Research Computing Orientation for UF Courses

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HiPerGator

The University of Florida Supercomputer for Research

- 16,384 cores (total of ~21,000 today)
- Infiniband interconnect
- 2.1PB fast, high-availability, storage

Course use of HiPerGator

- Coursework should be done through course account
  - All course accounts are deleted at the end of the semester
  - http://www.rc.ufl.edu/help/account-request/
- Course is allocated 32-cores
  - Design projects with this in mind
  - Time your work with this in mind
- Support requests should go through course TA
  - If TA cannot solve the issue, the TA should open support requests

Galaxy: Data intensive biology *for everyone*

- Accessible, reproducible, transparent computational biology
- galaxy.rc.ufl.edu

Tools

ssh client to connect to hipergator.rc.ufl.edu

e.g.: Terminal, PuTTY

SFTP client to move files to/from your computer

e.g.: Cyberduck, FileZilla

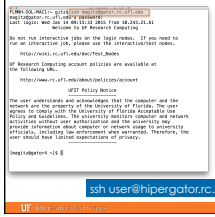
Text editor to prepare files

Especially on Windows, be sure to convert DOS line breaks to Unix, and don't use *Word*

Both have SFTP built in

e.g.: TextWrangler, Notepad++

SSH Clients

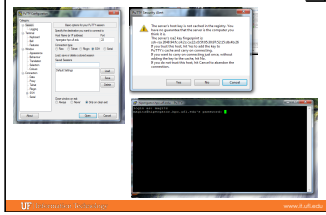


Mac/Linux: Terminal

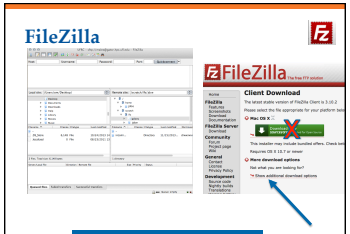
Windows: PuTTY

ssh user@hipergator.rc.ufl.edu

PuTTY



FileZilla

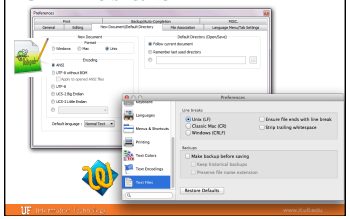


Tutorial at: http://wiki.rc.ufl.edu/doc/FileZilla

Text Editors

- ***Not*** Microsoft Word or other word processor
- Contextual coloring
- Built-in SFTP Client
- Regular expression find/replace
- **Unix line breaks**

Unix line breaks



Storage

- /home/$USER
  - 20GB limit
  - scripts, code, small data
  - Do NOT use for job input/output
- /scratch/lfs/$USER
  - 2TB limit per group
  - ALL input/output from jobs should go here

- All storage systems are for research and coursework data only
- Nothing is backed up
- All course accounts are deleted at the end of the semester

Cluster basics

User interaction

Login server (Head node)

Scheduler

Tell the scheduler what you want to do

Compute resources

Your job runs on the cluster

Development servers

- Do not run applications on the login servers
  - Account will be suspended

User interaction

Login

Do not run interactive jobs on the login nodes.

UF HPC Center Account Policies can be found here:

http://www.hpc.ufl.edu/about/policies/account

[magic@gator1 ~]$

- Use the development servers for testing and interactive use:
  - `ssh dev1` or `ssh dev2`

Scheduling a job

- Need to tell scheduler what you want to do
  - **How many CPUs** you want and how you want them grouped
  - **How much RAM** your job will use
  - **How long** your job will run
  - The commands that will be run

Scheduler

Tell the scheduler what you want to do

UF Research Computing

- Ordinary Shell Script

```
#!/bin/bash

date
module load test_app
test_app -i file.txt
```

Read the manual for your application

Commands typed on the command line can be put in a script.

Research Computing

- Submission Script

```
#!/bin/bash
#PBS -N My_Job_Name
#PBS -M Joe_Shmoe@ufl.edu
#PBS -m abe
#PBS -o My_Job_Name.log
#PBS -e My_job_Name.err
#PBS -l nodes=1:ppn=1
#PBS -l pmem=900mb
#PBS -l walltime=00:05:00

cd $PBS_O_WORKDIR
date
module load test_app
test_app -i file.txt
```

Optional Directives

Required Directives

Scheduler

Tell the scheduler what you want to do

Nodes and processors

Single processor apps:

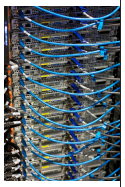
`#PBS -l nodes=1:ppn=1`

Threaded (& MPI) apps:

`#PBS -l nodes=1:ppn=8`

MPI apps:

`#PBS -l nodes=2:ppn=64`



HiPerGator

The University of Florida Supercomputer for Research

- ***Sharing Resources:***
  - Remember courses are limited to 32 cores total
  - `showq -w group=gms6001`

RAM

`#PBS -l pmem=900mb`

- Lots to consider, but do your best at estimating RAM needed for job
- Over about 4GB of RAM, "costs" toward CPU allocation

Wasted RAM leads to idle CPUs and low job throughput

End-of-job emails:

```
#PBS -M Joe_Shmoe@ufl.edu
#PBS -m abe
```

```
PBS Job Id: 358634.moab.ufhpc
Job Name:   NR.25.nex
Exec host:  c7a-s1/60
Execution terminated
Exit_status=0
resources_used.cput=07:16:09
resources_used.mem=251348kb
resources_used.vmem=318916kb
resources_used.walltime=07:16:52
```

RAM– bigmem queue

- For jobs asking for over 16GB per core (pmem)
- `#PBS -q bigmem`
- 1TB node

Walltime

`#PBS -l walltime=00:50:00`

- Fairly straight forward
- As with all resource requests, accuracy helps ensure ***your*** jobs and all other jobs will run sooner

	Maximum	Short	Long
Courses	7 days	<12 hrs	3 days

Scheduler

Tell the scheduler what you want to do

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- Job Management
  - `qsub <file_name>`: job submission
  - `qstat -u <user>`: check queue status
  - `showq -r -u <user>`: shows job efficiency
  - `qdel <JOB_ID>`: job deletion
  - `checkjob -v <job number>` (shows PE value)
  - `pbs_info -f my_job.pbs` (get job PE and group resources before submitting a job)

So what is this "module" thing?

- **lmod**—Implementation of Environment Modules developed at TACC
- Allows easy management of user's environment

Lmod: Environmental Modules System

The standard way

```
PATH=$PATH:/some/long/path/to/application
export $PATH
LD_LIBRARY_PATH=$LD_LIBRARY_PATH:/long/path/to/
place/I/probably/cant/find
export $LD_LIBRARY_PATH
```

- Need to track down paths to applications, libraries, etc.
- Multiple compilers, and MPI implementations
- Manage dependencies
- Multiple versions of apps

Module discovery

- `module spider`
  - List everything
- `module spider cl`
  - List applications that have cl in name
- `module spider amber/12`
  - List details about this version of AMBER
- `module key molecular`
  - Keyword search for applications

Multiple versions

```
[magitz@submit1 ~]$ module spider gaussian
Rebuilding cache file, please wait ... done

-----------------------------------------------------------------------------
gaussian:
-----------------------------------------------------------------------------
  Description:
    A software for electronic structure modeling

  Versions:
     gaussian/e01
     gaussian/g03
     gaussian/g09
-----------------------------------------------------------------------------
To find detailed information about gaussian please enter the full name.
For example:

  $ module spider gaussian/g09
-----------------------------------------------------------------------------
```


Multiple variants of a version

```
[magitz@submit1 ~]$ module spider mrbayes/3.2.1
Rebuilding cache file, please wait ... Done
-----------------------------------------------------------------------------
mrbayes: mrbayes/3.2.1

-----------------------------------------------------------------------------
Description:
      Bayesian inference of phylogeny

    This module can be loaded directly: module load
mrbayes/3.2.1

    Additional variants of this module can also be loaded
after the loading the following modules:

      intel/2012, openmpi/1.6
```


Module loading

- `module load raxml`
- `module load intel raxml`
- `module load intel openmpi raxml`
- `module load intel/12 openmpi/1.6 raxml/3.2`
- `module unload raxml`

Training sessions

- Thursdays@ 12:50 and online http://wiki.hpc.ufl.edu/doc/Training

UF Research Computing

- Help and Support (Continued)
  - http://wiki.rc.ufl.edu
    - Documents on hardware and software resources
    - Various user guides
    - Many sample submission scripts
  - http://rc.ufl.edu/support
    - Frequently Asked Questions
    - Account set up and maintenance