LONI QB3 System Overview

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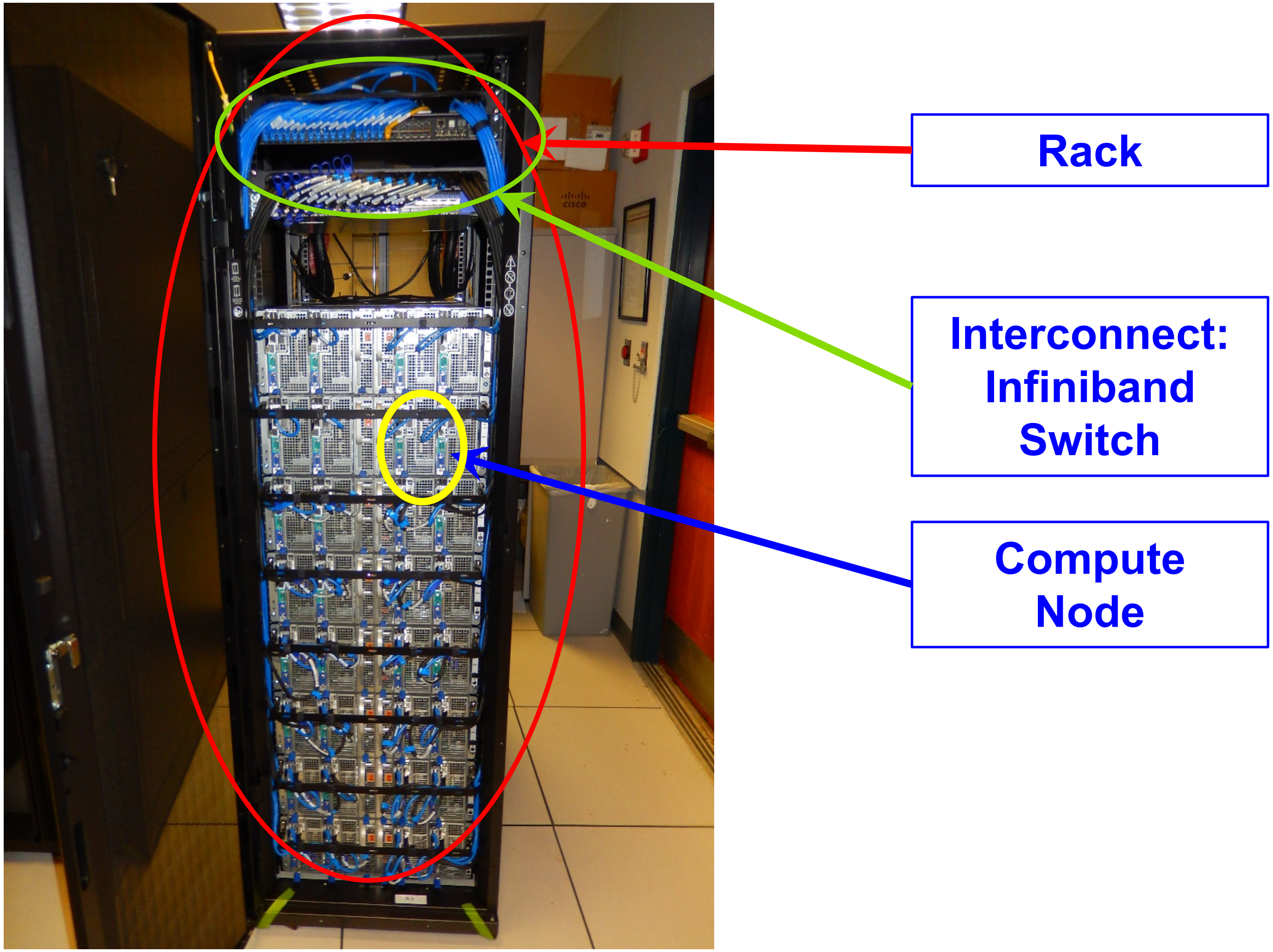
Outline

- **Things to be covered in the training**
  - Available HPC resources
    - LONI resources
    - Account and allocations
  - HPC software environment
    - General cluster architecture
    - How to access LONI clusters
    - How to check file systems, allocation balance
    - How to transfer files between cluster and local PC
    - The software management tool Module

Supercomputer Cluster Racks

Inside A Cluster Rack

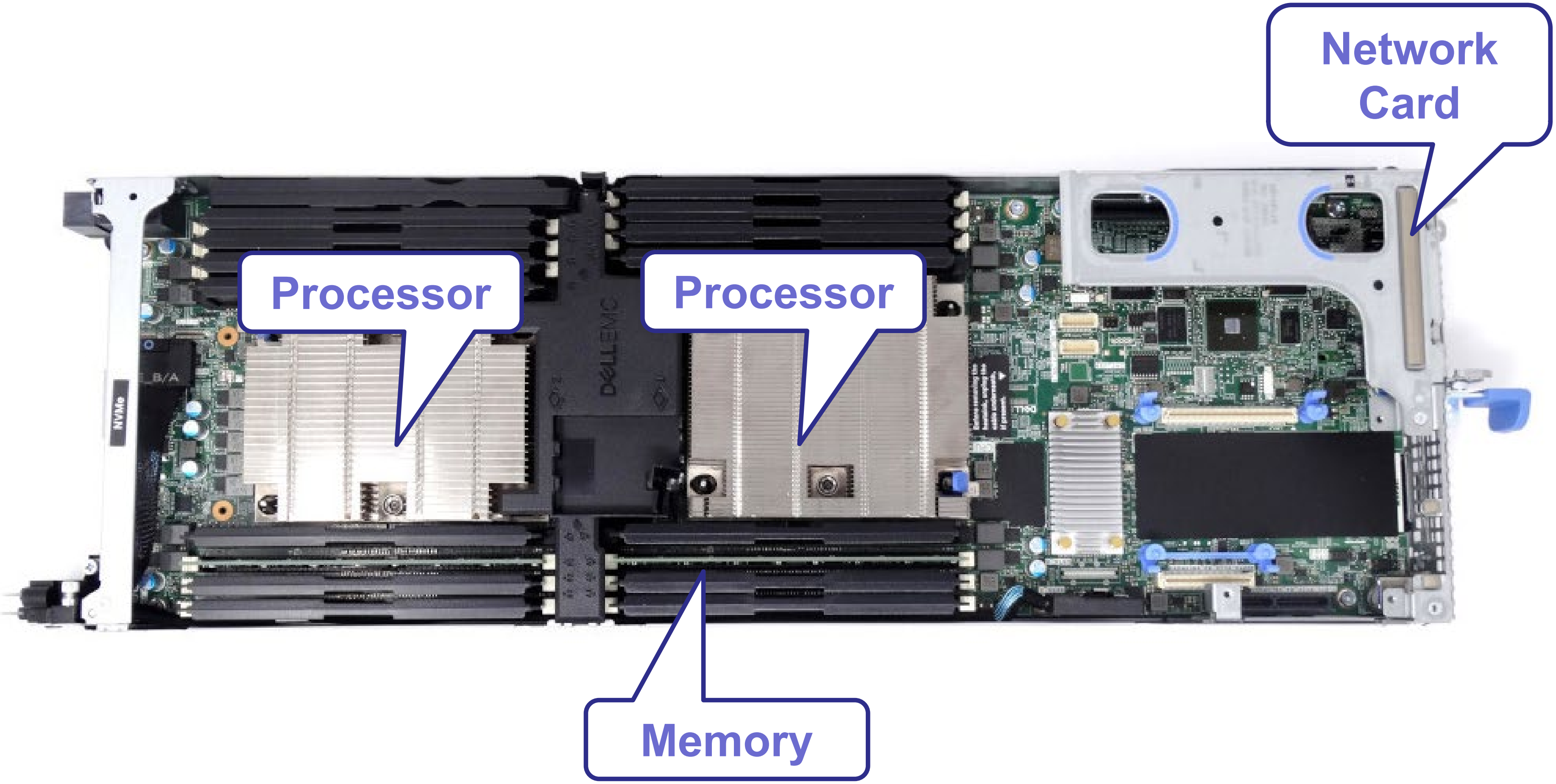


Rack

Interconnect: Infiniband Switch

Compute Node

Inside A Compute Node



Louisiana Optical Network Infrastructure (LONI)

- A state-of-the-art fiber optic network that runs throughout Louisiana and connects Louisiana and Mississippi research universities.
- $40M Optical Network, 10Gb Ethernet over fiber optics.

LONI-Louisiana Optical Network Infrastructure

- **LONI connects supercomputers at Louisiana's universities:**
  - Louisiana State University
  - Louisiana Tech University
  - LSU Health Sciences Center in New Orleans
  - LSU Health Sciences Center in Shreveport
  - Southern University
  - Tulane University
  - University of Louisiana at Lafayette
  - University of New Orleans
  - Grambling State University
  - Southeastern Louisiana University

  …
- **Full list: https://loni.org/about/participants/**

Available LONI Resources

QB2	
Hostname	qb2.loni.org
Peak Performance/TFlops	1,500
Compute nodes	504
Processor/node	2 10-Core
Processor Speed	2.8GHz
Processor Type	Intel Ivy Bridge-EP Xeon 64bit
Nodes with Accelerators	480
Accelerator Type	NVIDIA Tesla K20x
OS	RHEL v6
Vendor	Dell
Memory per node	64 GB
Location	Information Systems Building, Baton Rouge
Detailed Cluster Description	
User Guide	
Available Software	

QB3	
Hostname	qbc.loni.org
Peak Performance/TFlops	857
Compute nodes	202
Processor/node	2 24-Core
Processor Speed	2.4GHz
Processor Type	Intel Cascade Lake Xeon 64bit
Nodes with Accelerators	8
Accelerator Type	NVIDIA Volta V100
OS	RHEL v7
Vendor	Dell
Memory per node	192 GB
Location	Information Systems Building, Baton Rouge
Detailed Cluster Description	
User Guide	
Available Software	

Ref: http://hpc.loni.org/resources/hpc/index.php

Account Eligibility-***LONI***

- **All faculty and research staff at a LONI Member Institution, as well as students pursuing sponsored research activities at these facilities, are eligible for an LONI account.**
- User accounts on LONI require a valid LONI Institutional email address, and a sponsor from one of the LONI Member Institutions.
- **ACCOUNT SPONSOR: The person who is responsible for your activities on the cluster.**
- Only faculty members from LONI Member Institutions can sponsor accounts.
- Students, postdoctoral researchers, or research associates may choose their advisor as their sponsor.
- Requests for accounts by research associates not affiliated with a LONI Member Institution will be handled on a case by case basis.
- For prospective LONI Users from a non-LONI Member Institution, you are required to have a faculty member in one of LONI Member Institutions as your Collaborator to sponsor you a LONI account.

How Do I Get a ***LONI*** Account?

- Visit https://allocations.loni.org/login_request.php
- Enter your **INSTITUTIONAL** Email Address.
- Check your email and click on the link provided (link is active for 24hrs only)
- Fill the form provided
- For LONI **CONTACT/COLLABORATOR** field enter the name of your research advisor/supervisor or course instructor who must be a Full Time Faculty member at a LONI member institution. Never enter HPC staff’s name.
- Click Submit button
- Your account will be activated once we have verified your credentials.

Account Management
- LONI User Portals

- **LONI User Portal: https://allocations.loni.org**
- **Same LONI account can be used for both QB2 and QB3**
- **The default Login shell is bash**
  - Supported Shells: bash, tcsh, ksh, csh, sh
  - Change Login Shell at the profile page
- **May keep the account after graduation under certain circumstances**

Allocation

- **An allocation is a block of service unit (SUs) that allows a user to run jobs on a cluster**
  - One SU is one core-hour
  - Example
    - 40 SUs will be charged for a job that runs 10 hours on 4 cores
- **LONI users: All LONI clusters need to be charged to a valid allocation.**
- **It is FREE to have allocation and use LONI resources, but there is a value of approximately $0.1/core-hour from other sources (e.g. taxpayer)**

Who Can Request Allocation?

- **Only Full Time LONI Faculty member at LONI member institutions can act as Principle Investigators (PI) and request LONI Allocations.**
  - Rule of Thumb: If you can sponsor user accounts, you can request allocations.
- **Everyone else will need to join an existing allocation of a PI, usually your advisor or course instructor (if your course requires an LONI account).**

- **As a non-PI, your goal is to help your PI understand the allocation policy and prepare the allocation request.**

Allocation Types

- **Startup: Allocations upto 50K SUs**
  - Can be requested at any time during the year.
  - **Begins on the first day of the quarter** in which we received the request
  - Only two active allocations per PI at any time.
- **Large (research): Allocations between 50K - 6M SUs.**
  - Decision will be made on January 1, April 1, July 1 and October 1 of each year
  - A request must be submitted one month before the decision day.
  - Users can have multiple Large Allocations.
  - Each requests is limited to 6 million SUs, and a PI may have a total of 12M SUs active at any given time
  - QB2 and QB3 use the same allocation and they are weighted equally

How to Request/join an Allocation

- **LONI: Login to your profile at https://allocations.loni.org**
- **Click on "Request Allocation" in the right sidebar**
- **Click "New Allocation" to request a New Allocation. (PI only)**
  - Fill out the form provided.
  - All requests require submission of a proposal justifying the use of the resources.
  - Click "Submit Request" button.
- **Click "Join Allocation" to join an existing Allocation (Non-PI).**
  - Search for PI using his/her email address, full name or LONI username
  - Click "Join Projects" button associated with the PI's information.
  - You will be presented with a list of allocations associated with the PI. Click "Join" for the allocation you wish to join.
  - Your PI will receive an email requesting him to confirm adding you to the allocation.
- **Please do not contact the helpdesk to do this.**

How Do I Reset My Password?

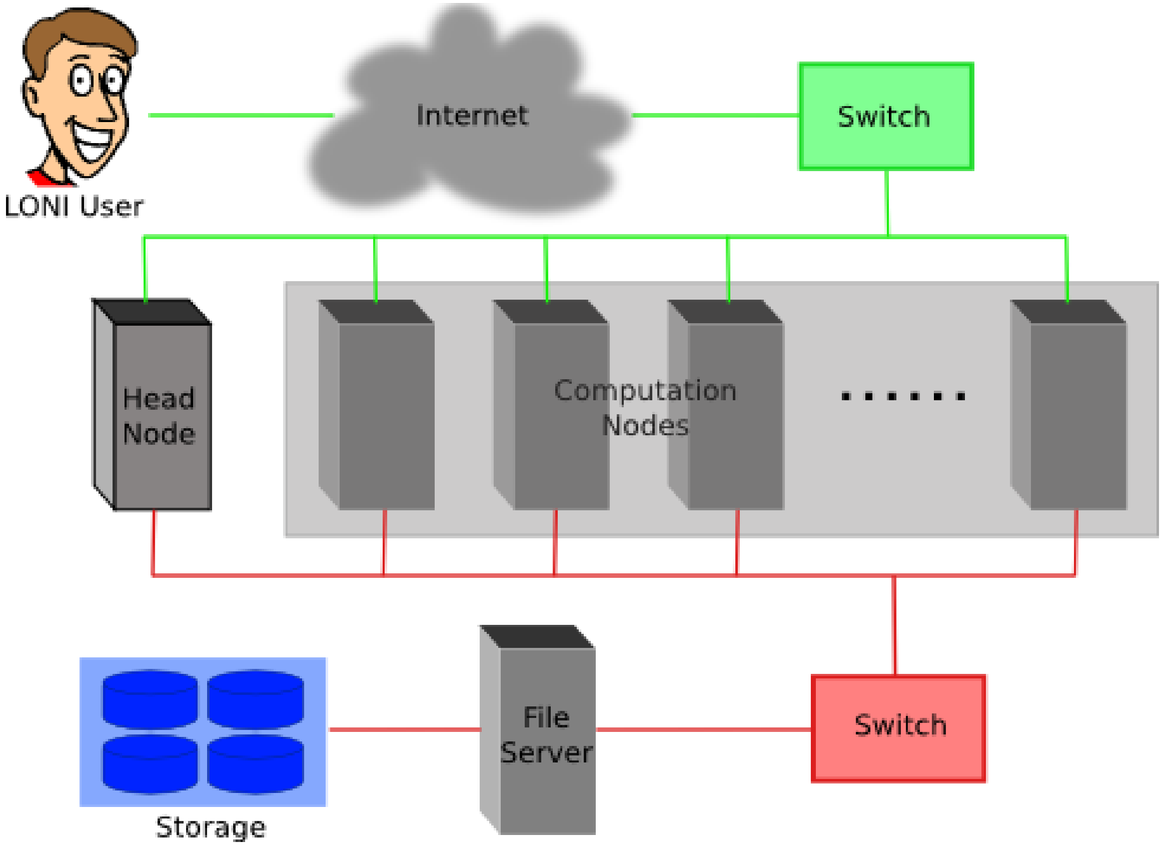
- LONI: Visit https://allocations.loni.org/user_reset.php
- Enter the email address attached to your account
- You will receive an email with link to reset your password, link must be used within 24 hours.
- Once you have entered your password, your password reset request needs to be manually reviewed. **IMPORTANT:**
  - **DO NOT** assume your new password is available to use right after the reset request submission
  - **DO NOT** submit the reset request multiple times if you didn't see your new password worked at once.
- The Password approval can take anything from 10 mins to a few hours depending on the schedule of the Admins and also time of day.
- You will receive a confirmation email stating that your password reset has been approved.

Password Security

- Passwords should be changed as soon as your account is activated for added security.
- Password must be at least 12 and at most 32 characters long, must contain three of the four classes of characters:
  - lowercase letters,
  - uppercase letters,
  - digits, and
  - other special characters (punctuation, spaces, etc.).
- Do not use a word or phrase from a dictionary,
- Do not use a word that can be obviously tied to the user which are less likely to be compromised.
- Do not tell your password to others including your advisor.

General Cluster Architecture

- Multiple compute nodes
- Multiple users
- Each user may have multiple jobs running simultaneously

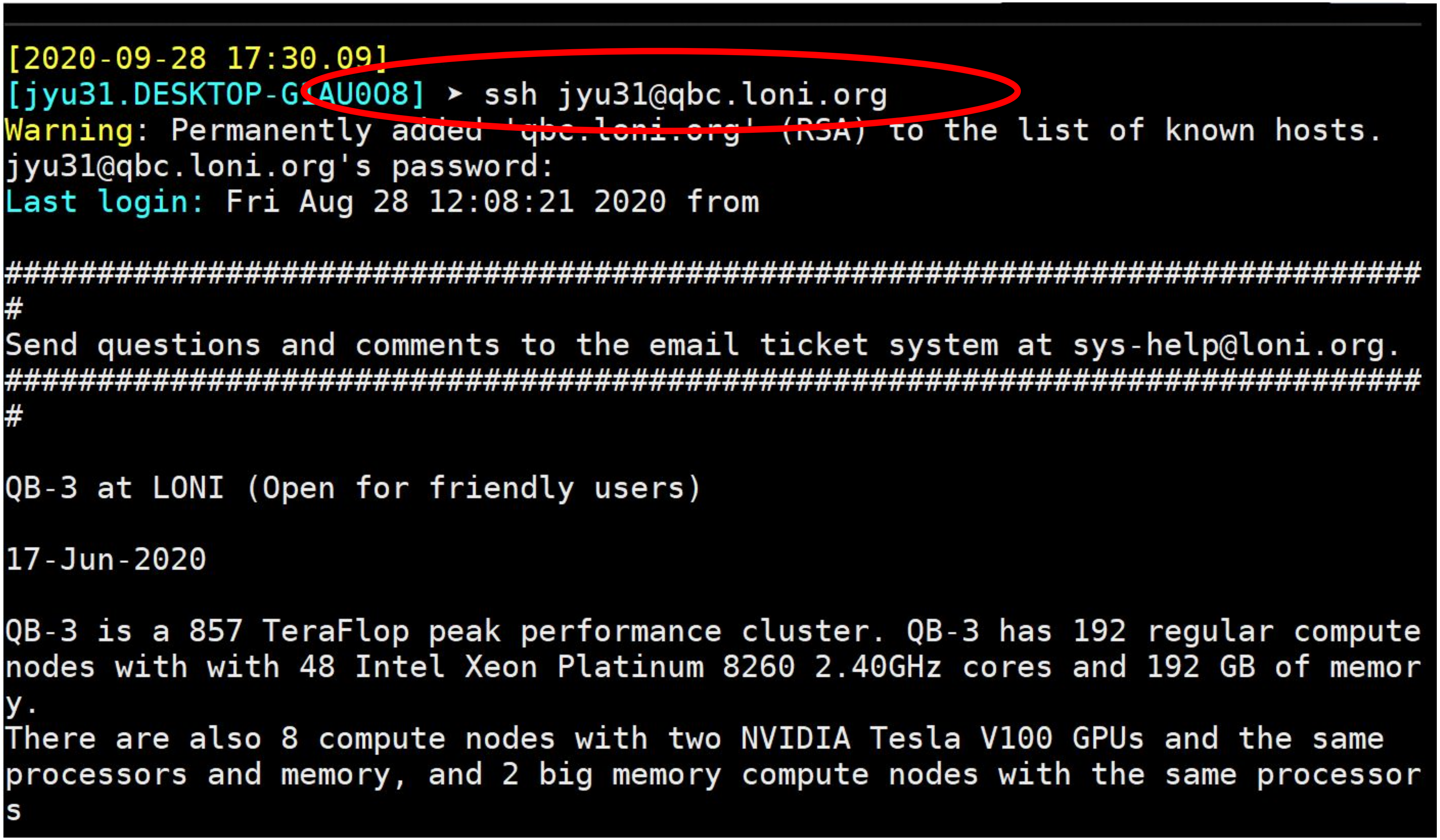


Accessing Cluster via SSH (Secure Shell)

- **On Linux and Mac**
  - use ssh on a terminal to connect
- **Windows box (ssh client):**
  - MobaXterm (recommended)
  - SSH Secure Shell Client
  - Putty (Better use Bitvise SSH Client from http://www.putty.org/)

- **Username and password**
- **Host name**
  - QB2: <cluster_name>.loni.org
    - <cluster_name> can be:
      - **qb.loni.org**
  - QB3: <cluster_name>.loni.org
    - <cluster_name> can be:
      - **qbc.loni.org**

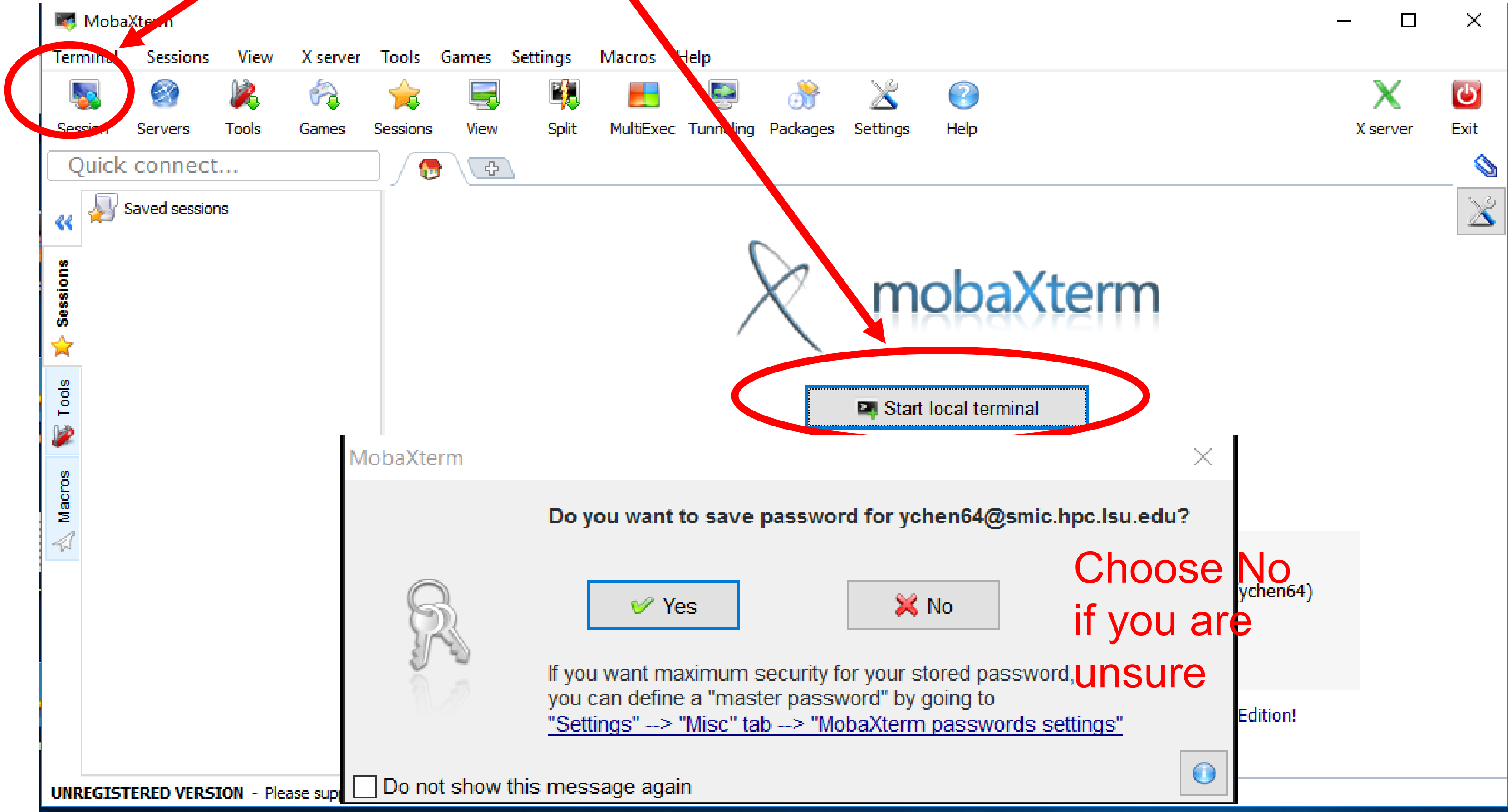
Accessing Cluster on Linux and Mac



```
[2020-09-28 17:30.09]
[jyu31.DESKTOP-G1AU008] ➤ ssh jyu31@qbc.loni.org
Warning: Permanently added 'qbc.loni.org' (RSA) to the list of known hosts.
jyu31@qbc.loni.org's password:
Last login: Fri Aug 28 12:08:21 2020 from

#############################################################################
#
Send questions and comments to the email ticket system at sys-help@loni.org.
#############################################################################
#

QB-3 at LONI (Open for friendly users)

17-Jun-2020

QB-3 is a 857 TeraFlop peak performance cluster. QB-3 has 192 regular compute
nodes with with 48 Intel Xeon Platinum 8260 2.40GHz cores and 192 GB of memor
y.
There are also 8 compute nodes with two NVIDIA Tesla V100 GPUs and the same
processors and memory, and 2 big memory compute nodes with the same processor
s
```

Accessing Cluster on Windows - MobaXterm

- **First time user, choose either one:**
  - use ssh on a terminal
  - start a new remote session -> SSH


MobaXterm
Terminal Sessions View X server Tools Games Settings Macros Help
Session Servers Tools Games Sessions View Split MultiExec Tunneling Packages Settings Help X server Exit
Quick connect...
Saved sessions
Sessions
Tools
Macros
mobaXterm
Start local terminal
ychen64)
Edition!
UNREGISTERED VERSION - Please sup

MobaXterm

Do you want to save password for ychen64@smic.hpc.lsu.edu?

✔ Yes ✖ No

If you want maximum security for your stored password, you can define a "master password" by going to "Settings" --> "Misc" tab --> "MobaXterm passwords settings"

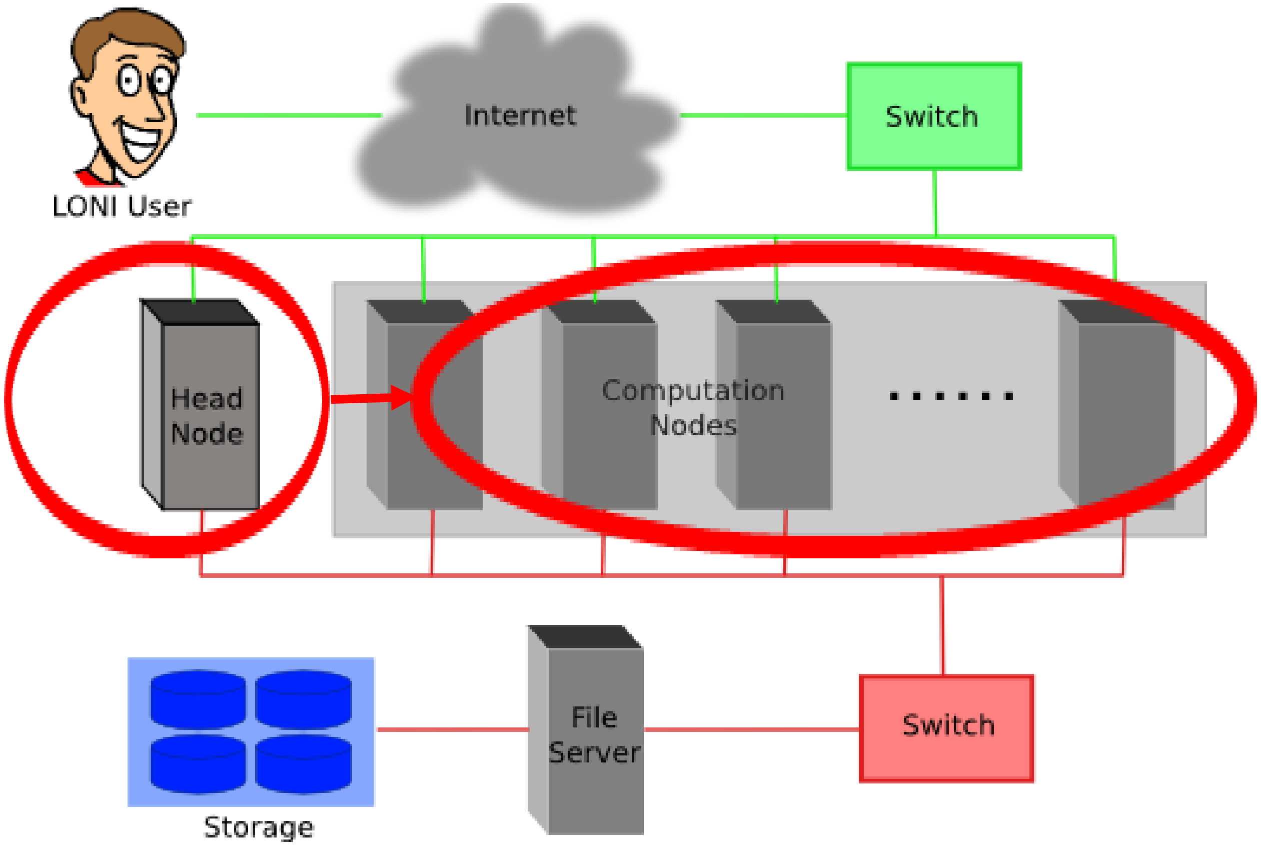
□ Do not show this message again

Choose No if you are unsure

Cluster Environment

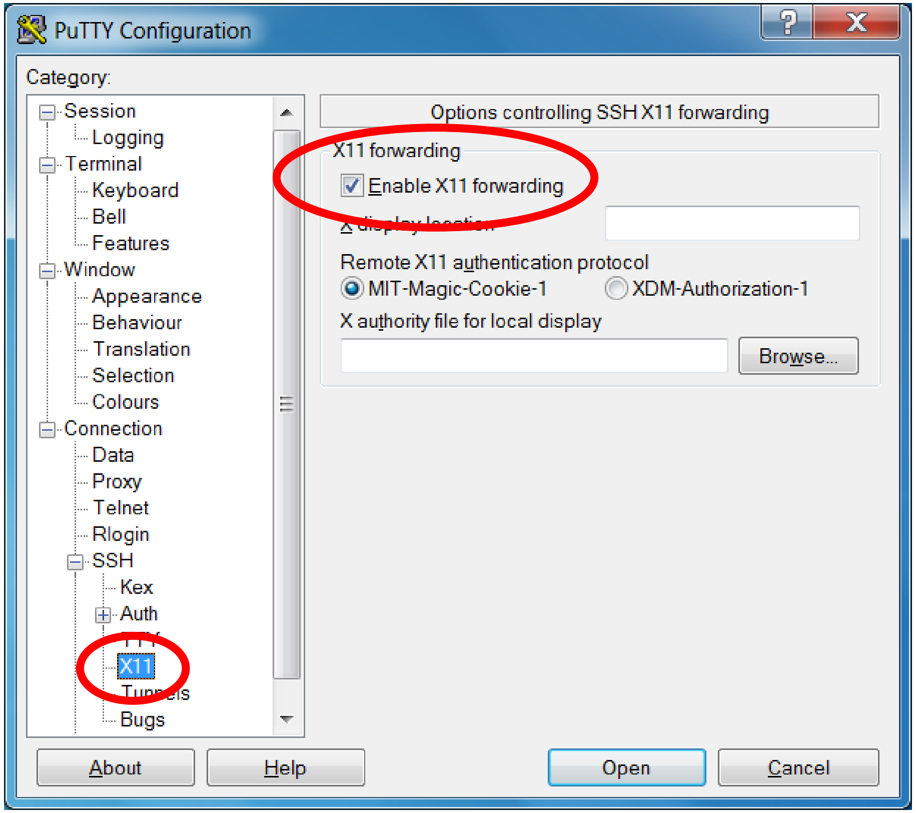
- Multiple compute nodes
- Multiple users
- Each user may have multiple jobs running simultaneously

DO NOT RUN YOUR JOB ON THE HEAD NODE!!!



Enable X11 Forwarding

- **On Linux or Mac, simply pass the -X option to the ssh command line**
  - `ssh -X username@qbc.loni.org`
- **On Windows using putty**
  - Connection->SSH->X11->Enable X11 forwarding
  - Install X server (e.g. Xming)
- **On Windows using MobaXterm**
  - X server already set up
  - Automatically start X server at start up (Settings -> X11)



PuTTY Configuration

Category:

Options controlling SSH X11 forwarding

X11 forwarding

☑ Enable X11 forwarding

X display location

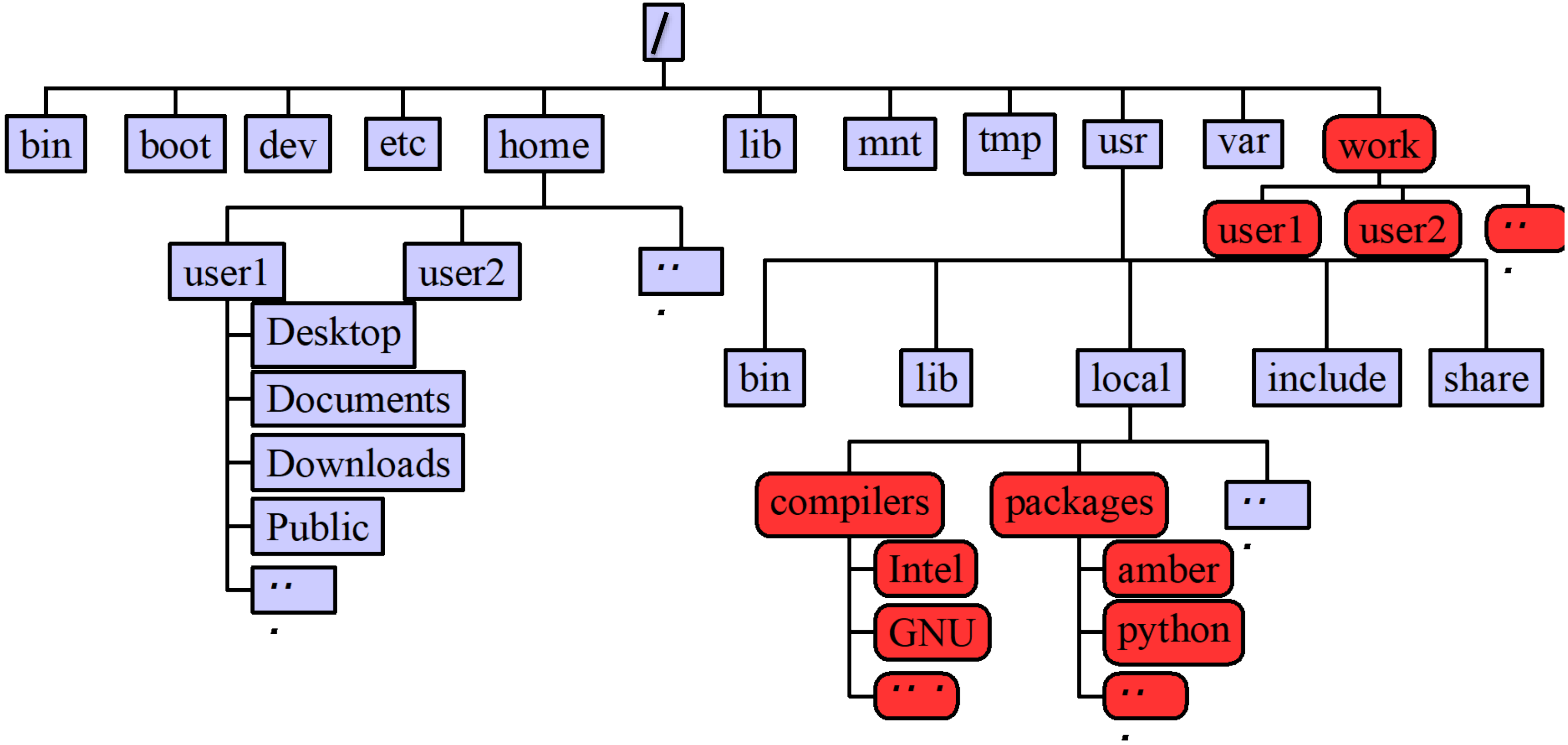
Remote X11 authentication protocol

● MIT-Magic-Cookie-1 ○ XDM-Authorization-1

X authority file for local display

File Systems

- All files are arranged in directories.
- These directories are organized into the file system.
- QB2 and QB3 have separate file systems.



File Systems

Directory (folder)	Distributed	Throughput	File life time	Best used for
Home	Yes	Low	Unlimited	Code in development, compiled executable
Work	Yes	High	60 days	Job input/output
Project	Yes	Medium/High	1 year	storage space for a specific project, NOT for archival purposes

- **Tips**
  - The work directory is not for long-term storage
    - Files are subject to be purged after 60-90 days
  - The work directory will be created 1 hour after the first cluster login
  - The project directory provides storage space for a specific project
    - **only PI** can apply storage allocation to use and renew periodically
    - NOT for archival purposes
    - An active allocation is needed
    - For more info about the storage allocation, see appendix or contact us

Disk Quota

Cluster	Home		Work		Local scratch
	Access point	Quota	Access Point	Quota	Access point
LONI	/home/$USER	5GB/ 10 GB	/work/$USER	N/A	/var/scratch

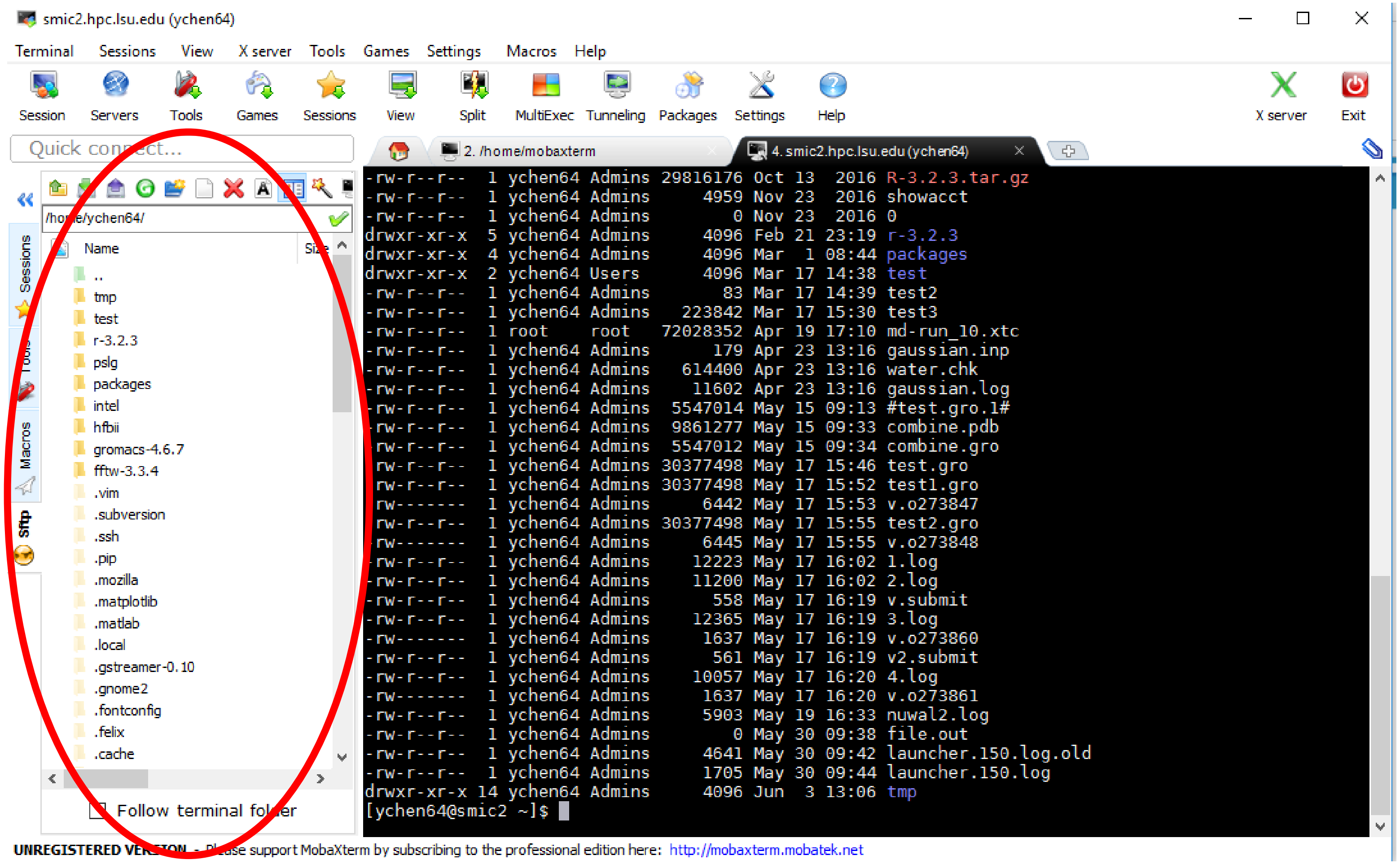
- **Never let you job write output to your home directory**
- **/home quota increased from 5 GB to 10 GB on QB3**
- **Check current disk quota and usage**
  - showquota

File Transfer (Linux/Mac)

- **From/to a Unix/Linux/Mac machine (including between the clusters)**
  - `scp` command
    - Syntax: `scp <options> <source> <destination>`
  - `rsync` command
    - Syntax: `rsync <options> <source> <destination>`
- **From a download link on a website (usually opened with a web browser)**
  - `Right click on the link and then copy the link location`
  - `wget command`

File Transfer (Windows)

- **From/to a Windows machine**
  - Use a client that supports the scp protocol (e.g. SSH Secure Shell Client)



smic2.hpc.lsu.edu (ychen64)
Terminal Sessions View X server Tools Games Settings Macros Help
Session Servers Tools Games Sessions View Split MultiExec Tunneling Packages Settings Help X server Exit
Quick connect...
2. /home/mobaxterm
4. smic2.hpc.lsu.edu (ychen64)
Sessions Tools Macros Sftp
/home/ychen64/
Name Size
..
tmp
test
r-3.2.3
pslg
packages
intel
hfbii
gromacs-4.6.7
fftw-3.3.4
.vim
.subversion
.ssh
.pip
.mozilla
.matplotlib
.matlab
.local
.gstreamer-0.10
.gnome2
.fontconfig
.felix
.cache
Follow terminal folder

```
-rw-r--r--  1 ychen64 Admins 29816176 Oct 13  2016 R-3.2.3.tar.gz
-rw-r--r--  1 ychen64 Admins     4959 Nov 23  2016 showacct
-rw-r--r--  1 ychen64 Admins        0 Nov 23  2016 0
drwxr-xr-x  5 ychen64 Admins     4096 Feb 21 23:19 r-3.2.3
drwxr-xr-x  4 ychen64 Admins     4096 Mar  1 08:44 packages
drwxr-xr-x  2 ychen64 Users      4096 Mar 17 14:38 test
-rw-r--r--  1 ychen64 Admins       83 Mar 17 14:39 test2
-rw-r--r--  1 ychen64 Admins   223842 Mar 17 15:30 test3
-rw-r--r--  1 root    root   72028352 Apr 19 17:10 md-run_10.xtc
-rw-r--r--  1 ychen64 Admins      179 Apr 23 13:16 gaussian.inp
-rw-r--r--  1 ychen64 Admins   614400 Apr 23 13:16 water.chk
-rw-r--r--  1 ychen64 Admins    11602 Apr 23 13:16 gaussian.log
-rw-r--r--  1 ychen64 Admins  5547014 May 15 09:13 #test.gro.1#
-rw-r--r--  1 ychen64 Admins  9861277 May 15 09:33 combine.pdb
-rw-r--r--  1 ychen64 Admins  5547012 May 15 09:34 combine.gro
-rw-r--r--  1 ychen64 Admins 30377498 May 17 15:46 test.gro
-rw-r--r--  1 ychen64 Admins 30377498 May 17 15:52 test1.gro
-rw-------  1 ychen64 Admins     6442 May 17 15:53 v.o273847
-rw-r--r--  1 ychen64 Admins 30377498 May 17 15:55 test2.gro
-rw-------  1 ychen64 Admins     6445 May 17 15:55 v.o273848
-rw-r--r--  1 ychen64 Admins    12223 May 17 16:02 1.log
-rw-r--r--  1 ychen64 Admins    11200 May 17 16:02 2.log
-rw-r--r--  1 ychen64 Admins      558 May 17 16:19 v.submit
-rw-r--r--  1 ychen64 Admins    12365 May 17 16:19 3.log
-rw-------  1 ychen64 Admins     1637 May 17 16:19 v.o273860
-rw-r--r--  1 ychen64 Admins      561 May 17 16:19 v2.submit
-rw-r--r--  1 ychen64 Admins    10057 May 17 16:20 4.log
-rw-------  1 ychen64 Admins     1637 May 17 16:20 v.o273861
-rw-r--r--  1 ychen64 Admins     5903 May 19 16:33 nuwal2.log
-rw-r--r--  1 ychen64 Admins        0 May 30 09:38 file.out
-rw-r--r--  1 ychen64 Admins     4641 May 30 09:42 launcher.150.log.old
-rw-r--r--  1 ychen64 Admins     1705 May 30 09:44 launcher.150.log
drwxr-xr-x 14 ychen64 Admins     4096 Jun  3 13:06 tmp
[ychen64@smic2 ~]$
```

UNREGISTERED VERSION - Please support MobaXterm by subscribing to the professional edition here: http://mobaxterm.mobatek.net

Application Software

- **Installed Software**
  - Mathematical and utility libraries
    - FFTW, HDF5, NetCDF, PETSc...
  - Applications
    - Amber, NWChem, NAMD, Gromacs, LAMMPS…
    - R, Python...
  - Visualization
    - VMD
  - Programming Tools
    - DDT, TAU...
- **List of software**
  - `http://www.hpc.lsu.edu/resources/software/index.php`
- **Installed by using Spack under** `/usr/local/packages`
- **User requested packages**
  - Usually installed in user home directory, unless request by a group of users, in which case it will be installed under `/project` or `/usr/local/packages`

Software Environment: Module

- **Environment variables**
  - `PATH`: where to look for executables
  - `LD_LIBRARY_PATH`: where to look for shared libraries
  - `LD_INCLUDE_PATH`: where to look for header and include files
- **Other environment variables sometimes needed by various software**
  - `LIBRARY_PATH, C_LIBRARY_PATH`
  - `LDFLAGS, LDLIBS`
- **Module**
  - An application that helps users set up their environment. Most supercomputing sites (including XSEDE) use modules. Much more convenient than setting variables in .bashrc
  - QB2 and QB3

Using Environment Modules

- **Environment Modules is a framework to manage what software is loaded into a user's environment. Its functionality includes**
  - List all software packages currently available in the Environment Modules system,
  - List all software packages loaded into a user's environment,
  - Load/Switch software packages into a user's environment
  - Unload a software package from a user's environment.

Modules: List All Available Packages

- **The command to list all available packages is:** `module avail/av`

```
[jyu31@qbc1 ~]$ module av
--------------- /usr/local/packages/Modules/modulefiles/apps ---------------
adios2/2.3.1/intel-19.0.5-mvapich-2.3.3            vmd/1.9.3/intel-19.0.5
amber/18/intel-19.0.5-mvapich-2.3.3
autodock-vina/1_1_2/intel-19.0.5
beast2/2.5.2/intel-19.0.5
blast/2.10.1/gcc-9.3.0
boost/1.69.0/intel-19.0.5
boost/1.72.0/gcc-9.3.0
bowtie/1.2.3/intel-19.0.5
bowtie2/2.3.5.1/gcc-9.3.0
bwa/0.7.17/intel-19.0.5
cmake/3.16.2/intel-19.0.5
```

- **The format of the listed packages is <package name>/<package version>. For example, gcc/9.3.0 is version 9.3.0 of gcc.**

Modules: List Currently Loaded Packages

- To see what packages are currently loaded into a user's environment, the command is: `module list`

```
[jyu31@qbc1 ~]$ module list
Currently Loaded Modulefiles:
 1) intel/19.0.5
 2) mvapich2/2.3.3/intel-19.0.5(default)
 3) gcc/9.3.0
 4) gromacs/2020.2/intel-19.0.5-mvapich-2.3.3
```

- The above listing shows that this user has 4 packages loaded

Modules: Load/Unload a Package

- **The command for loading a package into a user's environment is:** `module load <package name>`**.**
- **The command for unloading a package is:** `module unload <package name>.`
- **If a specific version of a package is desired, the command can be expanded to:** `module load <package name>/<package version>`**.**

```
[jyu31@qbc1 ~]$ module av intel
--------------- /usr/local/packages/Modules/modulefiles/apps ----------------
intel-mpi/2019.5.281  intel/19.0.5  intel/19.1.2
[jyu31@qbc1 ~]$ module load intel
[jyu31@qbc1 ~]$ icc -v
icc version 19.1.2.254 (gcc version 4.8.5 compatibility)
[jyu31@qbc1 ~]$ module unload intel
[jyu31@qbc1 ~]$ module load intel/19.0.5
[jyu31@qbc1 ~]$ icc -v
icc version 19.0.5.281 (gcc version 4.8.5 compatibility)
```

Modules: Unload All Loaded Packages

- **To unload all loaded module files, use the purge method:**

```
[jyu31@qbc1 ~]$ module list
Currently Loaded Modulefiles:
 1) intel/19.0.5
 2) mvapich2/2.3.3/intel-19.0.5(default)
 3) gcc/9.3.0
 4) gromacs/2020.2/intel-19.0.5-mvapich-2.3.3
[jyu31@qbc1 ~]$ module purge
[jyu31@qbc1 ~]$ module list
No Modulefiles Currently Loaded.
[jyu31@qbc1 ~]$
```

Modules: Dependencies

- **Note that Modules will load any prerequisites (dependencies) for a package when that package is loaded.**

```
[jyu31@qbc1 ~]$ module list
No Modulefiles Currently Loaded.
[jyu31@qbc1 ~]$ module av gromacs
--------------- /usr/local/packages/Modules/modulefiles/apps ----------------
gromacs/2018.8/intel-19.0.5-cuda-mvapich-2.3.3
gromacs/2020.2/intel-19.0.5-mvapich-2.3.3
[jyu31@qbc1 ~]$ module load gromacs/2020.2/intel-19.0.5-mvapich-2.3.3
Autoloading intel-19.0.5
Autoloading mvapich2/2.3.3/intel-19.0.5
Autoloading gcc/9.3.0

Loading gromacs/2020.2/intel-19.0.5-mvapich-2.3.3
  Loading requirement: intel/19.0.5 mvapich2/2.3.3/intel-19.0.5 gcc/9.3.0
[jyu31@qbc1 ~]$ module list
Currently Loaded Modulefiles:
 1) intel/19.0.5
 2) mvapich2/2.3.3/intel-19.0.5(default)
 3) gcc/9.3.0
 4) gromacs/2020.2/intel-19.0.5-mvapich-2.3.3
```

Modules: Display the module changes

- **The display/show command will detail all changes that will be made to the user's environment:** `module disp <package name>`**.**

```
[jyu31@qbc1 ~]$ module disp python/3.7.6
-------------------------------------------------------------------
/usr/local/packages/Modules/modulefiles/apps/python/3.7.6:

module-whatis   {Description: Python is a programming language that lets you work
more quickly and integrate your systems more effectively. - Homepage:
http://python.org/}
conflict        python
prepend-path    CPATH /usr/local/packages/python/3.7.6/include
prepend-path    MANPATH /usr/local/packages/python/3.7.6/share/man
prepend-path    PATH /usr/local/packages/python/3.7.6/bin
prepend-path    PKG_CONFIG_PATH /usr/local/packages/python/3.7.6/lib/pkgconfig
prepend-path    PYTHONPATH /usr/local/packages/python/3.7.6/lib/python2.7/site-
packages
setenv          LHPC_ROOTPYTHON /usr/local/packages/python/3.7.6
setenv          LHPC_VERSIONPYTHON 3.7.6
-------------------------------------------------------------------
```

Modules: Load Automatically on Login

- **On HPC and LONI clusters, Modules can be loaded automatically on login by adding the appropriate module load commands to a user's** `~/.bashrc` **or** `~/.modules (recommended)` **file**
- **The following example shows a .modules file that automatically loads** `python-3.7.6`

```
[jyu31@qbc1 ~]$ cat ~/.modules
#
# This is the default .modules file for smic.
# It is used to customize your Modules environment
# variables such as PATH and LD_LIBRARY_PATH.
#
# To learn more about Modules, use 'module --help'.
#
# Default software
#module load mvapich2

# Add additional software here
module load python/3.7.6
```

Creating Your Own Module File

- **An example of a simple module file** `(~/my_module/gitkey):`

```
#%Module
proc ModulesHelp { } {
    puts stderr { my compiled version of git.
    }
}
module-whatis {version control using git}
set GIT_HOME /home/fchen14/packages/git-master/install
prepend-path    PATH            $GIT_HOME/bin
```

- **Add the path to the key to the MODULEPATH environment variable:**

```
$ export MODULEPATH=~/my_module:$MODULEPATH
```

- **Then try to use**:

```
$ module load gitkey
$ which git
$ module unload gitkey
$ which git
```

Next Sessions

- **10:15 - 10:30**
  - Break
- **10:30 - 11:30**
  - Job management with Slurm
- **11:30 - 12:30**
  - Performance benchmarks and tuning
- **12:30 - 02:00**
  - Lunch break
- **02:00 - 04:00**
  - Q&A + On-ramp sessions (breakout sessions)