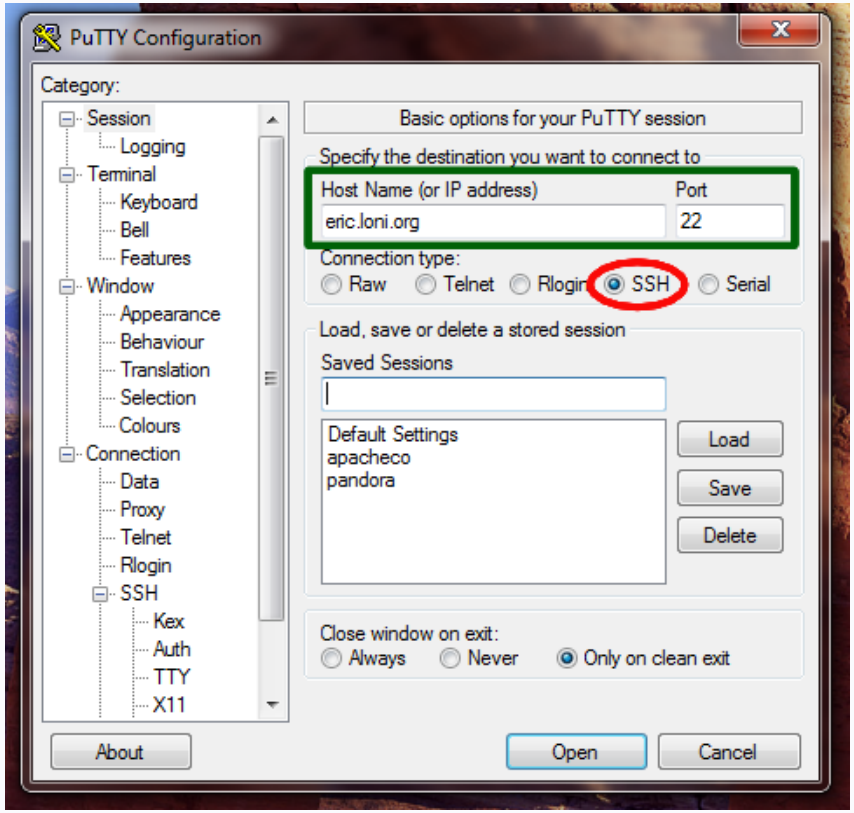

Applications Places System
81 °F Fri Jul 22, 16:13 Alexander Pacheco
eric : etrain00
File Edit View Bookmarks Settings Help
[apacheco@apacheco ~]$ ssh -X etrain00@eric.loni.org
etrain00@eric.loni.org's password:
Last login: Fri Jul 22 15:59:19 2011 from apacheco.cct.lsu.edu
Eric @
Send questions and support i
Eric is a 5 TF, 128 node (512 proces
accounts. Eric has its own /home dis
use your /work directory for batch j
limit the number of files per direct
Finally, DO NOT run compute jobs on
terminated.
[etrain00@eric2 ~]$ gview
GaussView 4.1.2 (on eric2)
File Edit View Calculate Results Windows Help
Carbon Tetrahedral
(Default Scheme)
Builder Fragment:
Carbon Tetrahedral
[Hot]
Build Select Placement
eric : etrain00
eric : etrain00
GaussView 4.1.2 (on e...
G1:M1:V1 - New (on e...

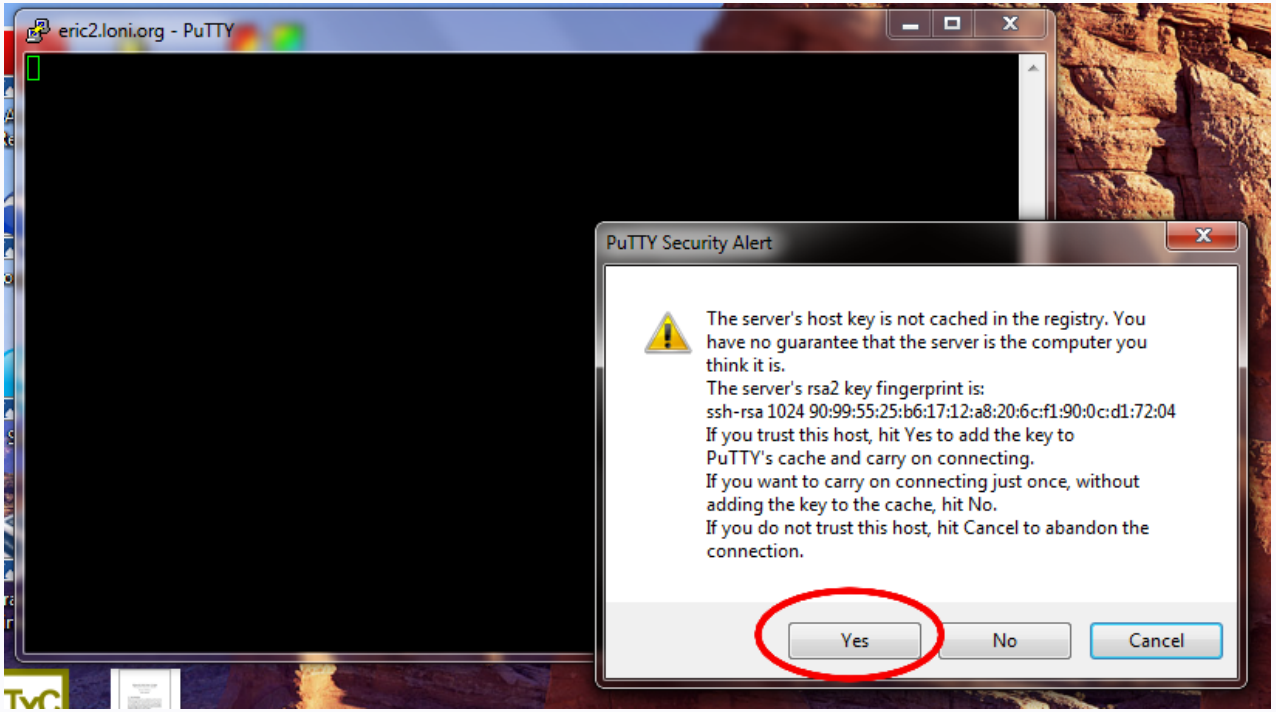

X11 Applications Edit Window Help
(Charged) Fri Jul 22 15:56
etrain00@eric2:~ — ssh — 159×51
etrain00@eric2:~ — ssh
bash
Alex-Pachecos-MacBook-Pro:~ apacheco$ ssh -X etrain00@eric.loni.org
etrain00@eric.loni.org's password:
Warning: No xauth data; using fake authentication data for X11 forwarding.
Last login: Fri Jul 22 07:52:42 2011 from apacheco-1.lsu.edu
Eric @ LSU
Send questions and support issues to: sys-help@loni.org
Eric is a 5 TF, 128 node (512 processor) Linux cluster using LONI LDAP accounts. Eric has its own /home disk. Quotas are set at 5 GB. Please use your /work directory for batch job I/O. It has a 100 GB limit. Please limit the number of files per directory to 10,000.
Finally, DO NOT run compute jobs on the headnodes. Any such jobs will be terminated.
[etrain00@eric2 ~]$ vmd
[1] 27101
[etrain00@eric2 ~]$
VMD 1.8.6 OpenGL Display
VMD
VMD Main
File Molecule Graphics Display Mouse Extensions Help
ID T A D F Molecule Atoms Frames Vol
zoom Loop step 1 speed
vmd console
Info) Please include this reference in published work using VMD:
Info) Humphrey, W., Dalke, A. and Schulten, K., 'VMD - Visual
Info) Molecular Dynamics', J. Molec. Graphics 1996, 14.1, 33-38.
Info) Multithreading available, 8 CPUs detected.
Info) Free system memory: 7100MB (89%)
Info) OpenGL renderer: NVIDIA GeForce GT 330M OpenGL Engine
Info) Features: STENCIL MSAA(16) MDE MTX NPOT PP PS
Info) GLSL rendering mode is NOT available.
Info) Textures: 2-D (4096x4096), Multitexture (8)
vmd >
y
x
z

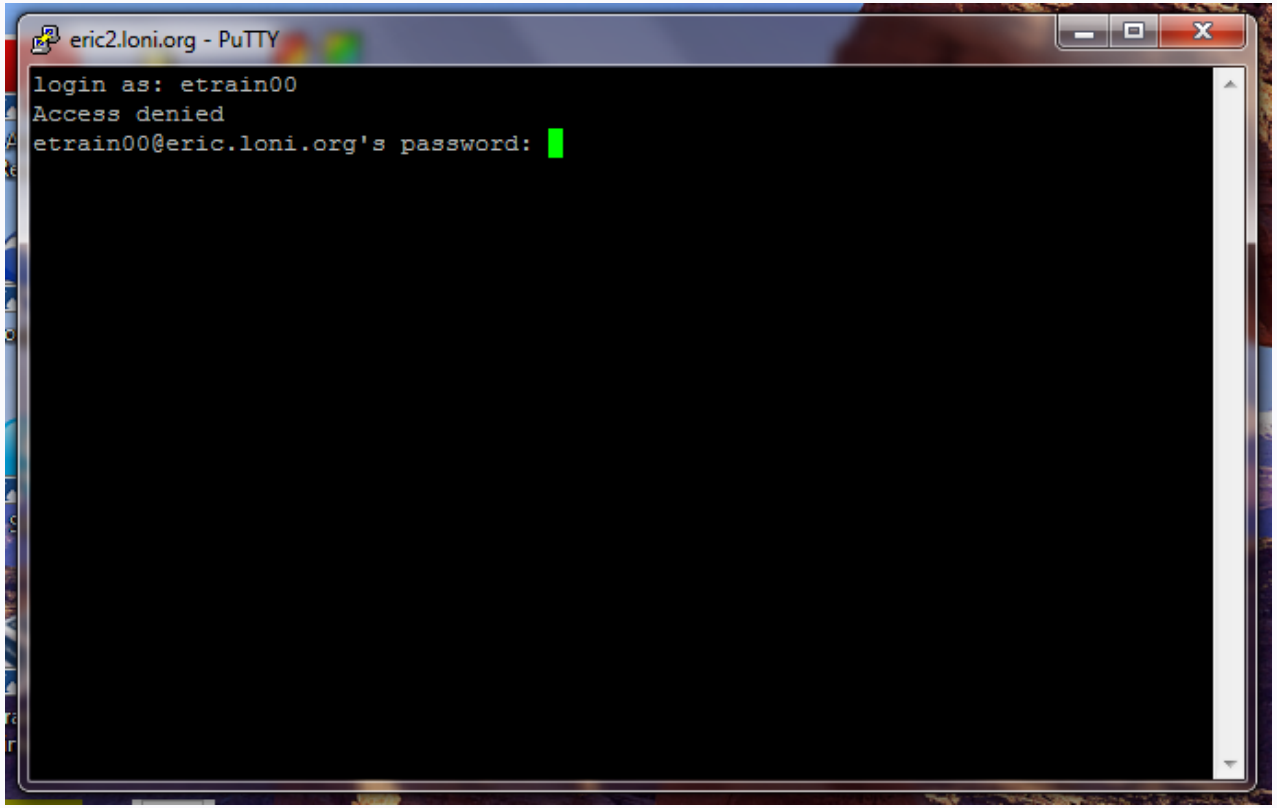
- Download and Install
  1. SSH Client: Putty
     `http://www.chiark.greenend.org.uk/~sgtatham/putty/`
  2. SSH+SFTP/SCP Client: Bitvise Tunnelier
     `http://www.bitvise.com/tunnelier`
  3. X-Server (if needed): X-ming
     `http://www.straightrunning.com/XmingNotes/`

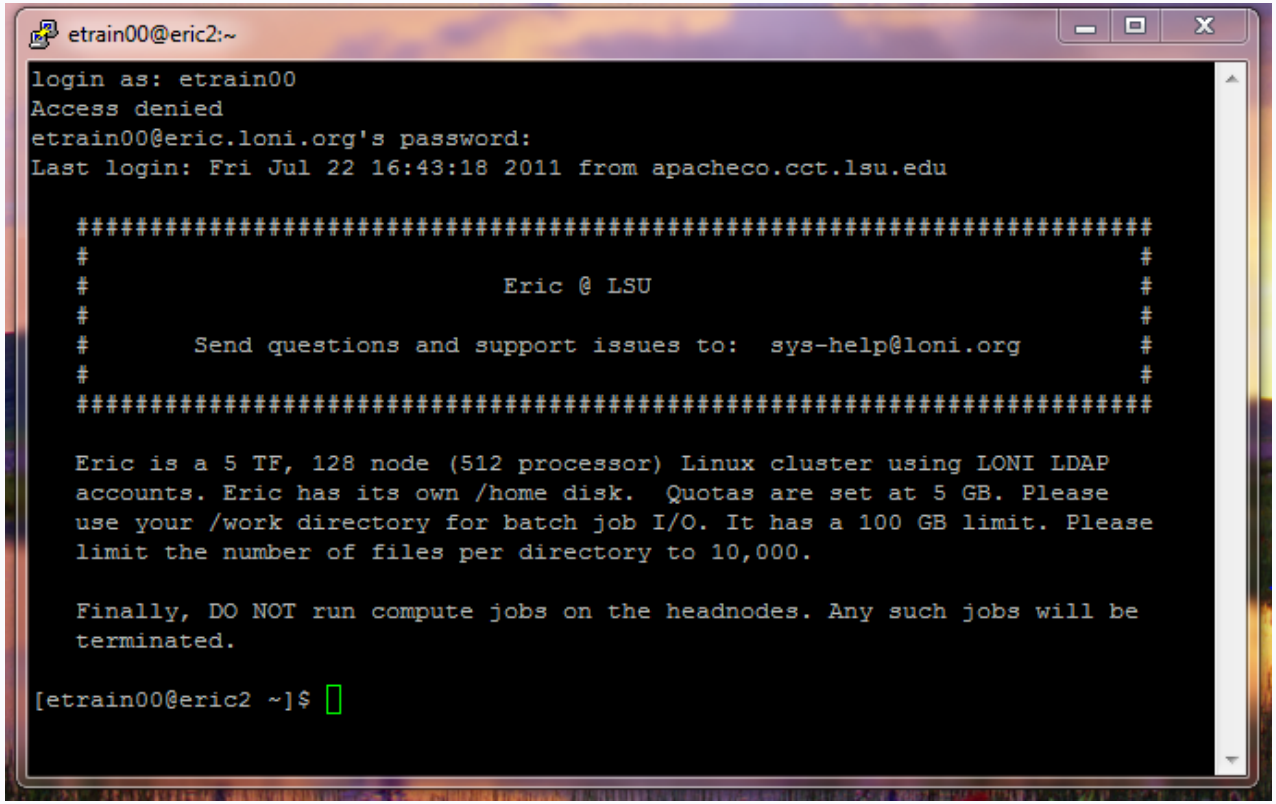

XLaunch
Xming

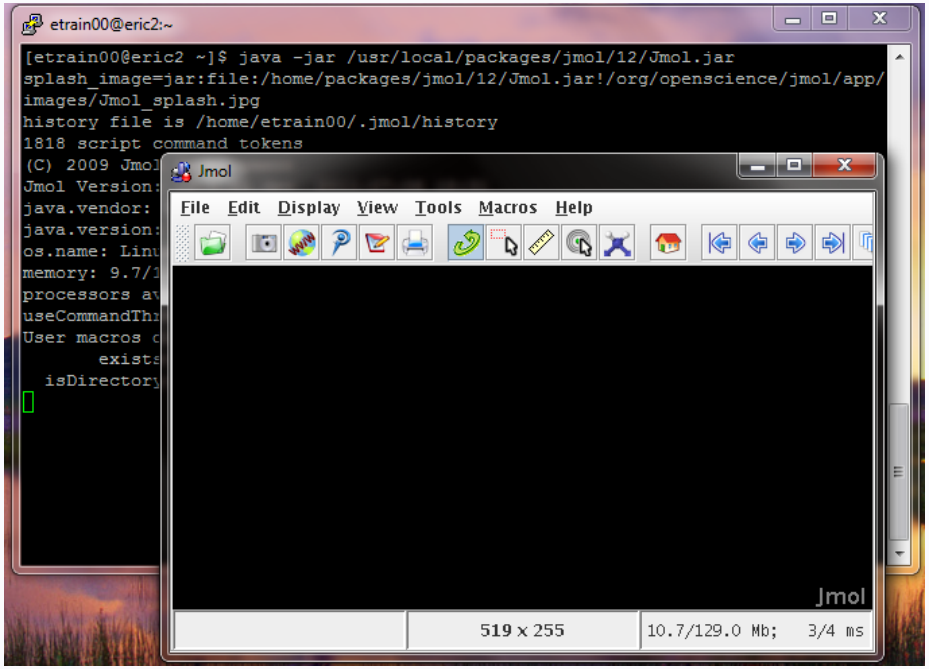

PuTTY Configuration
Category:
Terminal
Keyboard
Bell
Features
Window
Appearance
Behaviour
Translation
Selection
Colours
Connection
Data
Proxy
Telnet
Rlogin
SSH
Kex
Auth
TTY
X11
Tunnels
Bugs
Options controlling SSH X11 forwarding
X11 forwarding
Enable X11 forwarding
X display location
Remote X11 authentication protocol
MIT-Magic-Cookie-1
XDM-Authorization-1
X authority file for local display
Browse...
About
Open
Cancel

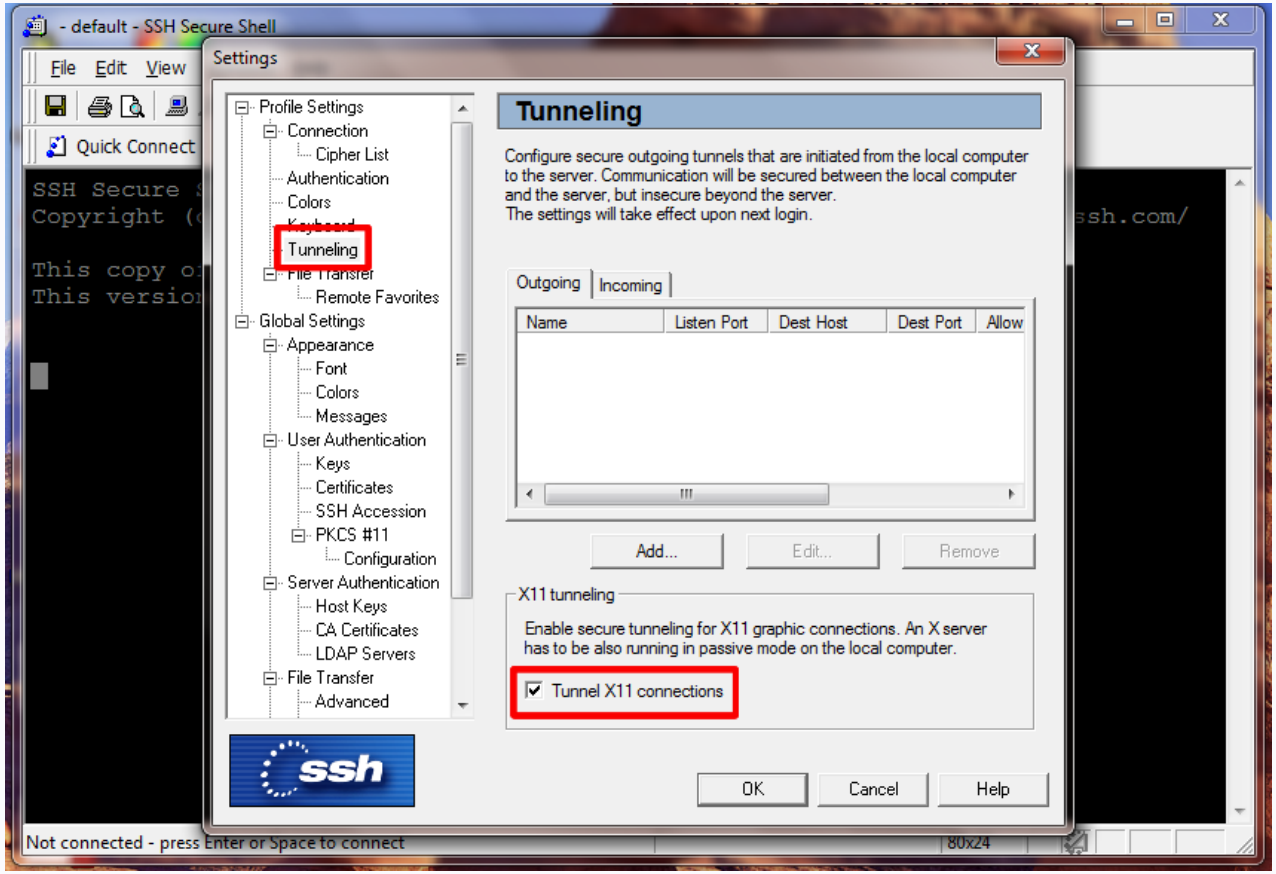

PuTTY Configuration
Category:
Session
Logging
Terminal
Keyboard
Bell
Features
Window
Appearance
Behaviour
Translation
Selection
Colours
Connection
Data
Proxy
Telnet
Rlogin
SSH
Kex
Auth
TTY
X11
Basic options for your PuTTY session
Specify the destination you want to connect to
Host Name (or IP address)
Port
eric.loni.org
22
Connection type:
Raw
Telnet
Rlogin
SSH
Serial
Load, save or delete a stored session
Saved Sessions
Default Settings
apacheco
pandora
Load
Save
Delete
Close window on exit:
Always
Never
Only on clean exit
About
Open
Cancel


eric2.loni.org - PuTTY
PuTTY Security Alert
The server's host key is not cached in the registry. You have no guarantee that the server is the computer you think it is.
The server's rsa2 key fingerprint is:
ssh-rsa 1024 90:99:55:25:b6:17:12:a8:20:6c:f1:90:0c:d1:72:04
If you trust this host, hit Yes to add the key to PuTTY's cache and carry on connecting.
If you want to carry on connecting just once, without adding the key to the cache, hit No.
If you do not trust this host, hit Cancel to abandon the connection.
Yes
No
Cancel

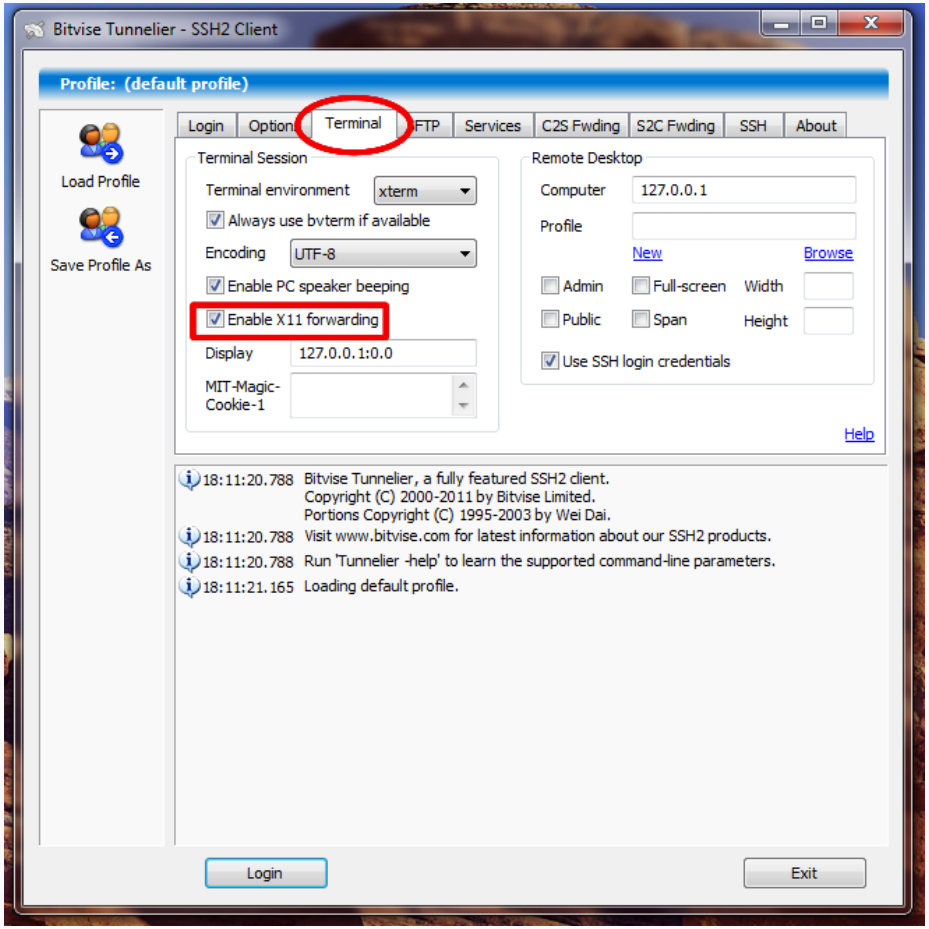

eric2.loni.org - PuTTY
login as: etrain00
Access denied
etrain00@eric.loni.org's password:


etrain00@eric2:~
login as: etrain00
Access denied
etrain00@eric.loni.org's password:
Last login: Fri Jul 22 16:43:18 2011 from apacheco.cct.lsu.edu
Eric @ LSU
Send questions and support issues to: sys-help@loni.org
Eric is a 5 TF, 128 node (512 processor) Linux cluster using LONI LDAP accounts. Eric has its own /home disk. Quotas are set at 5 GB. Please use your /work directory for batch job I/O. It has a 100 GB limit. Please limit the number of files per directory to 10,000.
Finally, DO NOT run compute jobs on the headnodes. Any such jobs will be terminated.
[etrain00@eric2 ~]$


etrain00@eric2:~
[etrain00@eric2 ~]$ java -jar /usr/local/packages/jmol/12/Jmol.jar
splash_image=jar:file:/home/packages/jmol/12/Jmol.jar!/org/openscience/jmol/app/
images/Jmol_splash.jpg
history file is /home/etrain00/.jmol/history
1818 script command tokens
(C) 2009 Jmol
Jmol Version:
java.vendor:
java.version:
os.name: Linu
memory: 9.7/1
processors av
useCommandThi
User macros d
exists
isDirectory
Jmol
File Edit Display View Tools Macros Help
Jmol
519 x 255
10.7/129.0 Mb; 3/4 ms


- default - SSH Secure Shell
File Edit View
Quick Connect
SSH Secure
Copyright
This copy o
This versio
ssh.com/
Not connected - press Enter or Space to connect
80x24
Settings
Profile Settings
Connection
Cipher List
Authentication
Colors
Keyboard
Tunneling
File Transfer
Remote Favorites
Global Settings
Appearance
Font
Colors
Messages
User Authentication
Keys
Certificates
SSH Accession
PKCS #11
Configuration
Server Authentication
Host Keys
CA Certificates
LDAP Servers
File Transfer
Advanced
Tunneling
Configure secure outgoing tunnels that are initiated from the local computer to the server. Communication will be secured between the local computer and the server, but insecure beyond the server.
The settings will take effect upon next login.
Outgoing
Incoming
Name
Listen Port
Dest Host
Dest Port
Allow
Add...
Edit...
Remove
X11 tunneling
Enable secure tunneling for X11 graphic connections. An X server has to be also running in passive mode on the local computer.
Tunnel X11 connections
ssh
OK
Cancel
Help

Configure Tunnelier/SSH Client to Tunnel X11 Connections



	Distributed File System	Throughput	File life time	Best used for
Home	Yes	Low	Unlimited	Code in development, compiled executable
Work	Yes	High	30 days	Job input/output
Local Scratch	No		Job Duration	Temporary files

- Tips
  - Never write job output to your home directory
  - Do not write temporary files to /tmp, use local scratch or work space
  - Work space is not for long term storage. Files are purged peridocally
  - Use `rmpurge` to delete large amount of files.

Cluster	Home		Work		Scratch
	Access Point	Quota	Access Point	Quota	Access Point
LONI Linux	/home/$USER	5GB	/scratch/$USER	100GB	/var/scratch
LONI AIX	/home/$USER	500MB	/work/default/$USER	20GB	/var/scratch

- No quota is enforced on the work space of QueenBee
- Work directory is created within an hour of first login
- Check current disk usage

  Linux: `showquota`

  AIX: `quota`

- Log in to any cluster
- Check your disk quota
  1. Linux: `showquota`
  2. AIX: `quota`
- Copy the traininglab directory

```
cp -r /home/apacheco/traininglab .
```

- If you are not familiar with working on a Linux/Unix system
  1. Loni Moodle course @ `https://docs.loni.org/moodle`: HPC104 or HPC105

- Environment variables
  - PATH: where to look for executables
  - LD_LIBRARY_PATH: where to look for shared libraries
  - Other custom environment variables needed by various software
- **SOFTENV** is a software that is used to set up these environment variables on all the clusters
  - More convenient than setting numerous environment variables in .bashrc or .cshrc

- Command `softenv` lists all packages that are managed by **SOFTENV**

```
[apacheco@eric2 ~]$ softenv
SoftEnv version 1.6.2
...
----------------------------------------------------------------------------

These are the macros available:

*   @default


These are the keywords explicitly available:

    +ImageMagick-6.4.6.9-intel-11.1
                                    @types: Applications Visualization @name:
                                     ...
    +NAMD-2.6-intel-11.1-mvapich-1.1
                                    @types: Applications @name: NAMD @version:
                                      ...
    +NAMD-2.7b2-intel-11.1-mvapich-1.1
                                    @types: Applications @name: NAMD @version:
                                      ...
```

- Use `-k` option with `softenv`

```
[apacheco@eric2 ~]$ softenv -k gaussian
SoftEnv version 1.6.2
...
Search Regexp: gaussian
------------------------------------------------------------------------

These are the macros available:

These are the keywords explicitly available:

    +gaussian-03                  @types: Applications Chemistry @name:
                                    Gaussian @version: 03 @build: @internal:
                                    ...
    +gaussian-09                  @types: Applications Chemistry @name:
                                    Gaussian @version: 09 @build: @internal:
                                    ...
    +gaussview-4.1.2              @types: Applications Chemistry @name:
                                    GaussView @version: 4.1.2 @build: - @about:
                                    ...

These are the keywords that are part of the software tree,
however, it is not suggested that you use these:
```

- Setting up environment variables to use a certain package in the current session only.
  - Remove a package: `soft add <key>`
  - Add a package: `soft add <key>`

```
[apacheco@eric2 ~]$ which g09
/usr/local/packages/gaussian09/g09/g09
[apacheco@eric2 ~]$ soft delete +gaussian-09
[apacheco@eric2 ~]$ which g09
/usr/bin/which: no g09 in (/home/apacheco/bin:...
[apacheco@eric2 ~]$ soft add +gaussian-03
[apacheco@eric2 ~]$ which g03
/usr/local/packages/gaussian03/g03/g03
```

- Setting up the environment variables to use a certain software package(s).
  - First add the key to `$HOME/.soft`.
  - Execute `resoft` at the command line.

```
[apacheco@eric2 ~]$ cat .soft
#
# This is the .soft file.
...
+mvapich-1.1-intel-11.1
+intel-fc-11.1
+intel-cc-11.1
+espresso-4.3.1-intel-11.1-mvapich-1.1
+gaussian-09
+lmto-intel-11.1
+nciplot-intel-11.1
+gaussview-4.1.2
+jmol-12
+vmd-1.8.6
+xcrysden-1.5.24-gcc-4.3.2
+tcl-8.5.8-intel-11.1
+gamess-12Jan2009R1-intel-11.1
+nwchem-5.1.1-intel-11.1-mvapich-1.1
+cpmd-3.11.1-intel-11.1-mvapich-1.1
@default
[apacheco@eric2 ~]$ resoft
```

- `soft-dbq` shows which variables are set by a SOFTENV key

```
[apacheco@eric2 ~]$ soft-dbq +amber-11-intel-11.1-mvapich-1.1

This is all the information associated with
the key or macro +amber-11-intel-11.1-mvapich-1.1.

------------------------------------------

Name: +amber-11-intel-11.1-mvapich-1.1
Description: @types: Applications @name: Amber @build: amber-11-intel-11.1-mvapich-1.1
  ...
Exists on: Linux

------------------------------------------

On the Linux architecture,
the following will be done to the environment:

  The following environment changes will be made:
    AMBERHOME = /usr/local/packages/amber/11/intel-11.1-mvapich-1.1
    LD_LIBRARY_PATH = ${LD_LIBRARY_PATH}:/usr/local/compilers/Intel/mkl-10.2/lib/em64t
    PATH = ${PATH}:/usr/local/packages/amber/11/intel-11.1-mvapich-1.1/exe

------------------------------------------
```

- Find the key for VISIT (a visualization package).
- Check what variables are set through the key.
- Set up your environment to use VISIT.
- Check if the variables are correctly set by using `which visit`.

- Find the key for VISIT (a visualization package).

  ```
  softenv -k visit
  ```

- Check what variables are set through the key.

  ```
  soft-dbq +visit
  ```

- Set up your environment to use VISIT.

  ```
  soft add +visit
  ```

- Check if the variables are correctly set by using `which visit`.

  ```
  /usr/local/packages/visit/bin/visit
  ```

Language	Linux Cluster			AIX Clusters
	Intel	PGI	GNU	XL
Fortran	ifort	pgf77,pgf90	gfortran	xlf,xlf90
C	icc	pgcc	gcc	xlc
C++	icpc	pgCC	g++	xlC

- Usage: <compiler> <options> <your_code>
  - Example: icc -O3 -o myexec mycode.c
- Some compilers options are architecture specific
  - Linux: EM64T, AMD64 or X86_64
  - AIX: power5,power7 or powerpc

Language	Linux Cluster	AIX Clusters
Fortran	mpif77,mpif90	mpxlf,mpxlf90
C	mpicc	mpcc
C++	mpiCC	mpCC

- Usage: <compiler> <options> <your_code>
  - Example: mpif90 -O2 -o myexec mycode.f90
- On Linux clusters
  - Only one compiler for each language
  - There is no intel_mpicc or pg_mpicc
- There are many different versions of MPI compilers on Linux clusters
  - Each of them is built around a specific compiler
  - Intel, PGI or GNU

- It is extremely important to compile and run you code with the same version!!!
- Use the default version if possible
- These MPI compilers are actually wrappers
  - They still use the compilers we've seen on the previous slide
    - Intel, PGI or GNU
  - They take care of everything we need to build MPI codes
    - Head files, libraries etc.
  - What they actually do can be reveal by the `-show` option

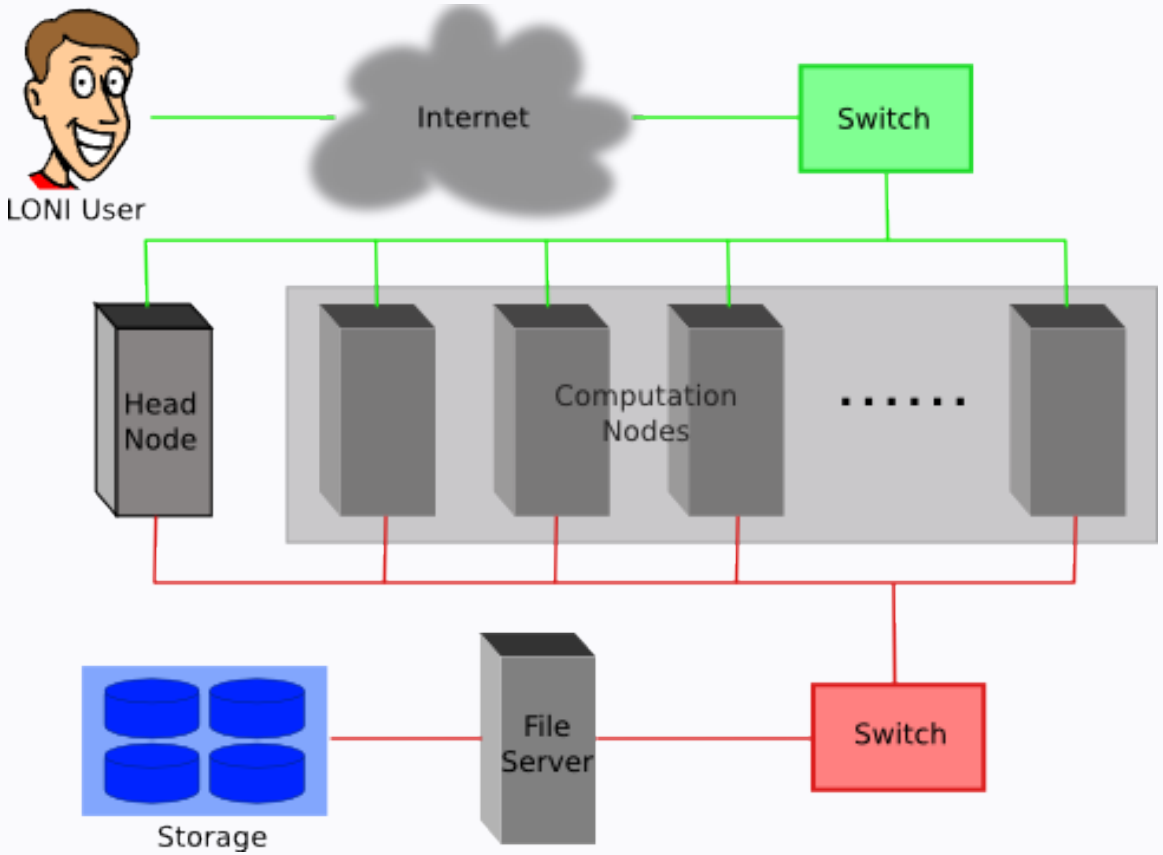
```
[apacheco@eric2 ~]$ mpif90 -show
ln -s /usr/local/packages/mvapich/1.1/intel-11.1/include/mpif.h mpif.h
ifort -fPIC -L/usr/local/ofed/lib64 -Wl,-rpath-link -Wl, \
   /usr/local/packages/mvapich/1.1/intel-11.1/lib/shared \
  -L/usr/local/packages/mvapich/1.1/intel-11.1/lib/shared \
  -L/usr/local/packages/mvapich/1.1/intel-11.1/lib \
  -lmpichf90nc -lmpichfarg -lmpich -L/usr/local/ofed/lib64 \
  -Wl,-rpath=/usr/local/ofed/lib64 -libverbs -libumad -lpthread -lpthread -lrt -limf
rm -f mpif.h
```

- Installed under `/usr/local/packages`
- Most of them managed by SOFTENV
  - Numerical and utility libraries
    - FFTW, HDF5, NetCDF, PetSc, Intel MKL
  - Computational Chemistry
    - Amber, CPMD, Gaussian, GAMESS, Gromacs, LAMMPS, NAMD, NWCHEM
  - Visualization
    - GaussView, VisIt, VMD
  - Profiling/debugging tools
    - DDT, Tau, TotalView
  - MPI Implementation
    - mvapich, mvapich2, mpich, openmpi
  - . . .

1. Serial Code
   - On Linux cluster, add the soft keys for either Intel (`+intel-fc-11.1`) or GCC (`+gcc-4.3.2`)
   - Compile `hello.f90` with a compiler of your choice
   - Run the executable from the command line
2. Parallel Code
   - On Linux cluster, find the appropriate key for mpi implementation of the above compiler
   - Compile `hello_mpi.f90`
   - Do Not run the parallel code, we'll use a script to submit to a job manager

1. Serial Code
   - On Linux cluster, add the soft keys for either Intel (`+intel-fc-11.1`) or GCC (`+gcc-4.3.2`)
   - Compile `hello.f90` with a compiler of your choice
     `ifort -o hello hello.f90`
   - Run the executable from the command line
     `./hello`
2. Parallel Code
   - On Linux cluster, find the appropriate key for mpi implementation of the above compiler
   - Compile `hello_mpi.f90`
     `mpif90 -o hellompi hello_mpi.f90`
   - Do Not run the parallel code, we'll use a script to submit to a job manager

- A cluster is a group of computers (nodes) that works together closely
- Type of nodes
  - Head node
  - Multiple Compute nodes
- Multi User Environment
- Each user may have multiple jobs running simultaneously.



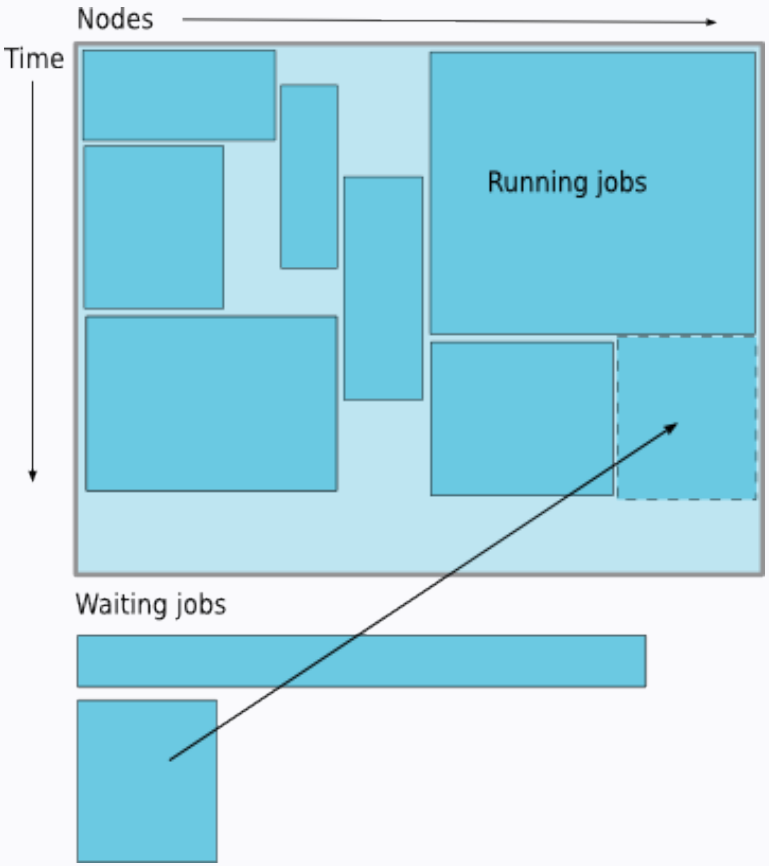
- A software that manages resources (CPU time, memory, etc) and schedules job execution
  - Linux Clusters: Portable Batch System (PBS)
  - AIX Clusters: Loadleveler
- A job can be considered as a user's request to use a certain amount of resources for a certain amount of time
- The batch queuing system determines
  1. The order jobs are executed
  2. On which node(s) jobs are executed

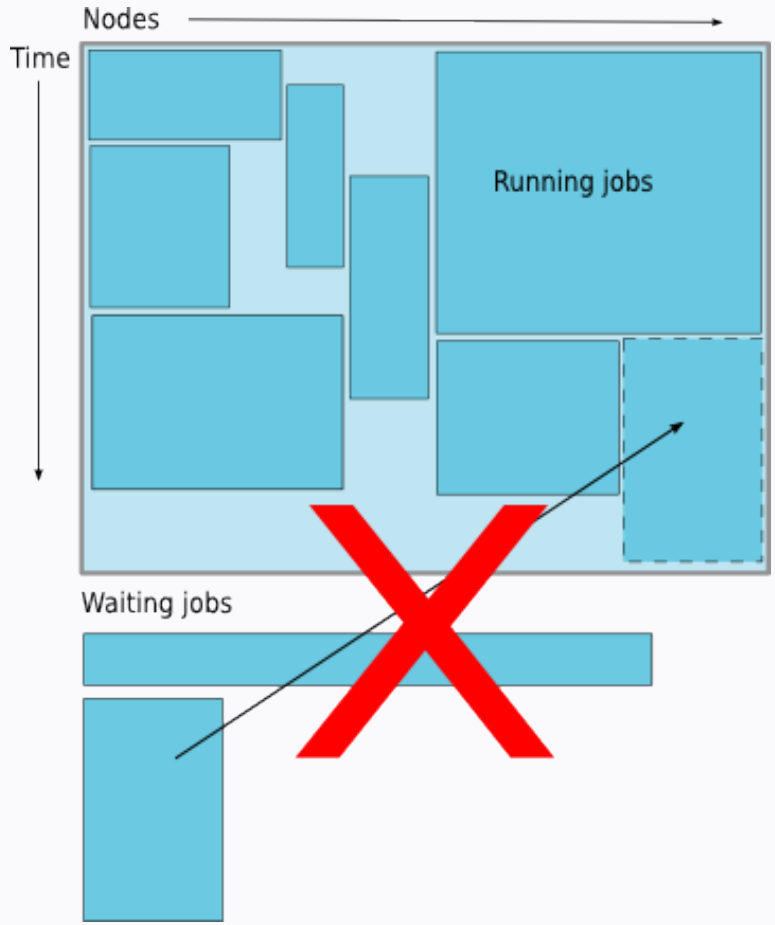
A Simplified View of Job Scheduling

- Map jobs onto the node-time space
  - Assuming CPU time is the only resource
- Need to find a balance between
  - Honoring the order in which jobs are received
  - Maximizing resource utilization

- A strategy to improve utilization
  - Allow a job to jump ahead of others when there are enough idle nodes
  - Must not affect the estimated start time of the job with the highest priority
- Enabled on all LONI clusters

How much time Should I request?





- Ask for an amount of time that is
  - Long enough for your job to complete
  - As short as possible to increase the chance of backfilling

- There are more than one job queue
- Each job queue differs in
  - Number of available nodes
  - Maximum run time
  - Maximum running jobs per user
- The main purpose is to maximize utilization

QueenBee

Queue	Max Run-time	Total number of nodes	Max running jobs per user	Max nodes per job	Use
workq	2 days	530	8	128	Unpreemptable
checkpt		668		256	preemptable
preempt		668	NA		Requires permission
priority		668	NA		Requires permission

Other Clusters

Queue	Max Run-time	Total number of nodes	Max running jobs per user	Max nodes per job	Use
single	14 days	16	64	1	Single processor jobs
workq	3 days	96	8	40	Unpreemptable
checkpt		128		64	preemptable
preempt		64	NA		Requires permission
priority		64	NA		Requires permission

- Queue querying
  - Check how busy the cluster is
- Job submission
- Job monitoring
  - Check job status (estimated start time, remaining run time, etc)
- Job manipulation
  - Cancel/Hold jobs

- `qfree`: show number of free,busy and queued nodes
- `qfreeloni`: run `qfree` on all LONI Linux clusters

```
[apacheco@eric2 ~]$ qfree
PBS total nodes: 128,  free: 49,  busy: 79,  down: 0,  use: 61%
PBS workq nodes: 96,  free: 40,  busy: 28,  queued: 0
PBS checkpt nodes: 104,  free: 40,  busy: 35,  queued: 0
PBS single nodes: 32,  free: 9 *36,  busy: 16,  queued: 366
[apacheco@eric2 ~]$ qfreeloni
-------- qb --------
PBS total nodes: 668,  free: 3,  busy: 647,  down: 18,  use: 96%
PBS workq nodes: 530,  free: 0,  busy: 278,  queued: 367
PBS checkpt nodes: 668,  free: 1,  busy: 369,  queued: 770
-------- eric --------
PBS total nodes: 128,  free: 49,  busy: 79,  down: 0,  use: 61%
PBS workq nodes: 96,  free: 40,  busy: 28,  queued: 0
PBS checkpt nodes: 104,  free: 40,  busy: 35,  queued: 0
PBS single nodes: 32,  free: 9 *36,  busy: 16,  queued: 366
-------- louie --------
PBS total nodes: 128,  free: 44,  busy: 83 *2,  down: 1,  use: 64%
PBS workq nodes: 104,  free: 40,  busy: 0,  queued: 0
PBS checkpt nodes: 128,  free: 44,  busy: 82,  queued: 50
PBS single nodes: 32,  free: 7 *26,  busy: 2,  queued: 0
-------- oliver --------
PBS total nodes: 128,  free: 74,  busy: 52,  down: 2,  use: 40%
PBS workq nodes: 62,  free: 8,  busy: 11,  queued: 0
...
```

Interactive Jobs

- Set up an interactive environment on compute nodes for users
  - Advantage: can run programs interactively
  - Disadvantage: must be present when job starts
- Purpose: testing and debugging code. **Do not run jobs on head node!!!**

```
qsub -I -V -l walltime=<hh:mm:ss>,nodes=<#
of nodes>:ppn=cpu -A <your allocation> -q
<queue name>
```

- On QueenBee, cpu=8
- Other LONI Clusters: cpu=4 (parallel jobs) or cpu=1 (single queue)
- To enable X-forwarding: add `-X`

Batch Jobs

- Executed using a batch script without user intervention
  - Advantage: system takes care of running the job
  - Disadvantage: can change sequence of commands after submission
- Useful for Production runs

```
qsub <job script>
llsubmit <job script>
```

PBS Job Script: Parallel Jobs


```
#!/bin/bash
#PBS -l nodes=4:ppn=4
#PBS -l walltime=24:00:00
#PBS -N myjob
#PBS -o <file name>
#PBS -e <file name>
#PBS -q checkpt
#PBS -A <loni_allocation>
#PBS -m e
#PBS -M <email address>

<shell commands>
mpirun  -machinefile $PBS_NODEFILE \
 -np 16 <path_to_executable> <options>
<shell commands>
```

```
Shell being used
# of nodes & processors
Maximum walltime
Job name
standard output
standard error
Queue name
Allocation name
Send mail when job ends
to this address

shell commands
run parallel job

shell commands
```

PBS Job Script: Serial Jobs


```
#!/bin/bash                                  Shell being used
#PBS -l nodes=1:ppn=1                        # of nodes & processors
#PBS -l walltime=24:00:00                    Maximum walltime
#PBS -N myjob                                Job name
#PBS -o <file name>                          standard output
#PBS -e <file name>                          standard error
#PBS -q single                               Use single queue
#PBS -A <loni_allocation>                    Allocation name
#PBS -m e                                    Send mail when job ends
#PBS -M <email address>                      to this address

<shell commands>                             shell commands
<path_to_executable> <options>               run parallel job
<shell commands>                             shell commands
```

- Write a job submission script to execute the `hellompi` program.
- Submit the script to the job manager.

Linux Clusters

- `showstart <job id>`
  - Check estimated time when job can start
- When can the estimated time change
  - Higher priority job gets submitted
  - Running jobs terminate earlier than time requested
  - System has trouble starting your job
- `qstat <options> <job id>`
  - Show information on job status
  - All jobs displayed if `<job id>` is omitted
  - `qstat -u <username>`: Show jobs belonging to `<username>`
  - `qstat -a <job id>`: Displat in an alternative format
- `qshow <job id>`
  - Show information of running job `<job id>`: node running on and CPU load

Linux Clusters

- `qdel <job id>`
  - Cancel a running or queued job
- `qhold <job id>`
  - Put a queued job on hold
- `qrls <job id>`
  - Resume a held job

- User's Guide
  - LONI: `https://docs.loni.org/wiki/Main_Page`
- Contact us
  - Email ticket system: sys-help@loni.org
  - Telephone Help Desk: 225-578-0900
  - Walk-in consulting session at Middleton Library
    - Tuesdays and Thursdays only
  - Instant Messenger (AIM, Yahoo Messenger, Google Talk)
    - Add "lsuhpchelp"

THE END

Questions, Comments ???