HPC User Environment, Job Management with PBS/Loadleveler

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Outline

Outline

- Two major architectures.

Linux Clusters

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

AIX Clusters

- Vendor: IBM
- OS: AIX
- CPU: Power 5/7

- 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
LSU HPC	Tezpur	15.3	LSU	Production	HPC
	Philip	3.5	LSU	Production	HPC

AIX Clusters

	Name	Peak TF/s	Location	Status	Login
LONI	Bluedawg	0.85	LaTech	Production	LONI
	Ducky	0.85	UNO	9/30/2011	LONI
	Lacumba	0.85	Southern	12/22/2011	LONI
	Neptune	0.85	Tulane	9/30/2011	LONI
	Zeke	0.85	ULL	9/30/2011	LONI
LSU HPC	Pelican	2.6	LSU	Production	HPC
	Pandora	6.8	LSU	Production	HPC

Account Management

- LONI account

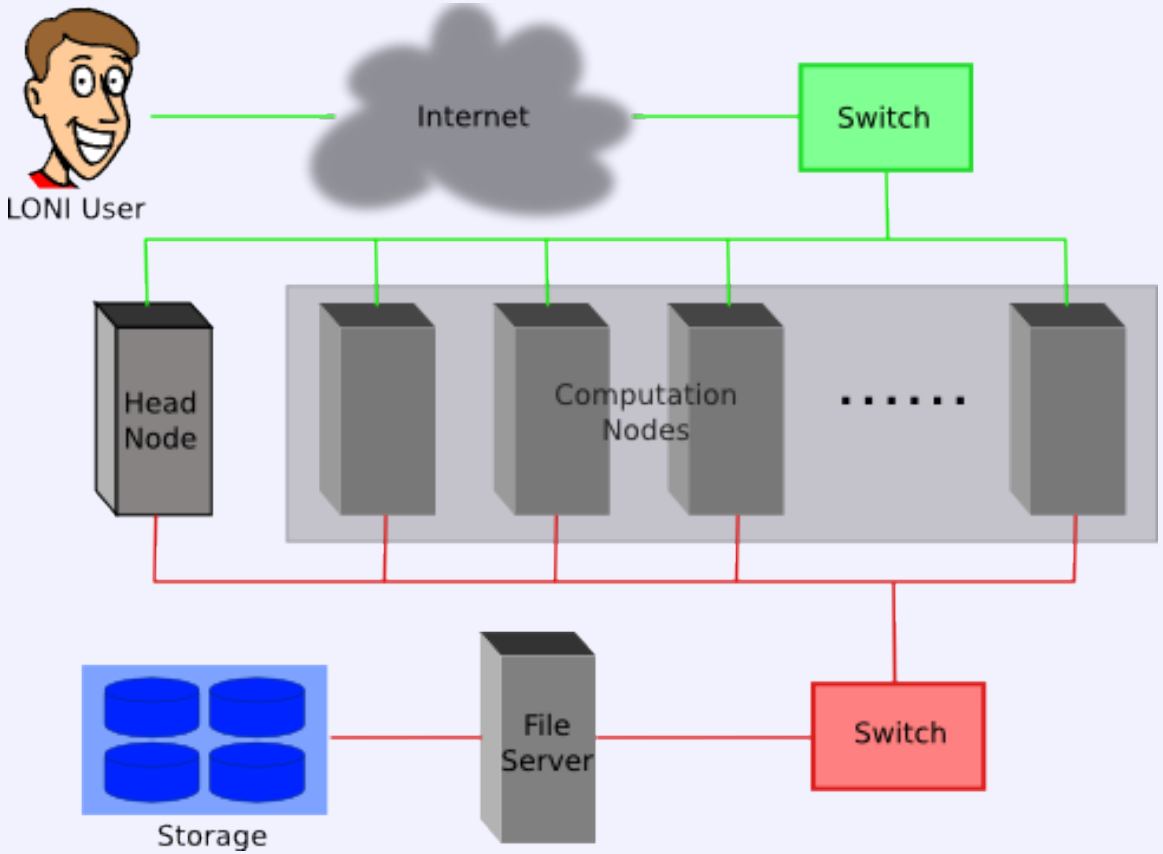
  `https://allocations.loni.org`
- LSU HPC account

  `https://accounts.hpc.lsu.edu`
- All LONI AIX clusters are being decommissioned.
- Newest cluster at LSU HPC is Pandora.

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

Cluster Architecture

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



LINUX Cluster Hardware

- 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
- Tezpur
  - 360 nodes, 4 Intel Xeon cores @ 2.33 GHz
  - 4 GB RAM
  - 32 TB storage
- Philip
  - 37 nodes, 8 Intel Xeon cores @ 2.93 GHz
  - 24/48/96 GB RAM
  - Shares storage with Tezpur

AIX Cluster Hardware

- LONI AIX clusters
  - 14 Power5 nodes, 8 IBM Power5 processors @ 1.9 GHz per node
  - 16 GB RAM
  - 280 GB storage
- Pelican
  - 16 Power5+ nodes, 16 IBM Power5+ processors @ 1.9 GHz per node
  - 32 GB RAM
  - 21 TB strorage
- Pandora
  - 8 Power7 nodes, 8 IBM Power7 processors @ 7.33 GHz per node
  - 128 GB RAM
  - 19 TB storage

Why is Cluster Hardware important?

- 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 c

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**

Technology Services

Usage: Max Memory

- The amount of installed memory less the amount that is used by the operating system and other utilities
- Max amount per node
  - Linux clusters: $\sim$6 GB for Queen Bee, $\sim$3 GB for others
  - AIX clusters: $\sim$13 GB
  - Pandora:$\sim$125 GBstorage

Outline

Accessing LONI & LSU HPC clusters

- LONI Host name: `<cluster name>.loni.org`
  - Eric: eric.loni.org
- LSU HPC Host name: `<cluster name>.hpc.lsu.edu`
  - Tezpur: tezpur.hpc.lsu.edu
- 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`
  - LSU HPC: `https://accounts.hpc.lsu.edu`
- Reset your password
  - LONI: `https://allocations.loni.org/user_reset.php`
  - LSU HPC: `https://accounts.hpc.lsu.edu/user_reset.php`

Connecting to Eric from a Linux box

```
[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 is
   #
   ##################################

   Eric is a 5 TF, 128 node (512 process
   accounts. Eric has its own /home disk
   use your /work directory for batch jo
   limit the number of files per directo

   Finally, DO NOT run compute jobs on
   terminated.

[etrain00@eric2 ~]$ gview
```

Connecting to Eric from a Mac box

```
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 ~]$
```

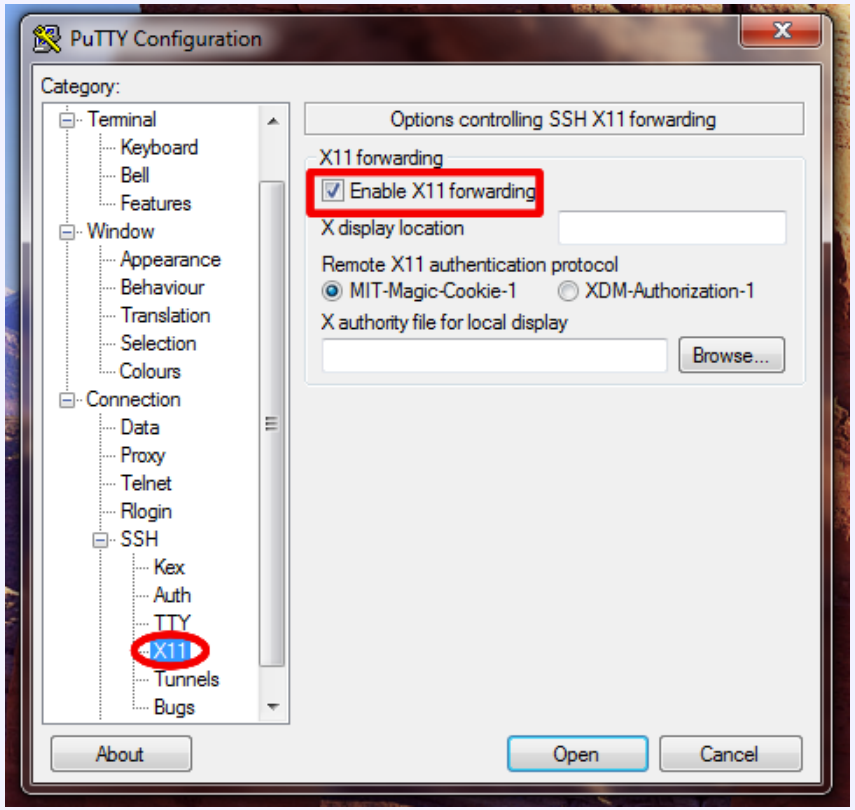
```
Info) Please include this reference in published work using VMD:
Info)    Humphrey, W., Dalke, A. and Schulten, K., `VMD - Visual
Info)    Molecular Dynamics', J. Molec. Graphics 1996, 14.1, 33-38.
Info) ----------------------------------------------------------------
Info) Multithreading available, 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 >
```

Connecting to Eric from a Windows box

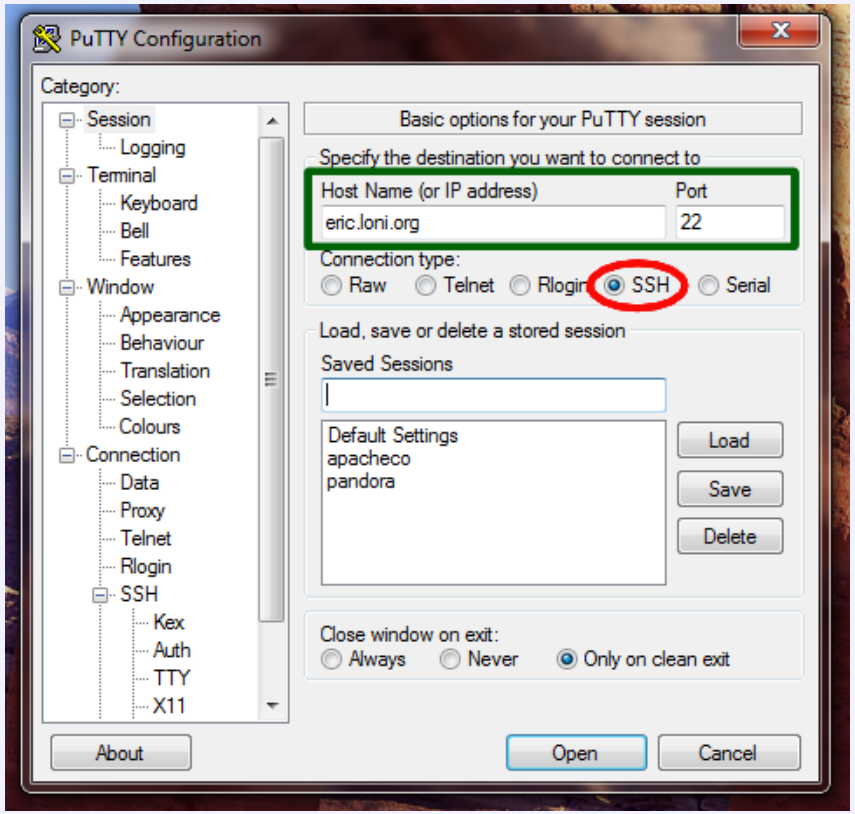
- Download and Install
  1. X-Server: X-ming
     `http://www.straightrunning.com/XmingNotes/`
  2. SSH Client: Putty
     `http://www.chiark.greenend.org.uk/~sgtatham/putty/`
  3. SSH+SFTP/SCP Client: Bitvise Tunnelier
     `http://www.bitvise.com/tunnelier`

Start X-ming

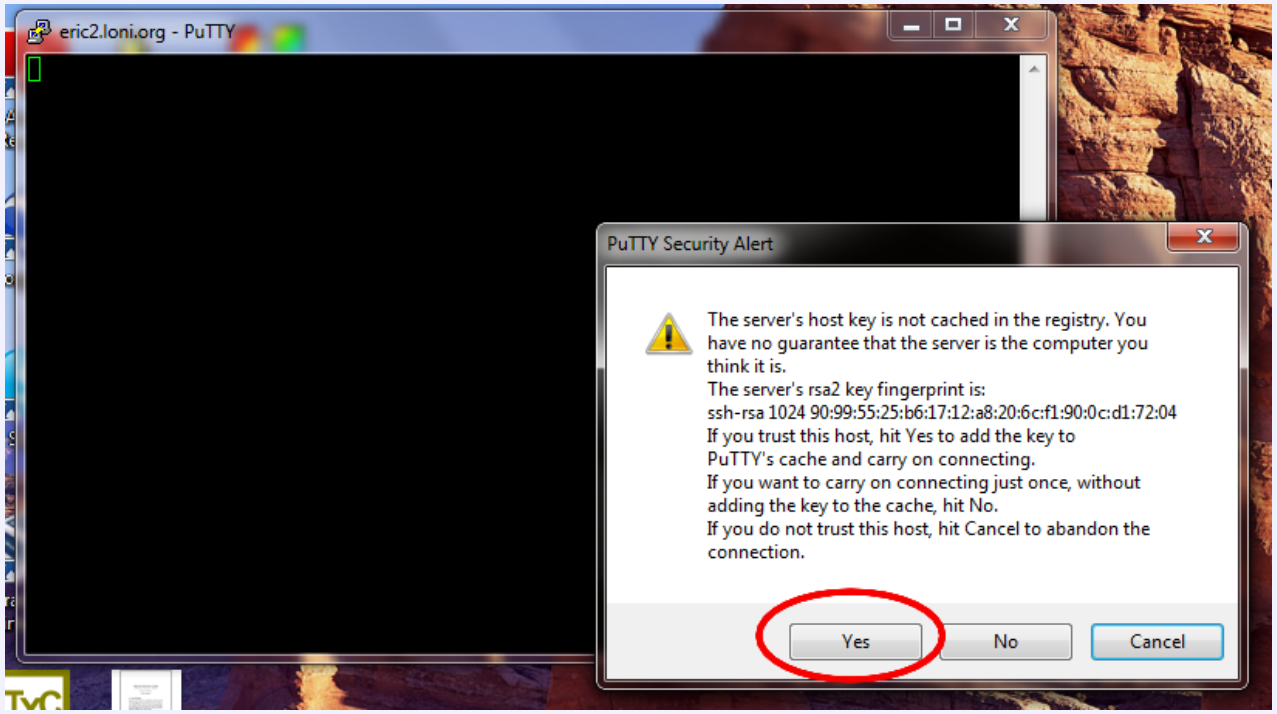
Putty with X11



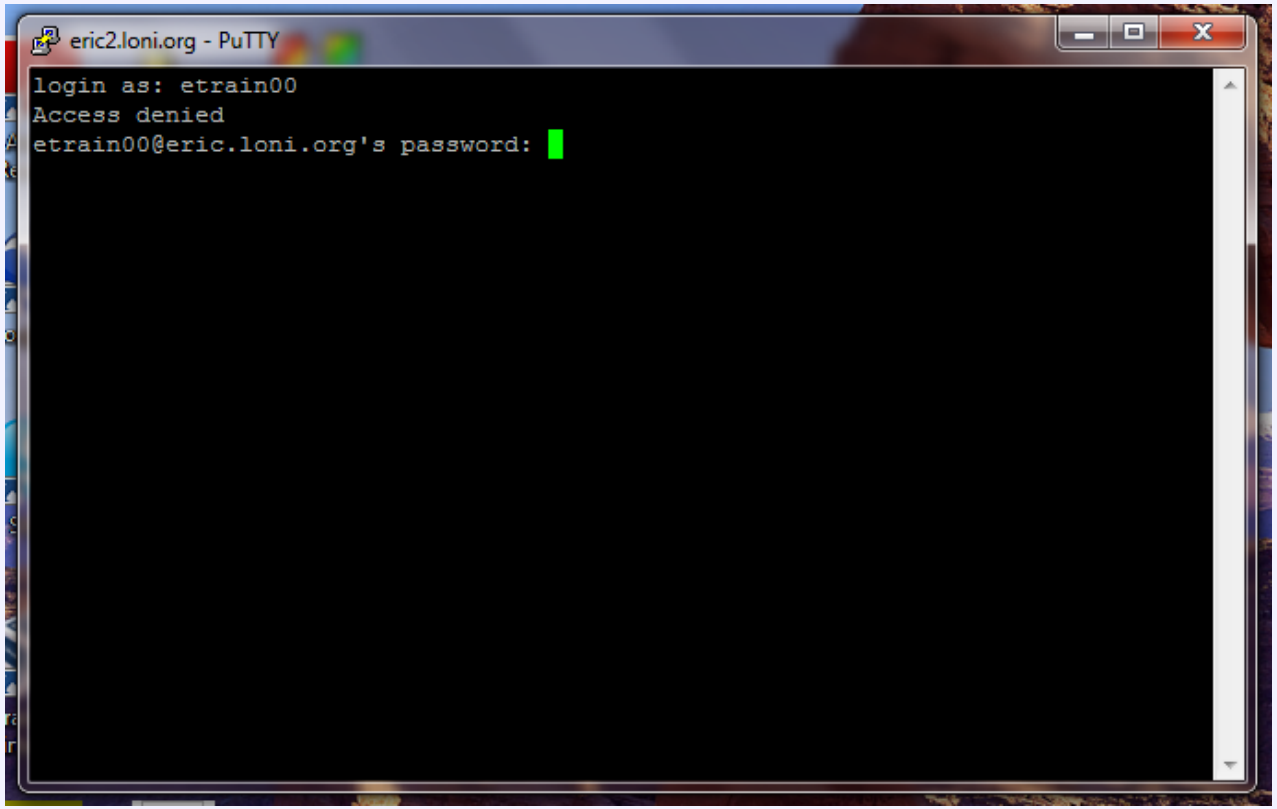
Putty with X11



Putty with X11



Putty with X11

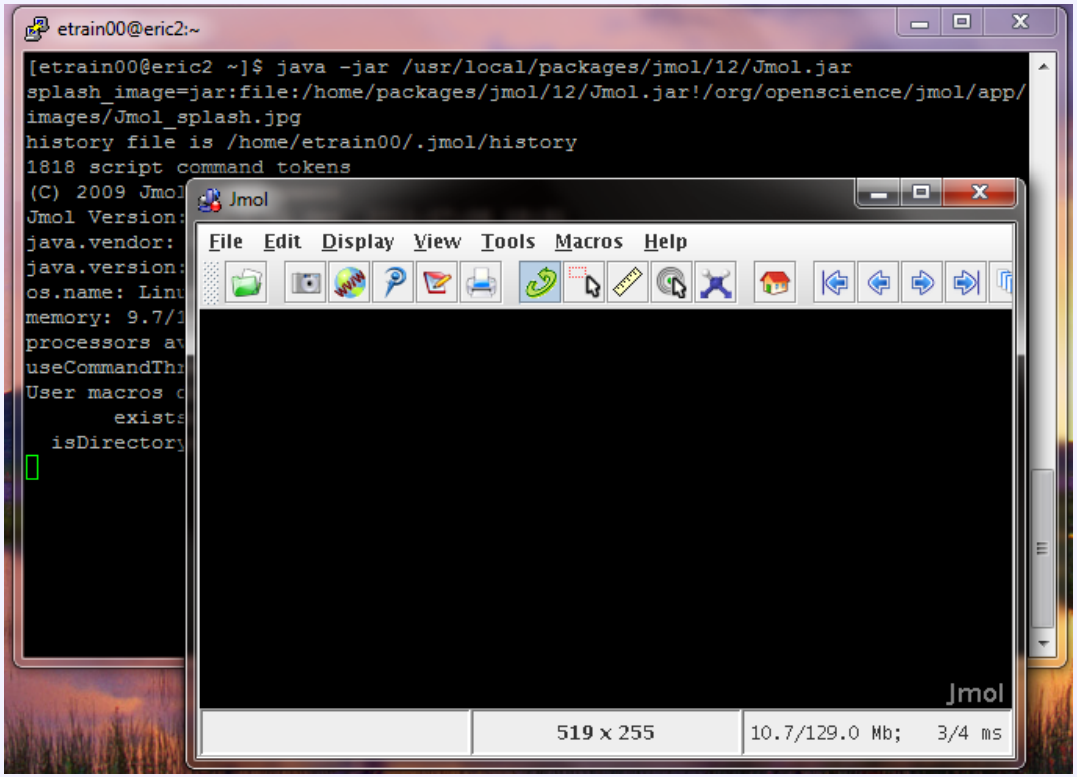


Putty with X11

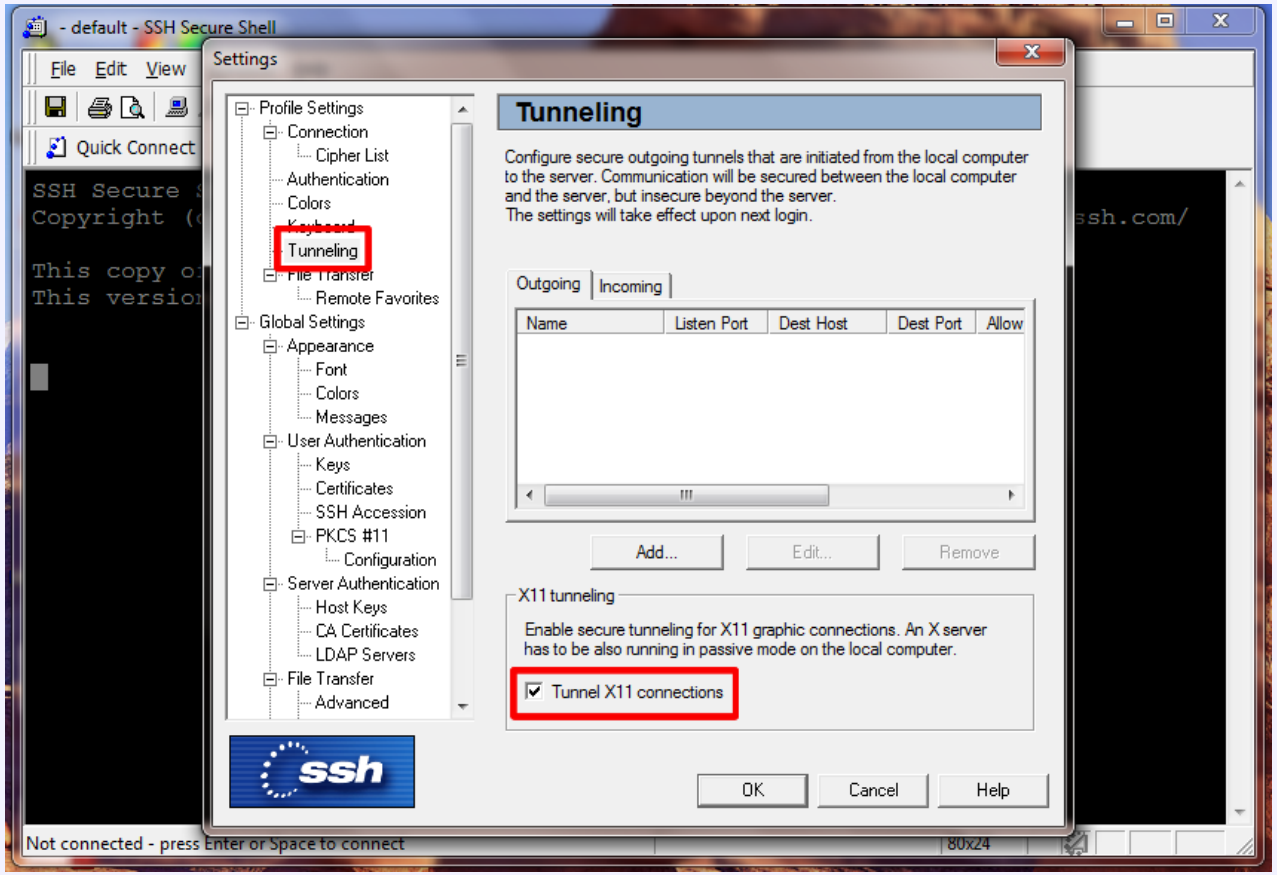
etrain00@eric2:~

```
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 ~]$
```

Putty with X11



Configure Tunnelier/SSH Client to Tunnel X11 Connections



Configure Tunnelier/SSH Client to Tunnel X11 Connections

Bitvise Tunnelier - SSH2 Client

Profile: (default profile)

Load Profile

Save Profile As

Login | Option | Terminal | FTP | Services | C2S Fwding | S2C Fwding | SSH | About

Terminal Session

Terminal environment: xterm

☑ Always use bvterm if available

Encoding: UTF-8

☑ Enable PC speaker beeping

☑ Enable X11 forwarding

Display: 127.0.0.1:0.0

MIT-Magic-Cookie-1

Remote Desktop

Computer: 127.0.0.1

Profile

New | Browse

☐ Admin ☐ Full-screen Width

☐ Public ☐ Span Height

☑ Use SSH login credentials

Help

18:11:20.788 Bitvise Tunnelier, a fully featured SSH2 client.
Copyright (C) 2000-2011 by Bitvise Limited.
Portions Copyright (C) 1995-2003 by Wei Dai.

18:11:20.788 Visit www.bitvise.com for latest information about our SSH2 products.

18:11:20.788 Run 'Tunnelier -help' to learn the supported command-line parameters.

18:11:21.165 Loading default profile.

Login | Exit

Information Technology Services

File Systems

	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.

Disk Quota

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
HPC Linux	/home/$USER	5GB	/work/$USER	NA	/var/scratch
HPC AIX	/home/$USER	5GB	/work/$USER	50GB	/scratch/local

- 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`

Exercise 1

- 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

Managing User Environment

- 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

Listing All packages

- 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:
                                      ...
```

Searching for a Specific Package

- 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 via Softenv: One Time Change

- 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 Environment via Softenv: Permanent Change

- 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
```

Querying a Softenv Key

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

```
[apacheco@eric2 ~]$ soft-dbq +espresso-4.3.1-intel-11.1-mvapich-1.1

This is all the information associated with
the key or macro +espresso-4.3.1-intel-11.1-mvapich-1.1.

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

Name: +espresso-4.3.1-intel-11.1-mvapich-1.1
Description: @types: Applications @name: Quantum Espresso @version: 4.3.1 @build: ...
Flags: none
Groups: none
Exists on: Linux

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

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

  The following environment changes will be made:
    ESPRESSO_PSEUDO = /usr/local/packages/espresso/4.3.1/intel-11.1-mvapich-1.1/pseudo
    ESPRESSO_ROOT = /usr/local/packages/espresso/4.3.1/intel-11.1-mvapich-1.1
    ESPRESSO_TMPDIR = /work/${USER}
    PATH = ${PATH}:/usr/local/packages/espresso/4.3.1/intel-11.1-mvapich-1.1/bin

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

Exercise 2: Use Softenv

- 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`.

Exercise 2: Use Softenv

- 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`

Compilers

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

Compilers for MPI programs I

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

Compilers for MPI programs II

- 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
```

Application Packages

- 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
  - ...

Exercise 3: Compiling a code

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

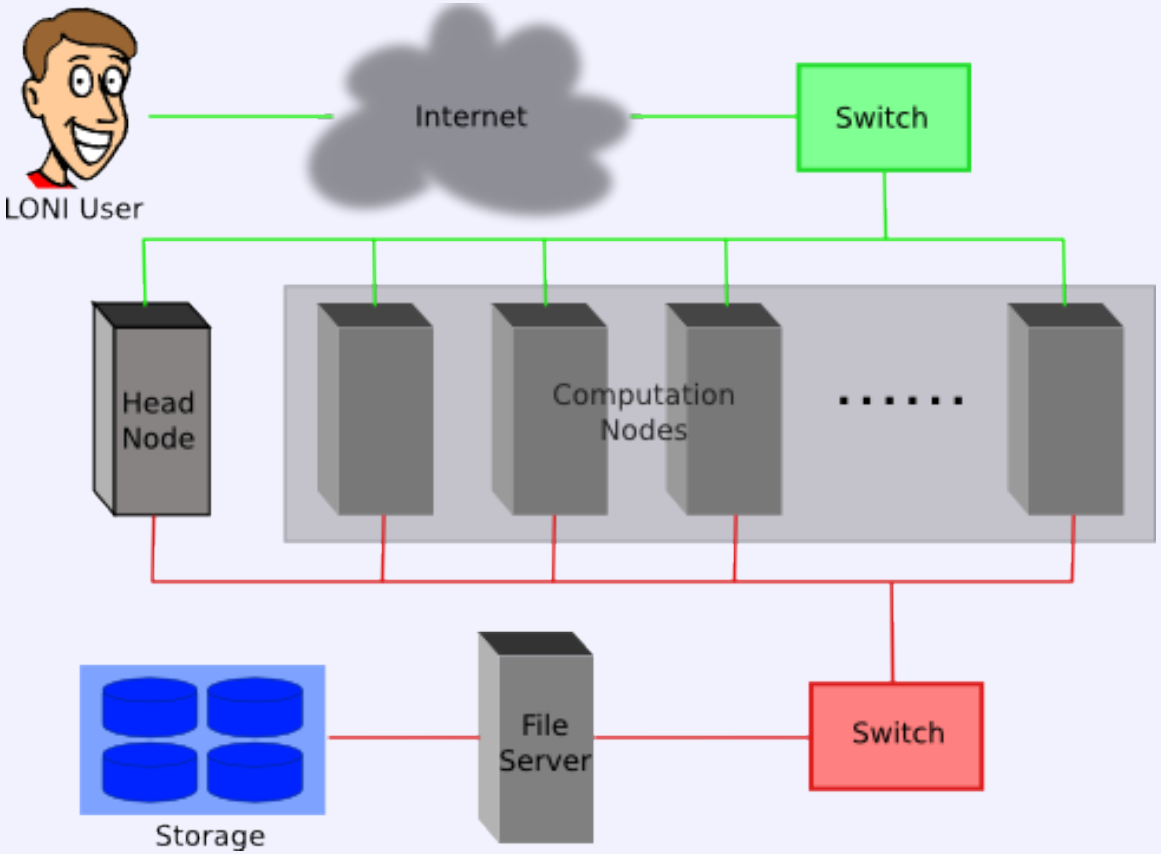
Exercise 3: Compiling a code

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
     xlf90 -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

Outline

The Cluster Environment

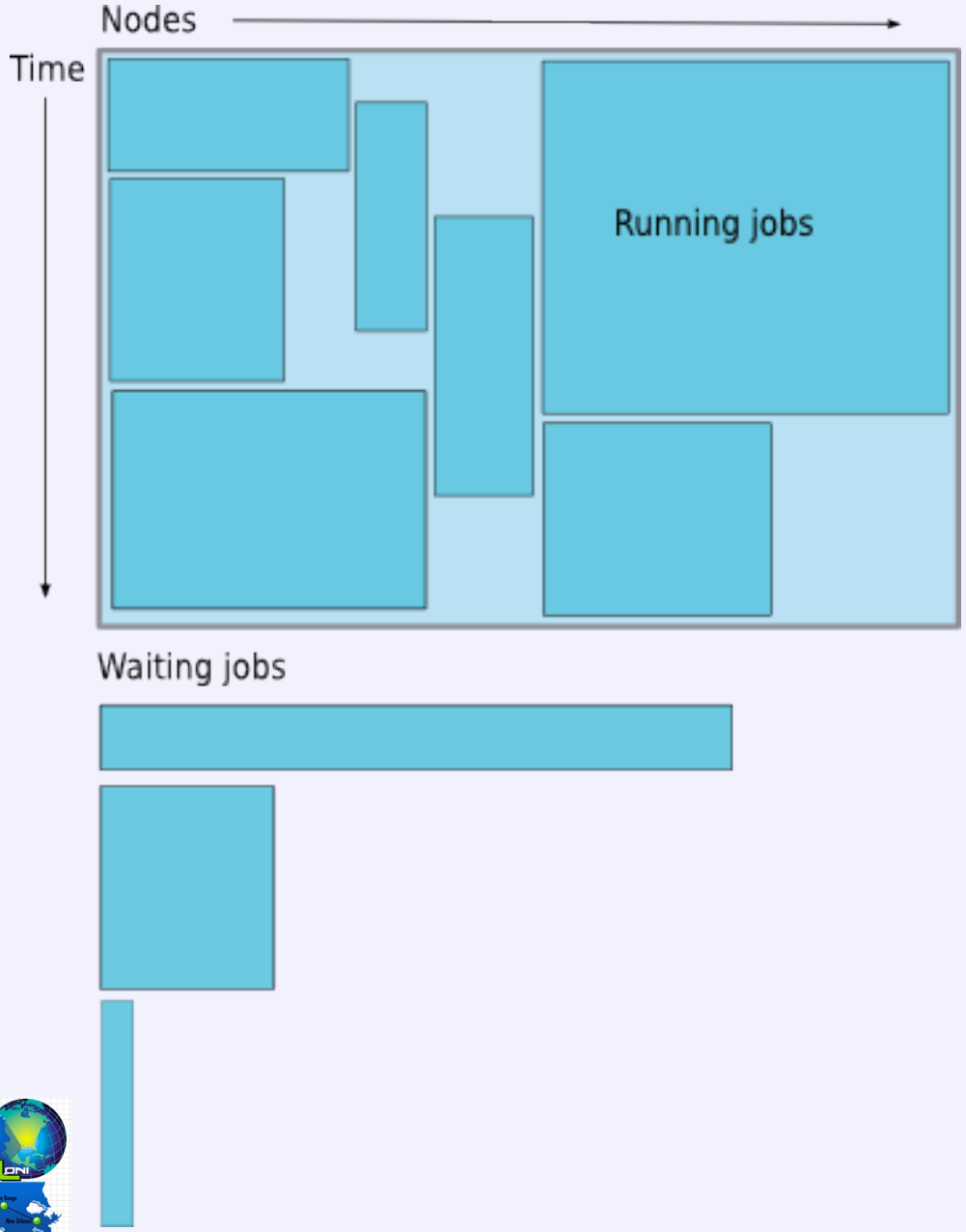
- A cluster is a group of computers (nodes) that works together closely
- Type of nodes
  - Head node
  - Multiple Compute nodes
- Multi User Environment
- Each user may have multiple jobs running simultaneously.



Batch Queuing System

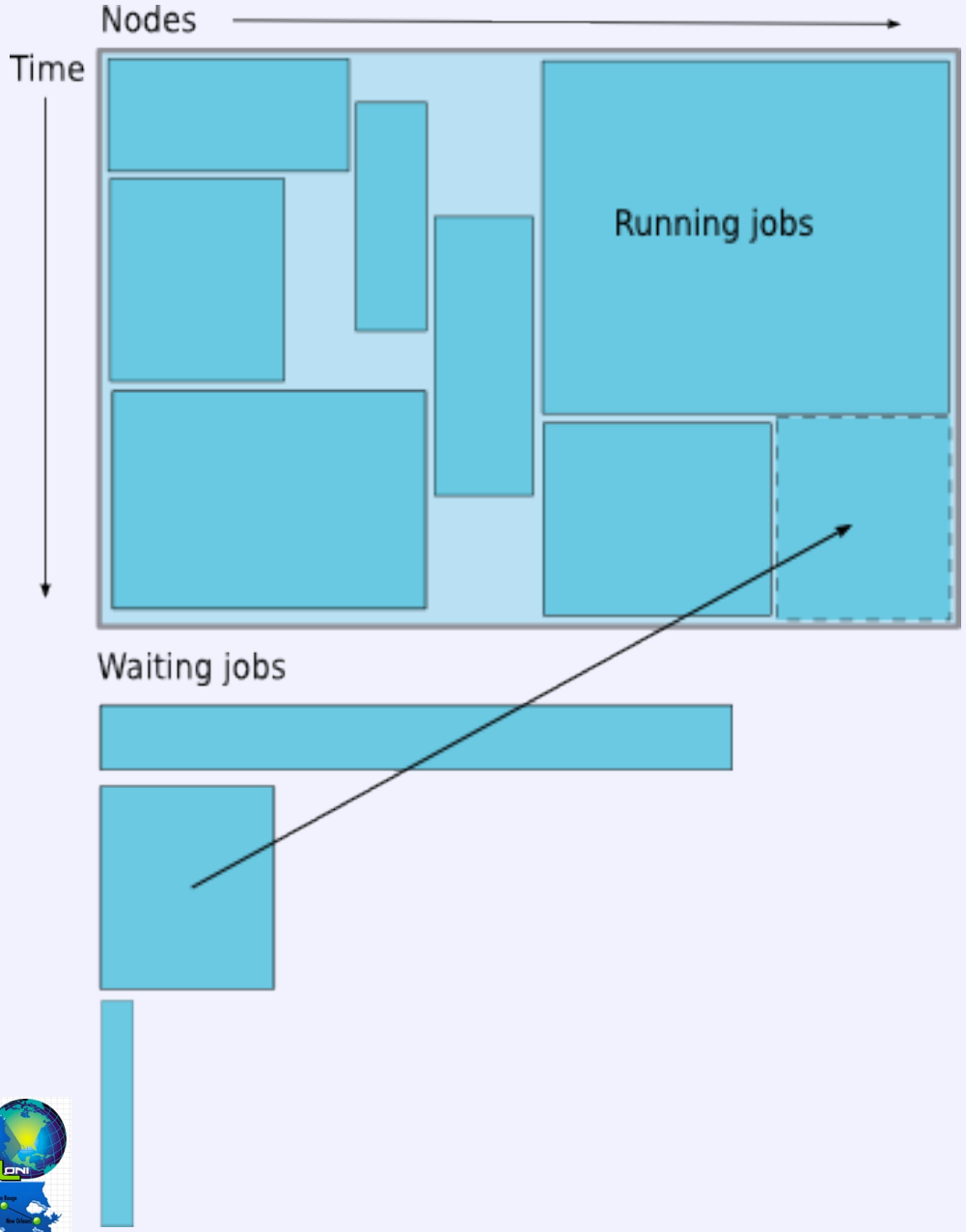
- A software that manages resources (CPU time, memory, etc) and schedules job execution
  - Linux Clusters: Portable Batch System (PBS)
  - AIX Clusters: Loadleveler
- A job can be considered as a user's request to use a certain amount of resources for a certain amount of time
- The batch queuing system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

A Simplified View of Job Scheduling



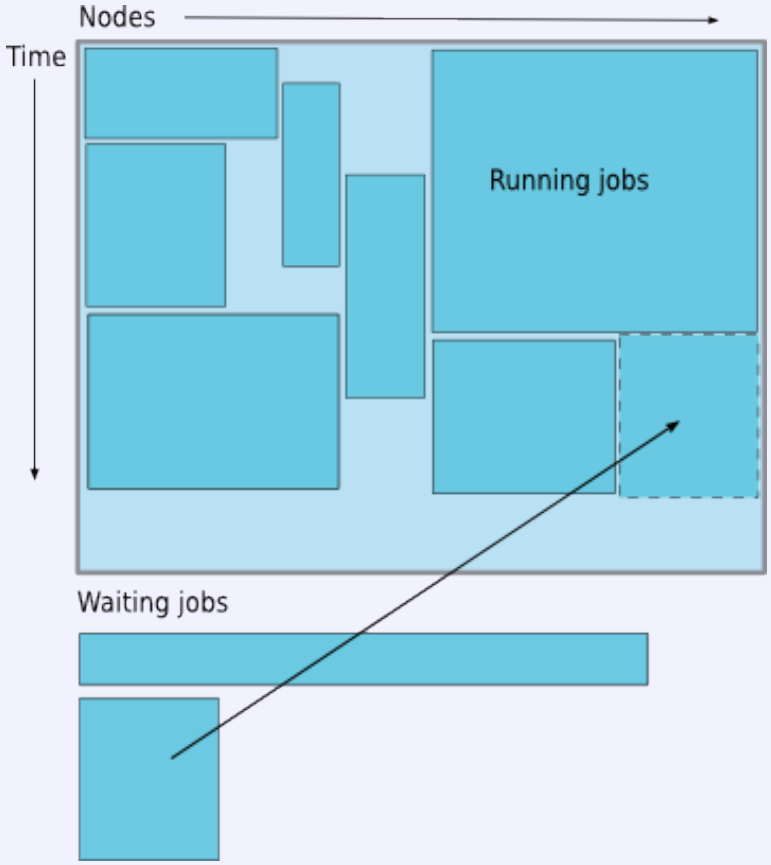
- Map jobs onto the node-time space
  - Assuming CPU time is the only resource
- Need to find a balance between
  - Honoring the order in which jobs are received
  - Maximizing resource utilization

Backfilling



- 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 and LSU HPC 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

Job Queues

- 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

Queue Characteristics: LONI Linux Clusters

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 Characteristics: LSU HPC Linux Clusters

Tezpur

Queue	Max Run-time	Total number of nodes	Max running jobs per user	Max nodes per job	Use
single	3 days	16	64	1	Single processor jobs
workq		180	8	90	Unpreemptable
checkpt		344		180	preemptable
preempt		NA			Requires permission
priority		NA			Requires permission

Philip

Queue	Max Run-time	Total number of nodes	Max running jobs per user	Max nodes per job	Use
single	3 days	24	12	1	Single processor jobs
workq		28		5	Unpreemptable
checkpt		28			preemptable
bigmem		5			
preempt		NA			Requires permission
priority		NA			Requires permission

Queue Characteristics: LSU HPC AIX Clusters

Pelican

Queue	Max Run-time	Total number of processors	Max running jobs per user	Max processors per job	Use
SP5L	4 hours	256	8	256	Short Jobs
MP5L	5 days			128	Medium Jobs
LP5L	7 days		4	64	Long Jobs

Pandora

Queue	Max Run-time	Total number of processors	Max running jobs per user	Max processors per job	Use
interactive	30mins	8	6	8	Interactive Jobs
workq	3 days	224		128	Standard Queue
single	7 days	64		32	Single Node Jobs

Basic Job Manager Commands

- 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

Queue Querying: Linux Clusters

- `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
...
```

- Command: `llclass`

```
apacheco@peg304$ llclass
Name                 MaxJobCPU     MaxProcCPU  Free   Max  Description
                    d+hh:mm:ss     d+hh:mm:ss Slots Slots
--------------- -------------- -------------- ----- -----  ---------------------
interactive          undefined      undefined     4     4  Interactive Parallel jobs running on in
SP5L                 unlimited      unlimited   154   256  Short (4 hours) Parallel queue on Power
MP5L                 unlimited      unlimited   154   256  Middle (5 days) Parallel queue on Power
LP5L                 unlimited      unlimited   154   256  Long (7 days) Parallel queue on Power5+
-------------------------------------------------------------------------------
"Free Slots" values of the classes "SP5L", "MP5L", "LP5L" are constrained by the MAX_STARTERS limi
pandora1:~ apacheco$ llclass
Name                 MaxJobCPU     MaxProcCPU  Free   Max Description
                    d+hh:mm:ss     d+hh:mm:ss Slots Slots
--------------- -------------- -------------- ----- ----- ---------------------
interactive          unlimited      unlimited     8     8 Queue for interactive jobs; maximum runt
workq                unlimited      unlimited    80   224 Standard queue for job submissions; maxi
single               unlimited      unlimited    32    64 Queue for single-node job submissions; m
-------------------------------------------------------------------------------
"Free Slots" values of the classes "workq", "single" are constrained by the MAX_STARTERS limit(s).
```

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                                  Shell being used
#PBS -l nodes=4:ppn=4                        # 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 checkpt                              Queue name
#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
mpirun  -machinefile $PBS_NODEFILE \         run parallel job
 -np 16 <path_to_executable> <options>
<shell commands>                             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
```

Loadleveler Job Script I

```
#!/bin/sh                                  Shell being used
#@ job_type = parallel                     Job Type
#@ output = $(jobid).out                   standard output
#@ error = $(jobid).err                    standard error
#@ notification = error                    notify on error
#@ notify_user = youremail@domain          to mail address
#@ class = checkpt                         job queue
#@ wall_clock_limit = 24:00:00             max walltime
#@ node_usage = shared                     node usage
#@ node = 2,2                              # of nodes
#@ total_tasks = 16                        total processors
#@ requirements = (Arch == "POWER5")       job requirements
#@ environment = COPY_ALL                  environment
#@ queue

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

Loadleveler Job Script II

```
#!/bin/sh                                  Shell being used
#@ job_type = serial                       Job Type
#@ output = $(jobid).out                   standard output
#@ error = $(jobid).err                    standard error
#@ notification = error                    notify on error
#@ notify_user = youremail@domain          to mail address
#@ class = checkpt                         job queue
#@ wall_clock_limit = 24:00:00             max walltime
#@ node_usage = shared                     node usage
#@ node = 1                                # of nodes
#@ total_tasks = 1                         total processors
#@ requirements = (Arch == "POWER5")       job requirements
#@ environment = COPY_ALL                  environment
#@ queue

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

Loadleveler Job Script III

- On Pandora:
  - `#@ resources = ConsumableMem(512 mb) ConsumableCPUS(1)` is required
  - `#@ requirements = (Arch == "POWER7")`
  - `#@ network.MPI_LAPI = sn_all,shared,US,HIGH`

Exercise 4: Job Submission

- Write a job submission script to execute the `hello_mpi` 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

AIX Clusters

- `llq <options> <job id>`
  - All jobs are displayed if `<job id>` is omitted
  - Display detailed information: `llq -l <job id>`
  - Check estimated start time: `llq -s <job id>`
  - Show jobs from a specific user: `llq -u <username>`

```
apacheco@l3f1n03$ llq
Id                        Owner      Submitted   ST PRI Class        Running on
------------------------- ---------- ----------- -- --- ------------ -----------
l3f1n03.14904.0           huiwu       7/16 15:45 R  50  checkpt      l3f1n09
l3f1n03.14908.0           srick       7/18 10:15 R  50  checkpt      l3f1n13
l3f1n03.14909.0           srick       7/18 10:18 R  50  checkpt      l3f1n04
l3f1n03.14911.0           huiwu       7/19 13:48 R  50  checkpt      l3f1n11
l3f1n03.14910.0           srick       7/18 10:18 R  50  checkpt      l3f1n06

5 job step(s) in queue, 0 waiting, 0 pending, 5 running, 0 held, 0 preempted
```

AIX Clusters

- `showllstatus.py`: Show job status and node running on

```
apacheco@peg304$ showllstatus.py
Node      Status    Load        Arch Node      Status    Load        Arch
ian1      Idle      1.02      Power4 pen09     Busy      16.28     Power5
pen01     Run       4.08      Power5 pen10     Busy      16.33     Power5
pen02     Run       2.01      Power5 pen11     Idle      0.00      Power5
pen03     Run       4.50      Power5 pen12     Idle      0.00      Power5
pen04     Run       7.04      Power5 pen13     Busy      16.21     Power5
pen05     Run       3.99      Power5 pen14     Run       2.50      Power5
pen06     Busy      16.30     Power5 pen15     Idle      0.00      Power5
pen07     Run       2.00      Power5 pen16     Idle      0.00      Power5
pen08     Run       4.07      Power5

Step ID          Owner         Status    Class     Hosts  Queue Date    Disp. Date
ian1.97678.0     nserno           R      MP5L        1    07/19 11:19   07/19 11:19
ian1.97677.0     nserno           R      MP5L        1    07/19 11:16   07/19 11:16
ian1.97672.0     cmcfer1          R      MP5L        1    07/19 08:38   07/19 08:38
ian1.97650.0     nserno           R      MP5L        1    07/18 13:30   07/18 13:30
ian1.97647.0     yuzhiyi          R      MP5L        4    07/18 10:27   07/18 10:27
ian1.97646.0     jgibs22          R      MP5L        1    07/18 10:09   07/18 10:09
ian1.97645.0     nserno           R      MP5L        1    07/17 13:20   07/17 21:40
ian1.97644.0     nserno           R      MP5L        1    07/17 13:20   07/17 17:20
ian1.97643.0     nserno           R      MP5L        1    07/17 13:20   07/17 16:51
```

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

AIX Clusters

- `llcancel <job id>`
  - Cancel a running or queued job
- `llhold <job id>`
  - Put a queued job on hold
- `llhold -r <job id>`
  - Resume a held job

Outline

Additional Help

- User's Guide
  - HPC: `http://www.hpc.lsu.edu/help`
  - 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"