# Introduction to Cluster Computing Using Maxwell


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Center for Advanced Computation and Data Systems

(CACDS)

http://cacds.uh.edu

http://support.cacds.uh.edu

University of Houston

Houston, TX

# Purpose of the Center

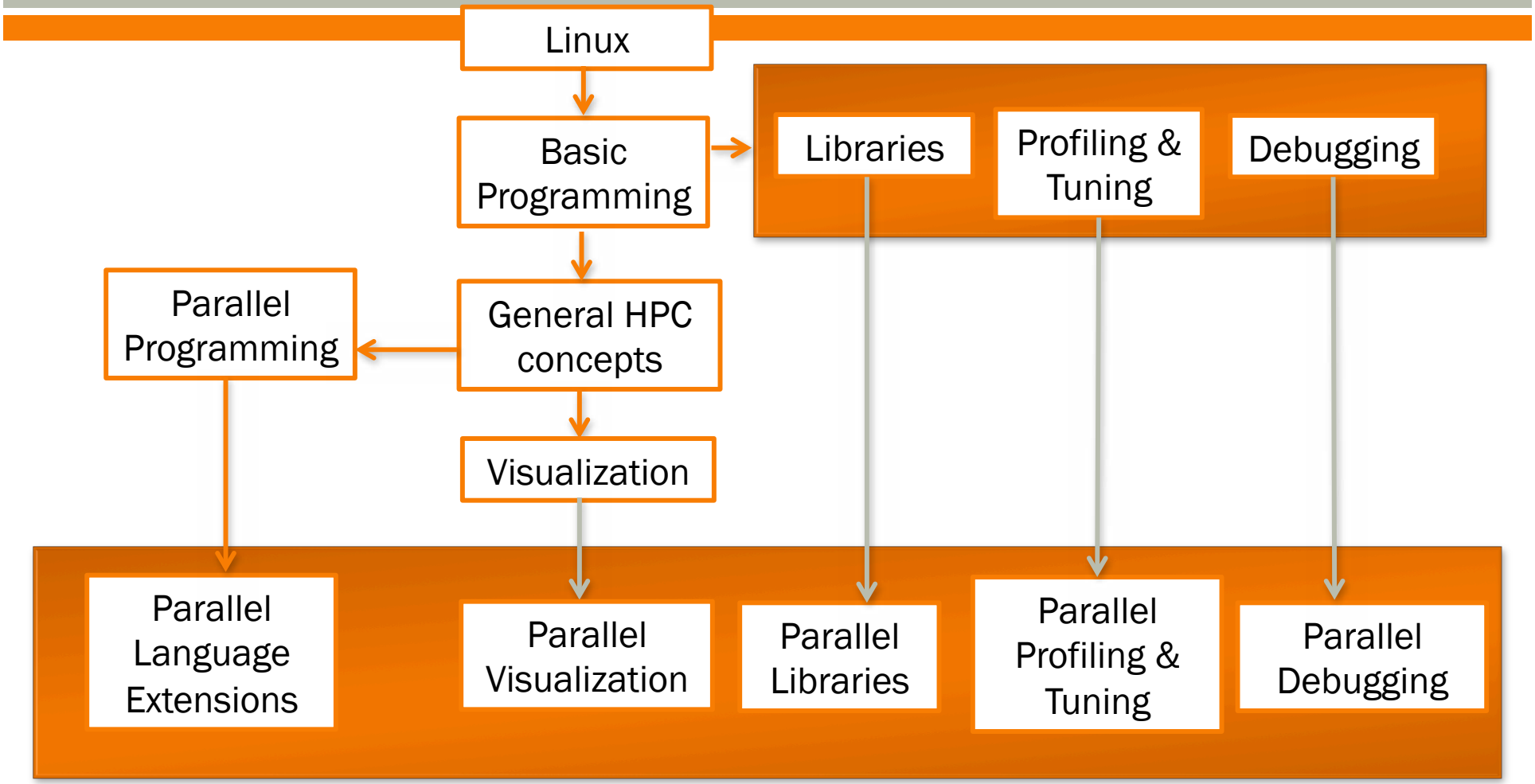
## CACDS Purpose Statement

- Provide access to high performance computing and data storage resources
- Offer expert training, consulting, and technical support services
- Consult on research design and production
- Assist in the development and/or execution of supported research activities

# Our Mission

- Advance the university's primary research thrusts in energy and health
- Support faculty research involving high performance computing (HPC), visualization, and computationally driven data-intensive science
- Provide consulting and training for UH faculty, staff and students
- Form relevant industry partnerships
- Facilitate collaborations between faculty as well as between faculty and external partners

# HPC User Training Road Map



# HPC Training
# Fall 2014

**Location: PGH 200**

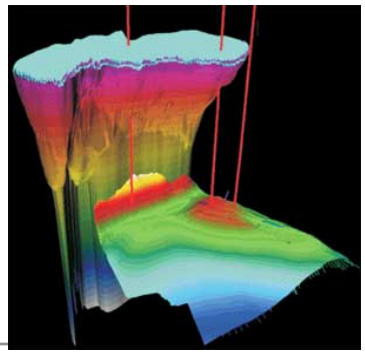
**48 seat class room**

- Linux
- Shell programming
- Cluster computing on Maxwell
- XSEDE Cyberinfrastructure and allocation process
- Python
- MATLAB
- C++
- Fortran
- Parallel Programming using OpenMP
- Parallel Programming using MPI
- Parallel numerical libraries

**Location: PGH 235**

**12 seat class room**

- Nvidia CUDA
  - introductory, intermediate and advanced
  - profiling, debugging & tuning
- OPENACC
  - intermediate, advanced
  - profiling, debugging & tuning
- Intermediate and Advanced MPI
  - profiling, debugging & tuning
- Intel Xeon Phi Programming
  - Native computing
    - OpenMP, Cilk++
  - Offload Execution
  - Symmetric Execution
  - profiling, debugging & tuning
- Visualization at scale
  - Paraview
  - VisIt



# Training Registration
# www.cacds.uh.edu/training

UNIVERSITY of HOUSTON
CENTER FOR ADVANCED COMPUTING & DATA SYSTEMS

ABOUT | RESEARCH | EDUCATION | RESOURCES | NEWS

## Training Courses

**EDUCATION**

Training Courses>>
- Events
- Lectures
- Workshops
- Technical Seminars

CACDS has launched several HPC training courses for members of the UH research community. Registration is required to take the courses. Please click the date you would like to attend under each course to register.

**CURRENT TRAINING**

| CLASS NAME |
| --- |
| Introduction to Linux |
| Introduction to Shell Programming |
| Introduction to Cluster Computing and Maxwell Cluster |
| Introduction to C++ Programming |
| Introduction to Python Programming |
| Introduction to Parallel Programming with OpenMP |
| GPGPU Parallel Programming with OpenACC |
| GPGPU Parallel Programming with CUDA |
| Introduction to Parallel Programming with MPI |
| Introduction to Matlab |
| Introduction to Intel Xeon Phi Programming |
| Introduction to High Performance Numerical Libraries |
| Visualization with VISIT I |
| Visualization with VISIT II |
| Visualization with Paraview I |

# Overview

- Accessing the Cluster
- Maxwell Specifications
- User Environment
- Compiling Programs
- Portable Batch System (PBS)
- Batch Jobs
- Interactive Jobs
- Killing & Suspending Jobs

# First Access Your Account

- Log into your accounts
  - Username or login = hpc_user**X**
  - Where x = sign in serial number 1 – 47
  - Password = **cacds2014**
  - Use your web browser
    - Firefox, Chromium or Google chrome
- Slides could be downloaded from URL below

/share/apps/tutorials/intro2maxwell.pdf

# Disclaimer

- Maxwell cluster is for research work under a UH PI
  - Faculty sponsored **RESEARCH** activity only
- You will be using a surrogate cluster for this training in place of the Maxwell Cluster
  - You would not be using Maxwell for this training
- We assuming you are already familiar with the Linux Operating Environment
  - If not try to attend any of the upcoming Linux hands on tutorials offered by CACDS
- After this training, if you do not already have an account on Maxwell feel free to request one, after authorization from your PI(UH Faculty)
  - http://www.rcc.uh.edu/cgi-bin/account.cgi (actual application page)

# Who Can Use Maxwell Cluster?

- Open to all UH faculty for research purposes
  - Students & postdocs –under UH faculty guidance
  - Collaborators –under UH faculty guidance

# What Happens Next?

- How to connect to the Maxwell Cluster:
  - For UNIX/Linux/Mac users
    - Open up terminal console and use Openssh secure shell client to connect
    - syntax:
      - ssh username@cusco.hpcc.uh.edu

Where username is your assigned login ID..

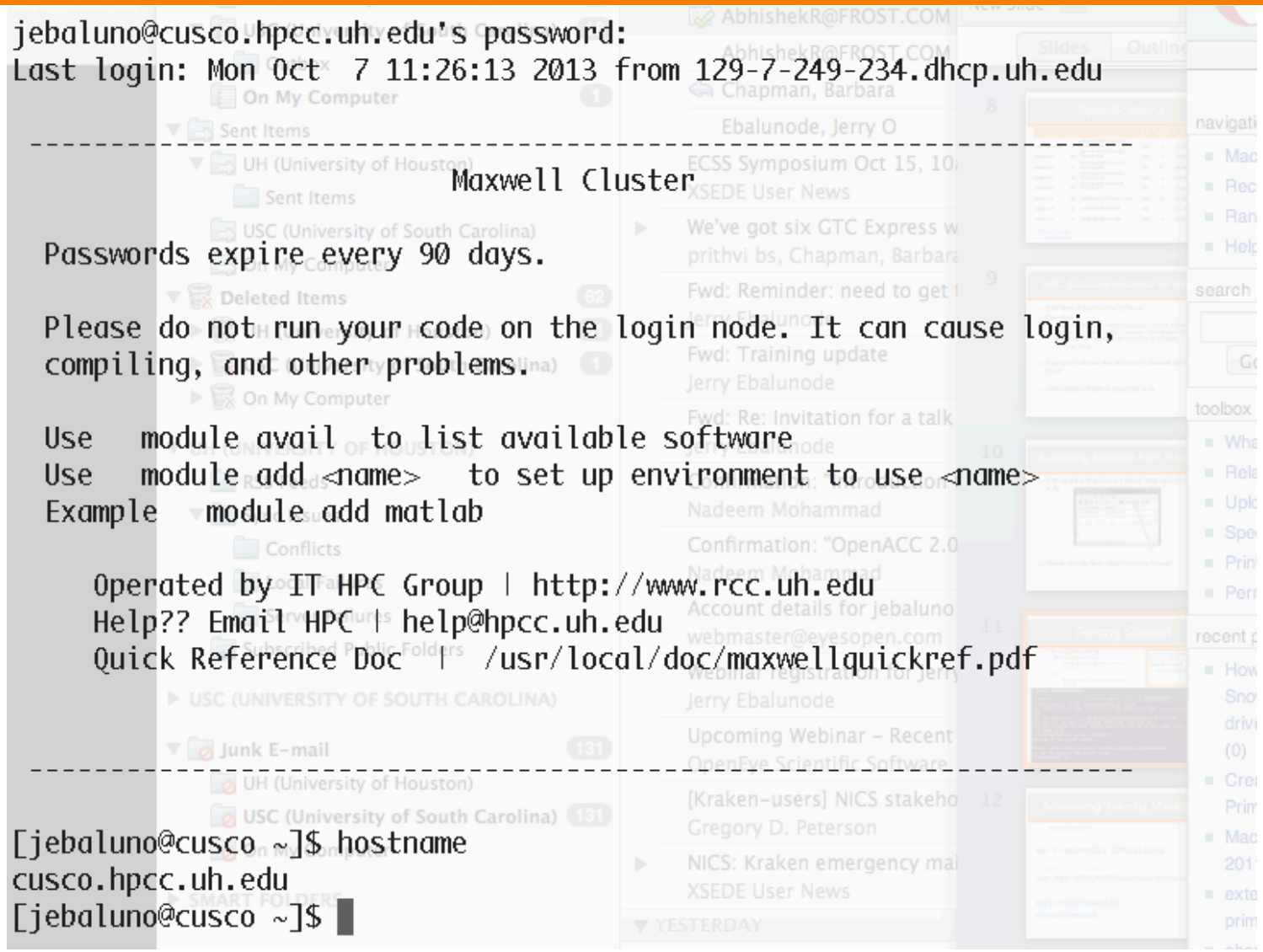
  - you might be prompted to accept finger print…
    - Just type “yes” followed be Enter key

  - For Windows users
    - Install Putty or any other compatible SSH client to connect
    - Putty URL = http://www.putty.org/

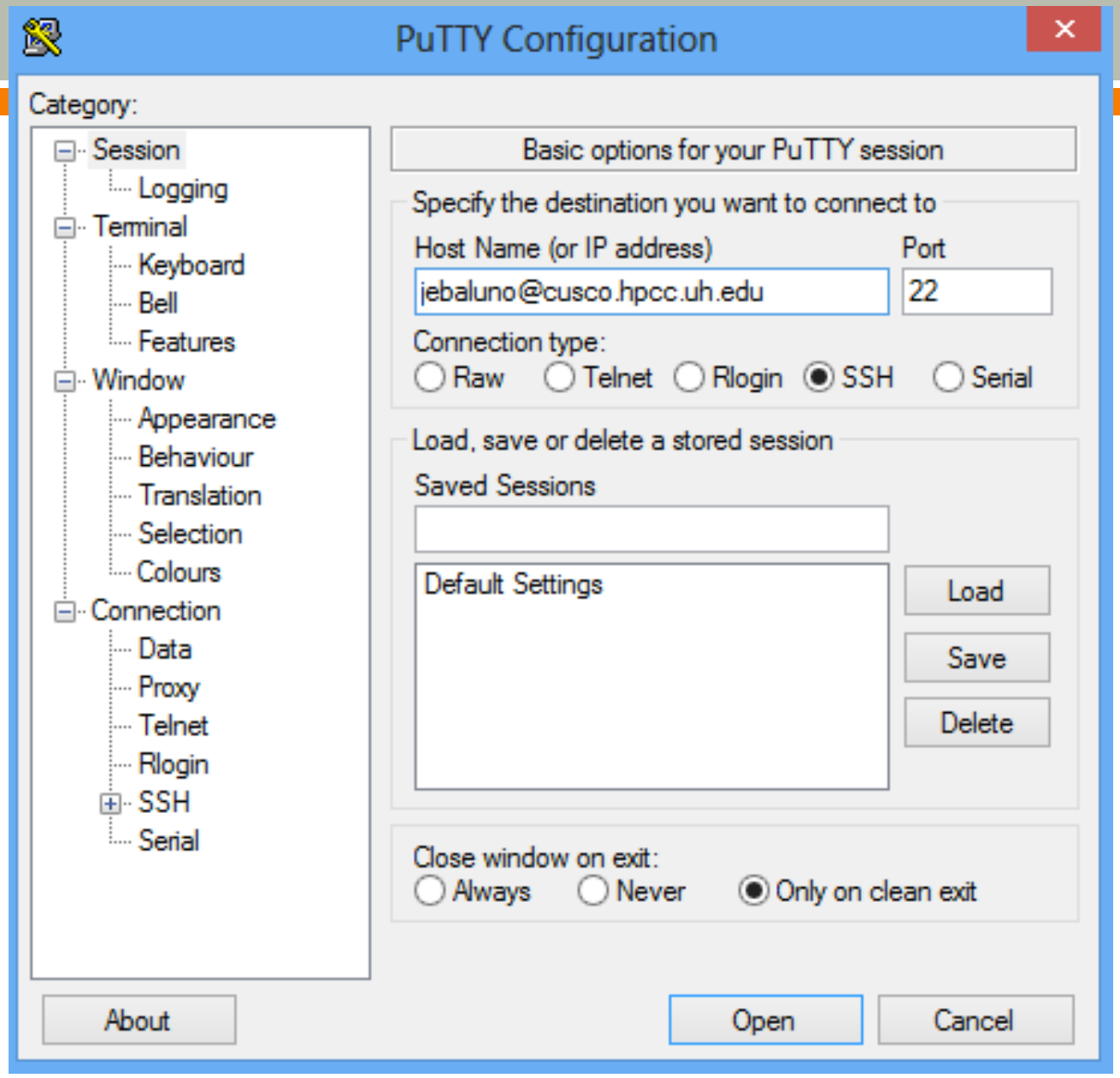
# Connecting via OpenSSH Client on UNIX based Systems

```
bash-4.2$ ssh  -Y    jebaluno@cusco.hpcc.uh.edu
The authenticity of host 'cusco.hpcc.uh.edu (129.7.54.9)' can't be established.
RSA key fingerprint is ac:3b:99:d0:6e:84:c0:d8:c9:16:60:d9:fe:e6:c7:71.
Are you sure you want to continue connecting (yes/no)? yes
Warning: Permanently added 'cusco.hpcc.uh.edu,129.7.54.9' (RSA) to the list of known hosts.

Use of University of Houston computing and network facilities requires
prior authorization.  Unauthorized access is prohibited.  Usage may be
subject to  security testing and monitoring.    Abuse   is  subject to
criminal   prosecution.   A  complete manual of  security policies and
procedures is   available at http://www.uh.edu/  in the Administration
directory.

jebaluno@cusco.hpcc.uh.edu's password:
```

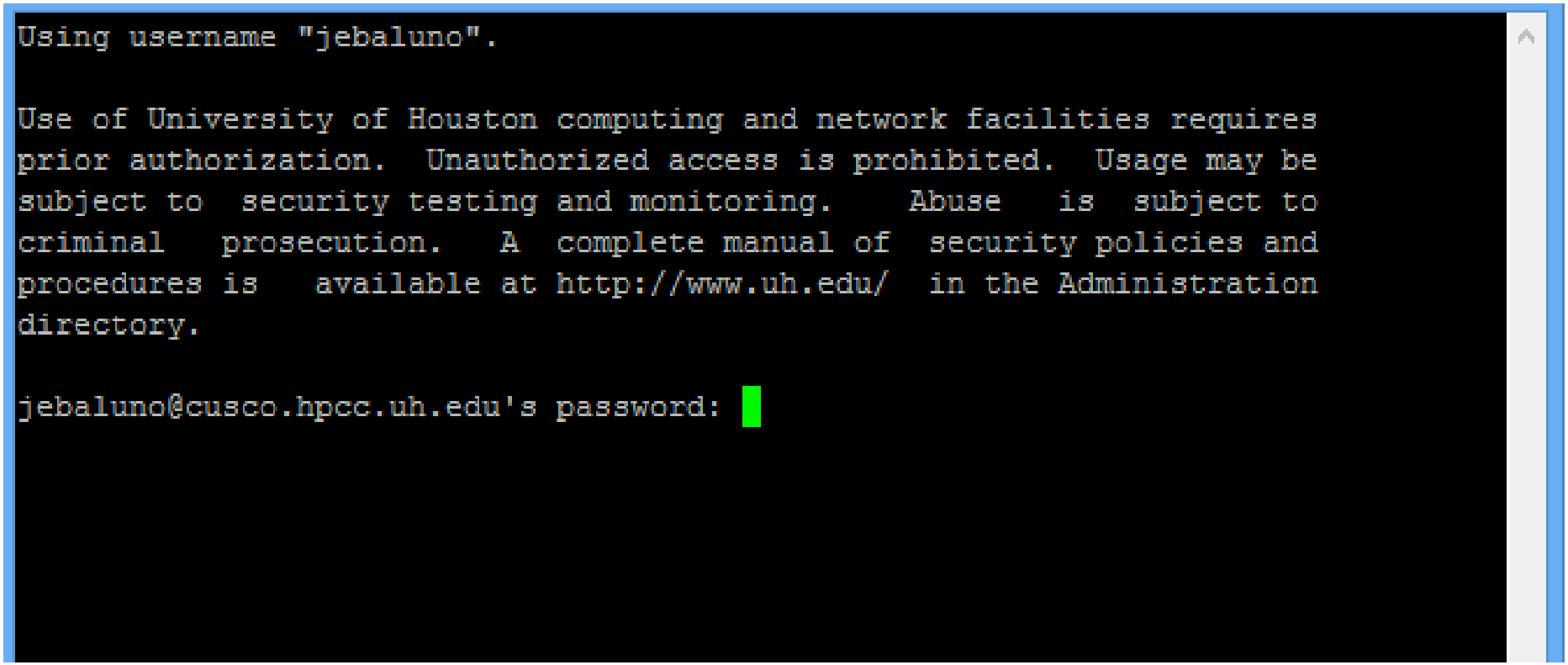
# Connecting via OpenSSH Client on UNIX based Systems



# Connecting via Putty  on Windows Systems



# Connecting via Putty on Windows Systems




Note: you will not be able see your password

# Accessing Tutorial Materials

First login into the cluster:

TYPE AND EXECUTE COMMANDS IN RED!!!

```
ssh  –Y  10.1.1.1
cd
cp /share/apps/tutorials/intro2maxwell.zip  ~

unzip intro2maxwell.zip

cd intro2maxwell
```

# The Maxwell Cluster

- Both Shared and Distributed systems
  - single core, multicore (multithreaded) and MPI jobs
- 434+ compute nodes (3756+ cpu cores)
  - http://baragon.hpcc.uh.edu/ganglia
  - 22+ Geforce GTX 570 Nvidia GPUs
  - 8+ Nvidia Tesla C2075 GPUs
- Operating system: Linux
  - Distribution: Redhat 6.5
- Gigabit network interconnect
- Data Storage:
  - Default: 10+ GB Home directory space per user
  - PI's could request for project directory space to host files needed for simulations
    - Justification might be required

# Specifications

| Name | Count | Processor Tyoe | Speed GHz | Total CPU Cores | Memory/ core | GPU |
|---|---|---|---|---|---|---|
| cusco (login node) | 1 | Quad-Core AMD Opteron(tm) Processor 2354 | 2.20 | 8 | 32+ GB | 0.00 |
| compute-X-Y | 183 | Quad-Core AMD Opteron(tm) Processor 2354 | 2.20 | 8 | 16+ GB | 0.00 |
| compute-X-Y | 25 | Quad-Core AMD Opteron(tm) Processor 8356 | 2.30 | 32 | 64+ GB | 0.00 |
| compute-X-Y | 39 | Quad-Core AMD Opteron(tm) Processor 2376 | 2.30 | 8 | 16.3+ GB | 0.00 |
| compute-X-Y | 112 | Dual Core AMD Opteron(tm) Processor 275 | 2.20 | 4 | 8+ GB | 0.00 |
| compute-X-Y | 28 | AMD Opteron(TM) Processor 6274 | 2.50 | 32 | 65+ GB | 0.00 |
| compute-X-Y | 22 | Intel(R) Xeon(R) CPU 5160 | 3.00 | 4 | 32+ GB | GeForce GTX 570 |
| compute-X-Y | 8 | Intel(R) Xeon(R) CPU 5160 | 3.00 | 4 | 32+ GB | Tesla C2075 |

X = Rack Number
Y = Node Number

# HPC Software Available on Maxwell

- Proprietary & Open-Source Software:
  - Examples:
    - Amber, Autodock, Bwa, NwChem, Espresso, Orca, R, Octave, Matlab, Gromacs, Lammps, NAMD, Turbomole, VASP, Rosetta, R, NAG, MKL , ASE, GSL, OpenMPI, Intel, Gnu and PGI compilers ….
    - and much more…
  - Proprietary software may be limited to licensed users e.g. Fluent, VASP
  - Open-source software is accessible to all

- PI could request for installation of additional software
  - PI's licensed propriety application can be installed too
- Software environment management via "modules"
  - Allows software to be accessed via an assigned module
  - Dynamic modification of a user's environment

# Computing Environment Setup Using Modules

- The module system is used to make software and related settings available easily
  - software environments can be **loaded** and **unloaded** dynamically

- To get a list of available software:
  `module avail`
  (also useful: module list)

- To clear-out all added modules:
  `module purge`

- To clear-out all specific modules:
  `module rm module1 module2 ....`

- To use specific software every time you log-in, place the
  module add command in your ~/.bashrc file i.e:
  `echo "module add intel openmpi" >> ~/.bashrc`

- Now add intel compiler and MPI runtime (Openmpi version to your environment)
  `module add openmpi`

# Compiling Programs

- CPU programs (compiled to execute on central processing unit)
  - Serial Programs
  - Parallel  Programs
- GPU programs (compiled to execute on graphics processing unit)
  - GPGPU Programs

# Compiling Programs: CPU Serial Program

- Example 1 Program in file: gethostname.c

```
#include <stdio.h>
#include <sys/utsname.h>
int main ( )
{
        struct utsname uts;
        uname (&uts);
        printf ("Process on node %s.\n",
        uts.nodename);
        return 0;
}
```

- To compile:
  - 1. choose compiler

    module add intel

    2. Compile

    icc gethostname.c –o gethostname.exe

# Compiling Programs: CPU Parallel Program

## Programs using Message Passing Interface (MPI)

- Example: 1 Program in file : gethostname.mpi.c

```
#include <stdio.h>
#include <sys/utsname.h>
#include <mpi.h>
int main (int argc, char *argv[]){
        struct utsname uts;
         int rank;
         MPI_Init (&argc, &argv);
         MPI_Comm_rank (MPI_COMM_WORLD, &rank);
         uname (&uts);
         printf ("Process %d on node %s.\n", rank, uts.nodename);
         MPI_Finalize ();
         return 0;
}
```

- To compile:
  - 1. choose compiler

    module add openmpi

    2. Compile

    mpicc gethostname.mpi.c -o gethostname.mpi.exe

# Compiling Programs: GPGPU Parallel Program

- Example 1 Program in file: sortkeys_basic_thrust.cu

```
#include <thrust/host_vector.h>
#include <thrust/device_vector.h>
#include <thrust/sort.h>
int main(void)
{      // generate 16 Million random numbers on the host
    thrust::host_vector<int> h_vec(1 << 24);
    thrust::generate(h_vec.begin(), h_vec.end(), rand);
    thrust::device_vector<int> d_vec= h_vec;  // transfer data to the device
    thrust::sort(d_vec.begin(), d_vec.end());  // sort data on the device (805 Mkeys/sec on GeForce GTX 480)
    thrust::copy(d_vec.begin(), d_vec.end(), h_vec.begin());  // transfer data back to host
    return 0;
}
```

- To compile:
  - 1. choose compiler

```
module  add  cuda-toolkit
```

2. Compile name = nvcc

```
nvcc  sortkeys_basic_thrust.cu   -o   sortkeys_basic_thrust.exe
```

# The Queue System (PBS)



- Portable Batch System (aka PBS) is the resource management service used on the Maxwell Cluster
- Enables you to make more efficient use of your time through scripting computational tasks
- PBS takes care of running these tasks and returning the results
- If the cluster is full, PBS holds your tasks and runs them when the resources are available
- PBS ensures fair sharing of cluster resources (policy enforcement)
  - PBS ensures optimal/efficient use of available resources

# PBS Commands

| Command(s) | Description |
|---|---|
| qstat | Check status of all jobs |
| qsub ./myjob | Submit batch jobs |
| qstat -u $USER | Check status of just your jobs |
| qsub -I | Submit an interactive job |
| qhold jobID<br>i.e. qhold 12345 | Put a job on hold (before it starts) |
| qrls jobID | Release a job from hold status |
| qdel #jobID | Delete a job, running or not |

# Using qsub with a Job Script

- Syntax/Format:
  - qsub [qsub params] [job script file]
- Examples:
  - qsub myjob

# PBS Batch Job Script File

- Very simple example:
- Serial job requesting 1 CPU, 2 GB memory, 60 hours of walltime

```
#!/bin/bash
#PBS   -N   jobname
#PBS   -l  mem=2gb,walltime=60:00:00
#PBS   -j  y

cd $PBS_O_WORKDIR

./my.program.exe [arguments for my program]
```

# Using Parallel Environment to Manage Memory and CPU Core Availability

- #PBS -l nodes=16:ppn=1 --use only one CPU core per node and use a total of 16 processes.
- #PBS -l nodes=8:ppn=2 --use only 2 CPU cores per node and use a total of 16 processes
- #PBS -l nodes=4:ppn=4 --use only 4 CPU cores per node and use a total of 16 processes
- #PBS -l nodes=8:ppn=8 --use only 8 CPU cores per node and use a total of 64 processes

# qsub Notification Parameters

- #PBS -M [e-mail address]
  - e-mail address can be a list of email addresses
  - separated by commas.

- #PBS -m bea or -m be or -m e
  - send an email when the job **b**egins, **e**nds, or is **a**borted.

Example:

```
#!/bin/bash
#PBS   -N   jobname
#PBS   -j  y
#PBS  -M   jerry@uh.edu
#PBS  -m   abe

cd $PBS_O_WORKDIR

./my.program.exe [arguments for my program]
```

# Sample Notification Email

**PBS JOB 3687125.cusco.hpcc.uh.edu**

root

Sent: Monday, October 7, 2013 at 6:27 AM

To: jebalunode@uh.edu

```
PBS Job Id: 3687125.cusco.hpcc.uh.edu
Job Name:   waterint-ACC-H17
Exec host:  compute-7-25/31+compute-7-25/30+compute-7-25/29+compute-7-25/28+compute-7-
25/27+compute-7-25/26+compute-7-25/25+compute-7-25/24+compute-7-25/23+compute-7-25/22+c
7-25/21+compute-7-25/20+compute-7-25/19+compute-7-25/18+compute-7-25/17+compute-7-
25/16+compute-7-25/15+compute-7-25/14+compute-7-25/13+compute-7-25/12+compute-7-25/11+c
7-25/10+compute-7-25/9+compute-7-25/8+compute-7-25/7+compute-7-25/6+compute-7-25/5+comp
25/4+compute-7-25/3+compute-7-25/2+compute-7-25/1+compute-7-25/0
Execution terminated
Exit_status=0
resources_used.cput=08:46:15
resources_used.mem=352472kb
resources_used.vmem=35667756kb
resources_used.walltime=00:33:07
```

# Handling Output Files

- When a job is started it takes its job name from the script file that was submitted.
  - The standard output and error output are sent to files named jobname.o987349 and jobname.e987349 (in your job directory )
- The following parameters modify this behavior:
  - -e [path] standard error output file.
  - -o [path] standard output file
  - -j y merge the error and standard output
- #PBS -N jobname name to be used for the job.

# Using qsub with a Job Script

- Syntax/Format:
  - **qsub [qsub params] [script file]**

- More examples on using parameters at the command line:
  - `qsub -N test1 myjob.sh`
  - `qsub -l nodes=2:ppn=2 -o test2.out -N test2 myjob.sh`
  - `qsub -l walltime=02:00:00,mem=4gb myjob.sh`
  - `qsub -l nodes=2:ppn=32,mem=64gb myjob.sh`
  - `qsub -q gpu -l nodes=1:ppn=4 my_gpu_job.sh`
- To see all available qsub options, just run qsub --help

# Using an Interactive Job

- Special kind of batch job
- Useful for debugging applications, short tests, or for computational steering


```
qsub -I
qsub -I -l  walltime=2:00:00
qsub -I -l walltime=2:00:00,nodes=2:ppn=8
qsub -I -l  walltime=2:00:00  -q gpu
```

# Job Queues

| Queue Name | Description |
|---|---|
| short | Queue to run short jobs ( =< 4 hours) |
| medium | Queue to run medium jobs ( 1 week allowed) |
| long | Queue to run very long jobs (2 weeks allowed) |
| gpu | Queue to run gpu jobs on GTX 570 equipped nodes (2 weeks allowed) |
| gpu-tesla | Queue to run gpu jobs on Testla C2075 equipped nodes (2 weeks allowed) |
| | |

USE “qstat -q” to probe the queues installed

Note gpu-tesla and gpu queue are not available/functional on the surrogate cluster

# PBS Script for Serial Program
## 1 CPU

- Example of a Serial Job Script

filename: job.gethostname.bash

```
#!/bin/bash
#PBS -N gethost
#PBS  -l mem=8gb,walltime=00:25:00
#PBS  -l nodes=1:ppn=1
#PBS  -M JohnDoe@gmail.com
#PBS -m bea

cd $PBS_O_WORKDIR

### Run gethostname

time   ./gethostname.exe
```

To submit the job run:
qsub job.gethostname.bash

# PBS Script for MPI Program

```
#!/bin/bash
#PBS -N gethostmpi
#PBS -l nodes=2:ppn=8,pmem=1gb
#PBS -S /bin/bash
#PBS -l walltime=00:05:00
#PBS -M monkeybrain@sc.edu
#PBS -m bea

cd $PBS_O_WORKDIR
##set up your environment
source /etc/profile.d/modules.sh

module add openmpi

mpirun –np  16 ./gethostname.mpi.exe > output.from.txt
```

See job filename:  job.gethostname.mpi.bash

To submit the  job run:
qsub job.gethostname.mpi.bash

# PBS Script for GPGPU Program

Give me a node with this kind of gpu

Example GPU Job Script

```
#!/bin/bash
#PBS -q gpu
#PBS -N sortrandomkeys
#PBS -l walltime=00:05:00,nodes=1:ppn=4
#PBS -M monkeybrain@gmail.com
#PBS –m bea

 cd $PBS_O_WORKDIR
##set up your environment
 source /etc/profile.d/modules.sh
module add cuda-toolkit
time    ./sortkeys_basic_thrust.exe
```

Load CUDA environment

See job filename: job.gpu.bash or job.gpu.sort.bash

# PBS Script for Executing Matlab script

## Using Proprietary Matlab runtime (sample I)

```
#!/bin/bash
#PBS -N matlabjob
#PBS -l nodes=1:ppn=1,pmem=1gb
#PBS -S /bin/bash
#PBS -l walltime=00:05:00

cd $PBS_O_WORKDIR

##set up your environment
source /etc/profile.d/modules.sh
module add matlab

matlab << EOF
a = 10;  b = 20; c = 30;
d = sqrt((a + b + c)/pi)
exit
EOF
```

See job filename: job.matlab1.bash

# PBS Script for Executing Matlab script

## Using Proprietary Matlab runtime (sample II)

```
#!/bin/bash
#PBS -N matlabjob
#PBS -S /bin/bash
#PBS -l walltime=20:05:00,pmem=1gb,nodes=1:ppn=4
#PBS -M monkeybrain@uh.edu
#PBS -m bea
##set up your environment
cd  $PBS_O_WORKDIR
source /etc/profile.d/modules.sh
module add matlab

## run matlab program compute pseudo inverse for  100  matrices of size 400x400
time    matlab    < matrix_inversion100_matlab.m
```

See job filename:  job.matlab2.bash

# PBS Script for Executing R script

```
#!/bin/bash
#PBS -N R-job
#PBS -S /bin/bash
#PBS -l walltime=0:05:00,pmem=1gb,nodes=1:ppn=1
#PBS -M monkeybrain@uh.edu
#PBS -m bea
##set up your environment
cd  $PBS_O_WORKDIR
source /etc/profile.d/modules.sh
module add R

## run R program
R –vanilla < sample.r
```

See job filename: job.R.bash

# PBS Script for NAMD2 Job Parallel MPI

```
#!/bin/bash
#PBS -l nodes=1:ppn=4
#PBS -l walltime=00:05:00
#PBS -l pmem=1gb
#PBS -N  namd
#PBS –V

cd $PBS_O_WORKDIR



module load namd

mpirun –v  namd2  apoa1.namd
```

See job filename:  job.namd.mpi.bash

# Killing Jobs

- One, or a few jobs:
  - qdel [jobID] [jobID] [jobID] …
- Kill all of your jobs:
  - qselect -u $USER | xargs qdel
- Kill all of your queued jobs:
  - qselect -u $USER -s Q | xargs qdel
- Kill all of your running jobs:
  - qselect -u $USER -s R | xargs qdel

# Try An Example Job

- Several job scripts files available to use for practice

- Edit job.**.bash files as needed, then run the job:
  - you can use gedit

- submit the job(s) i.e.
  - qsub job.**.bash
  - where ** represents the job pattern you are going to submit

job.gethostname.bash job.gethostname.mpi.bash job.gpu.bash job.matlab.bash job.namd.bash

# Homework

- Examine the  job files and fix potential glitches
- Submit the jobs.
- Record the runtime or execution time and send me these timings as well as the job log files

# Maxwell User Support

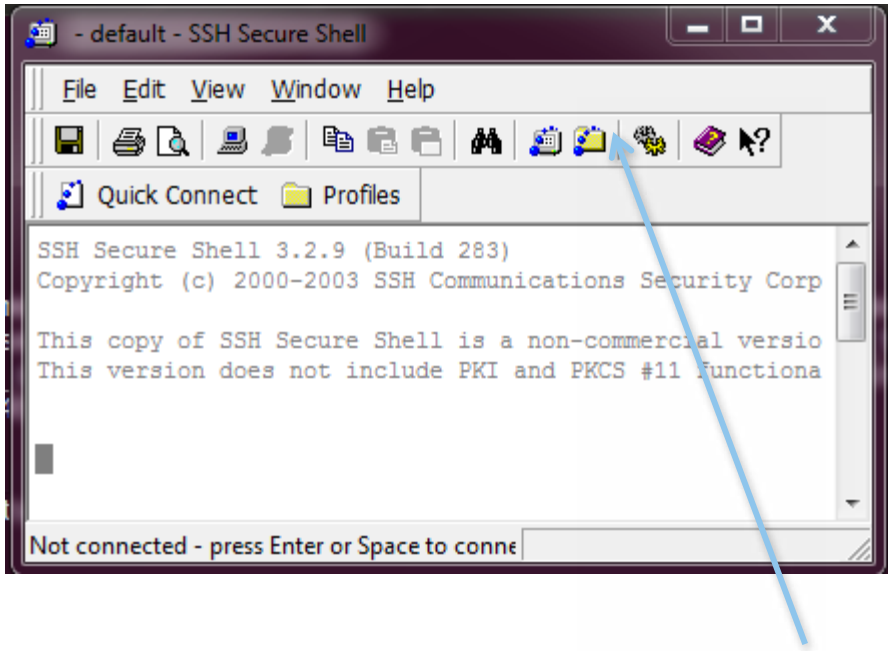
- Computational scientists are available for
  - consultation and training
  - We can help with porting  your homebrew code and domain applications to run on the cluster
  - We can also help with developing proposals that involve use of HPC (i.e. make use of Maxwell resources).
- "Help" requests or technical questions can be submitted to the Maxwell admin staff and anyone who can help will respond.
- Visit ➔ http://support.cacds.uh.edu
  - To Open A Support Ticket

# Acknowledgements


- Center for Advanced Computation and Data Systems
  - Tony Curtis
  - Barbara Chapman

# Accessing Maxwell from Windows

- Command-line interface, any Secure Shell (ssh) client  i.e. putty



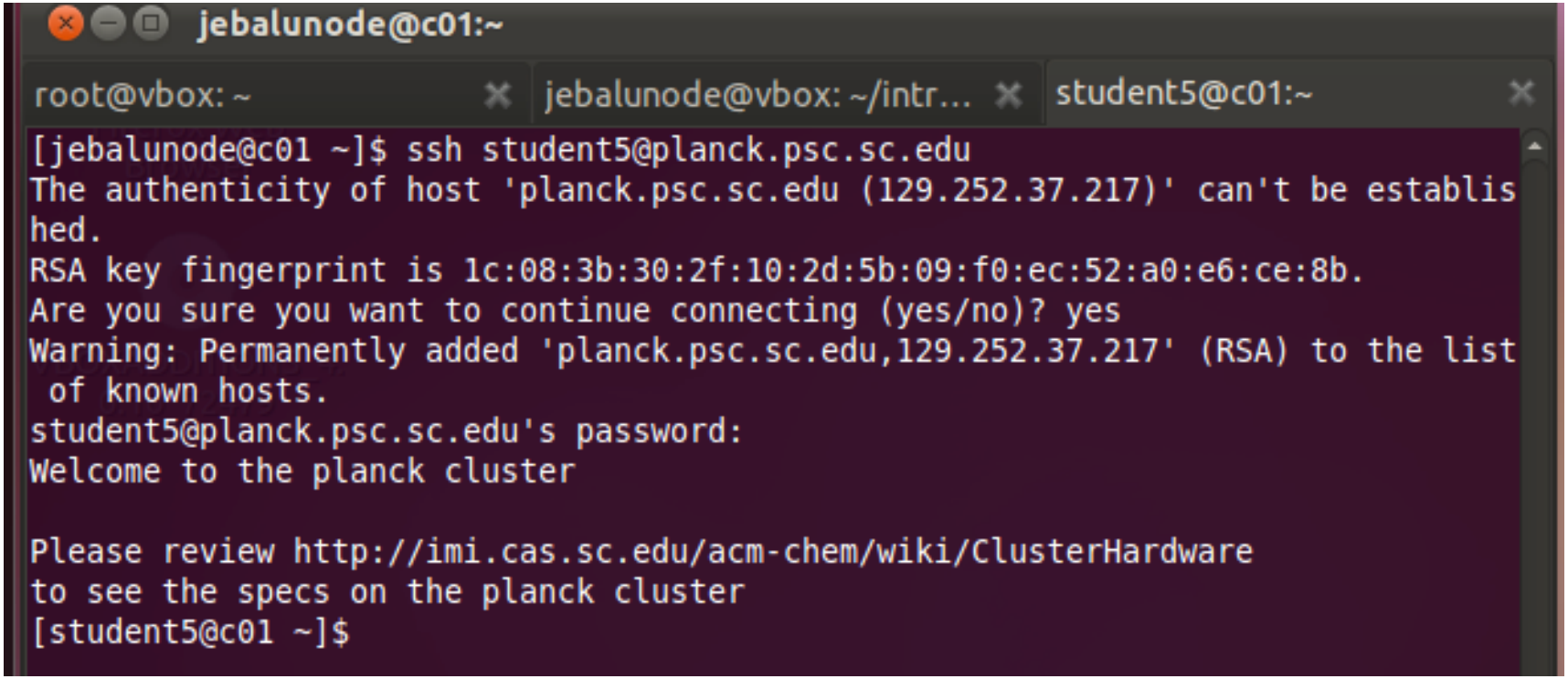

- Transfer files to/from using FileZilla (or Winscp)

# Getting Started

- Open up a gnome terminal
  - Multiple ways to do this:
    - Click on the gnome-terminal icon on the top panel
  - Or
    - On mouse right click and select terminal and click

User name = student0XX
where XX = 1 → 48
Password = provided

- ssh [username]@208.117.189.1



# Serial Task Management

Use **pbsdsh** to distribute groups of serial tasks within the PBS environment.

Within your “master” script (the one you submit with qsub):

```
pbsdsh -v $PBS_O_WORKDIR/subscript.bash
```

This runs subscript.bash on each core in your allocation:

```
#!/bin/bash
cd $PBS_O_WORKDIR
myexe < ${PBS_VNODENUM}.inp > ${PBS_VNODENUM}.out
```