

# 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

# Tools

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



e.g.: Terminal, PuTTY

SFTP client to move files  
to / from your computer

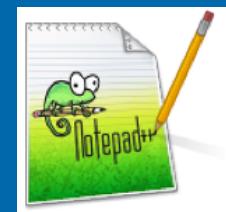


e.g.: Cyberduck, FileZilla

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

```
FLMNH-SOL-MAC1:~ gitz$ ssh magitz@gator.rc.ufl.edu
magitz@gator.rc.ufl.edu's password:
Last login: Wed Jan 14 09:15:33 2015 from 10.243.21.61
        Welcome to UF Research Computing

Do not run interactive jobs on the login nodes. If you need to
run an interactive job, please use the interactive/test nodes.

http://wiki.rc.ufl.edu/doc/Test\_Nodes

UF Research Computing account policies are available at
the following URL.

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

UFIT Policy Notice
-----
The user understands and acknowledges that the computer and the
network are the property of the University of Florida. The user
agrees to comply with the University of Florida Acceptable Use
Policy and Guidelines. The university monitors computer and network
activities without user authorization and the university may
provide information about computer or network usage to university
officials, including law enforcement when warranted. Therefore, the
user should have limited expectations of privacy.
-----
[magitz@gator4 ~]$
```



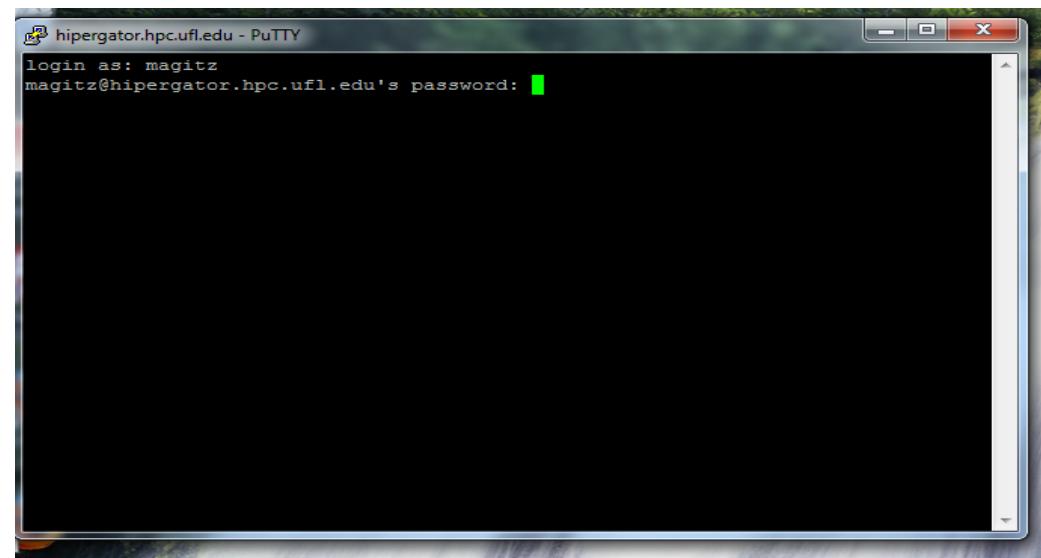
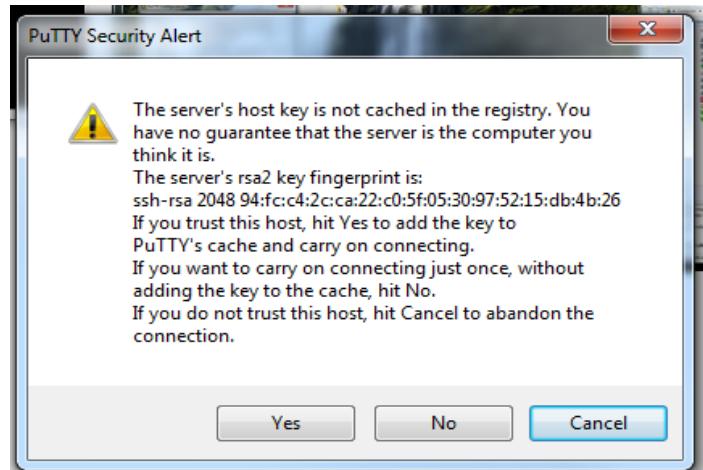
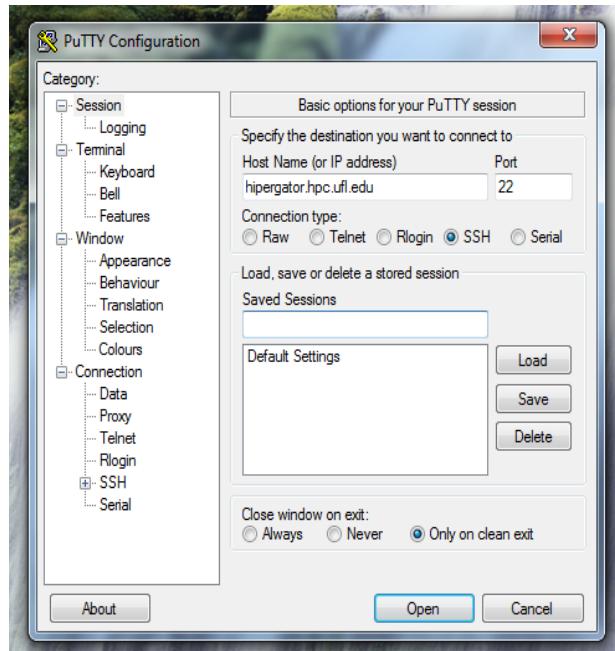
Mac/Linux: Terminal



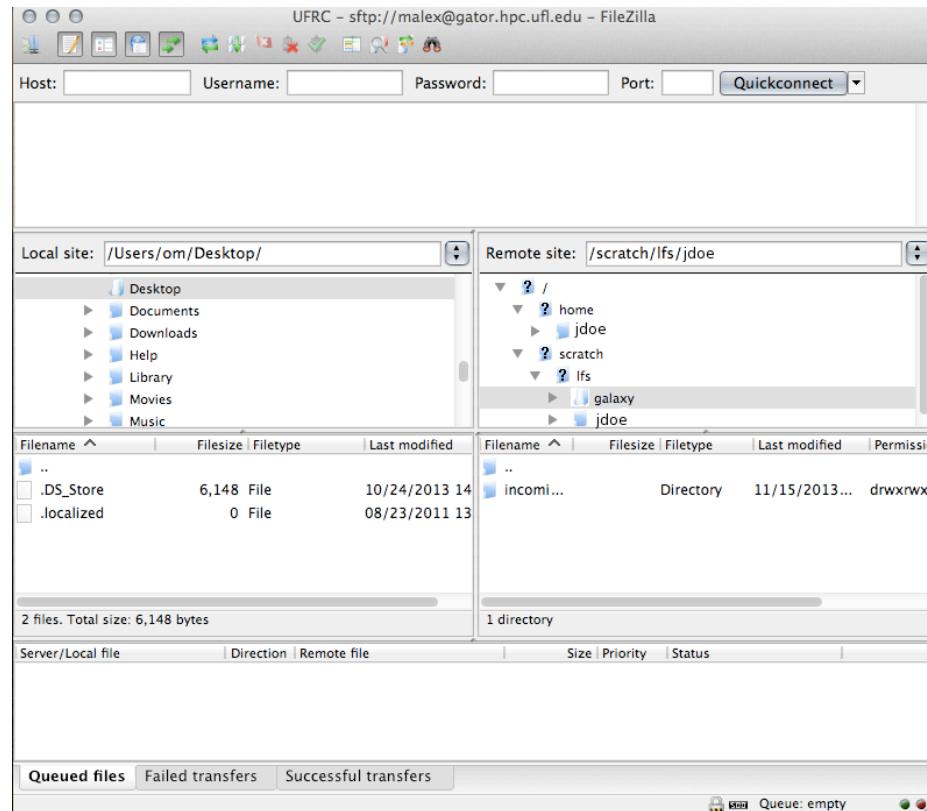
Windows: PuTTY

ssh user@hipergator.rc.ufl.edu

# PuTTY



# FileZilla



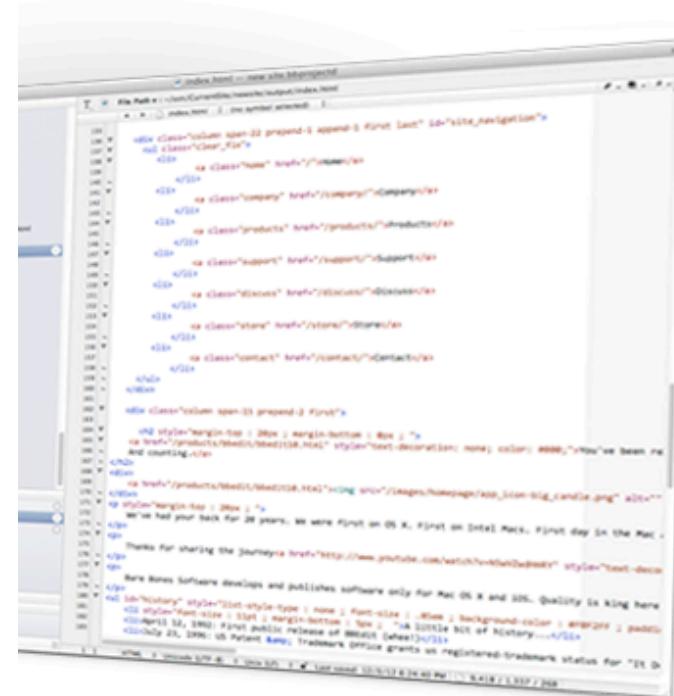
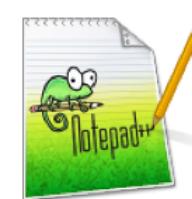
The screenshot shows the official FileZilla Client download page. The header features the FileZilla logo and the text "The free FTP solution". On the left, a sidebar lists links: Home, FileZilla (Features, Screenshots, Download, Documentation), FileZilla Server (Download), Community (Forum, Project page, Wiki), General (Contact, License, Privacy Policy), and Development (Source code, Nightly builds, Translations). The main content area is titled "Client Download" and states "The latest stable version of FileZilla Client is 3.10.2". It asks users to "Please select the file appropriate for your platform below". A section for "Mac OS X" includes a download button with a green arrow icon and the text "Download Now" with a note "sourceforge.net is not affiliated with or endorsed by Open Source". A large red "X" is overlaid on this button. Below it, text says "This installer may include bundled offers. Check below" and "Requires OS X 10.7 or newer". A link "More download options" is shown with a blue arrow pointing towards it from the bottom right.

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

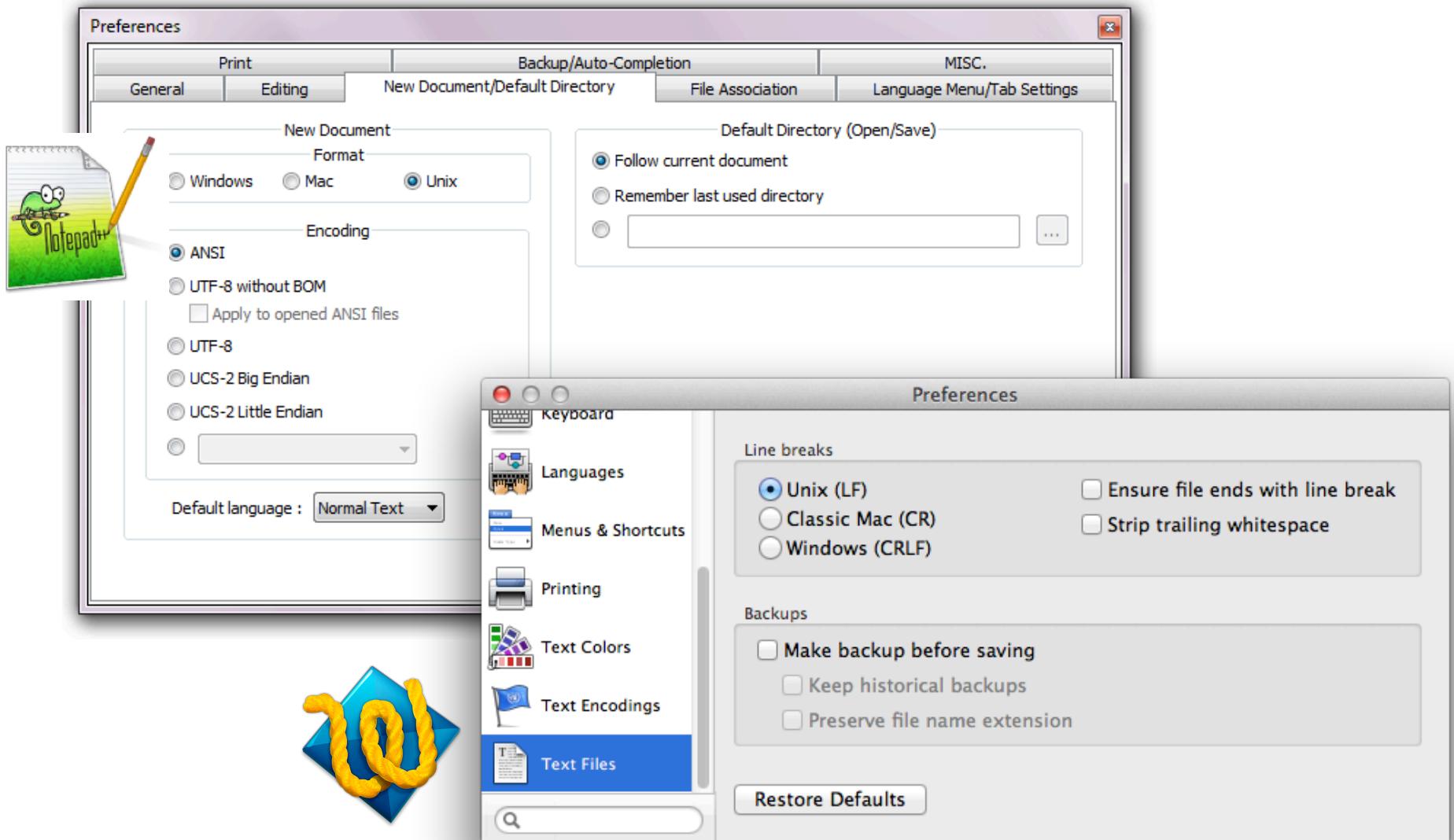
# Text Editors

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

- ▶ **Unix line breaks**



# Unix line breaks



# Storage

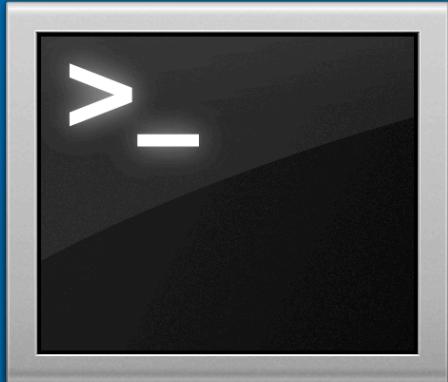
- ▶ /home/\$USER
  - 20GB limit
  - scripts, code, small data
  - Do NOT use for job input/output
  
- ▶ /scratch/lfs/\$USER
  - 2TB limit per group
  - ALL input/output from jobs should go here



- 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

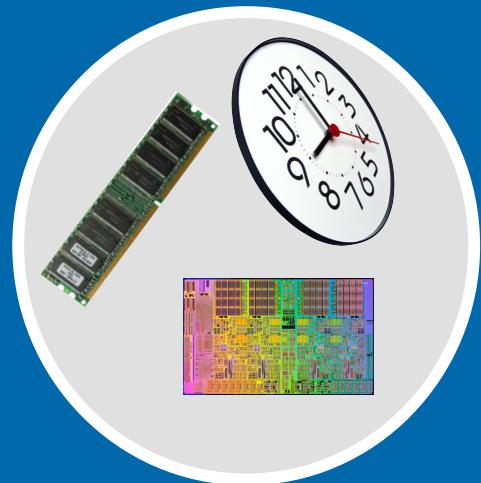
# Cluster basics

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



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  
[magitz@gator1 ~]$
```

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

# GUI Servers

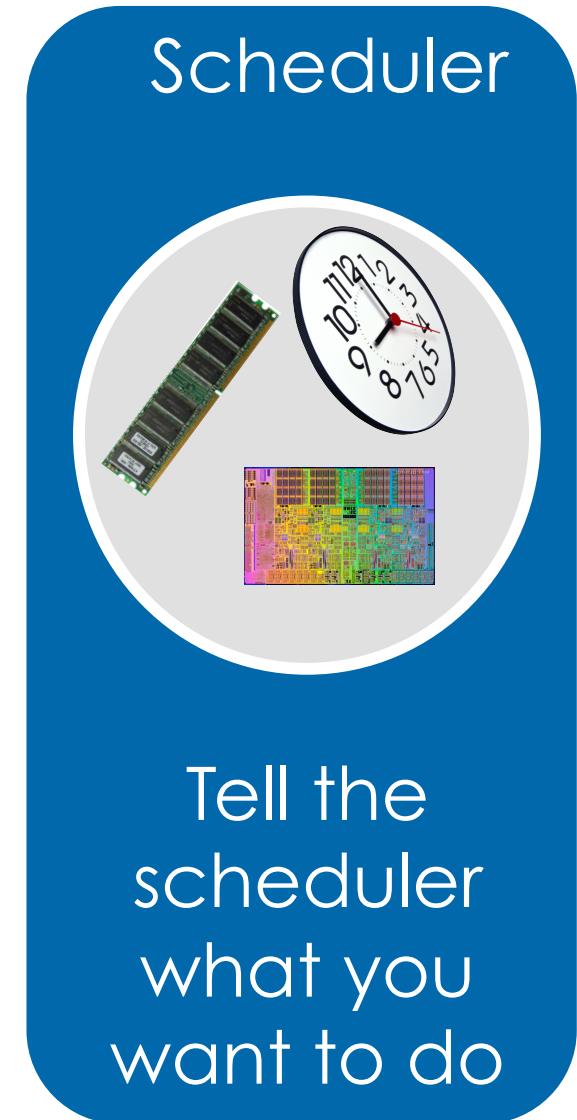
- ▶ gui1.rc.ufl.edu or gui.rc.ufl.edu  
ssh -Y user@gui1.rc.ufl.edu

## On Windows, use MobaXterm or PuTTY w/ Xming

- ▶ dev1 and dev2  
ssh -Y user@gator.rc.ufl.edu  
ssh -Y dev1
- ▶ Interactive job  
ssh -Y user@gator.rc.ufl.edu  
qsub -X -I -l nodes=1:ppn=4,pmem=1gb, walltime=1:00:00

# 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



# UF Research Computing

## ▶ Ordinary Shell Script

```
#!/bin/bash

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

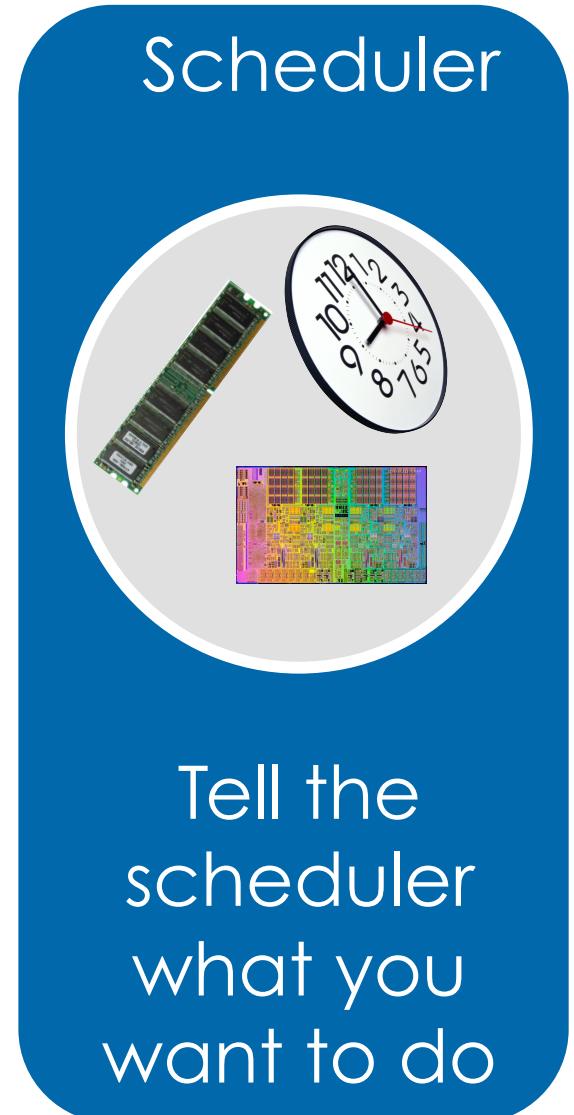
Read the manual  
for your application

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

# Research Computing

## ▶ Submission Script

```
#!/bin/bash  
{  
    Required Directives  
    #PBS -N My_Job_Name  
    #PBS -M Joe_Shmoef@ufl.edu  
    #PBS -m abe  
    #PBS -o My_Job_Name.log  
    #PBS -e My_job_Name.err  
}  
{  
    Optional Directives  
    #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
```



# Nodes and processors

Single processor apps:

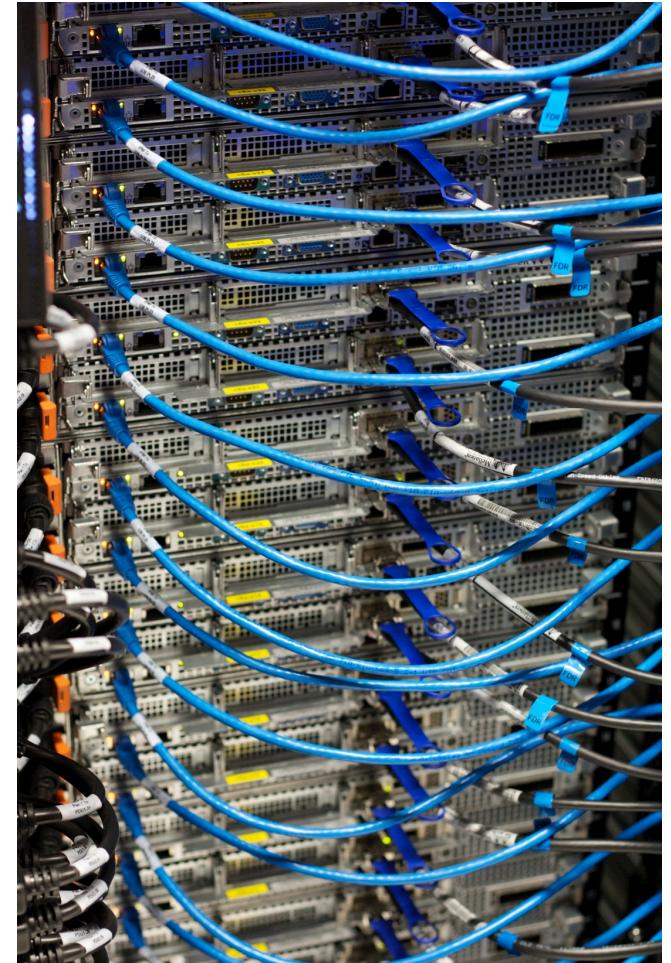
```
#PBS -l nodes=1:ppn=1
```

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=phz5155`



# 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_Shmoef@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

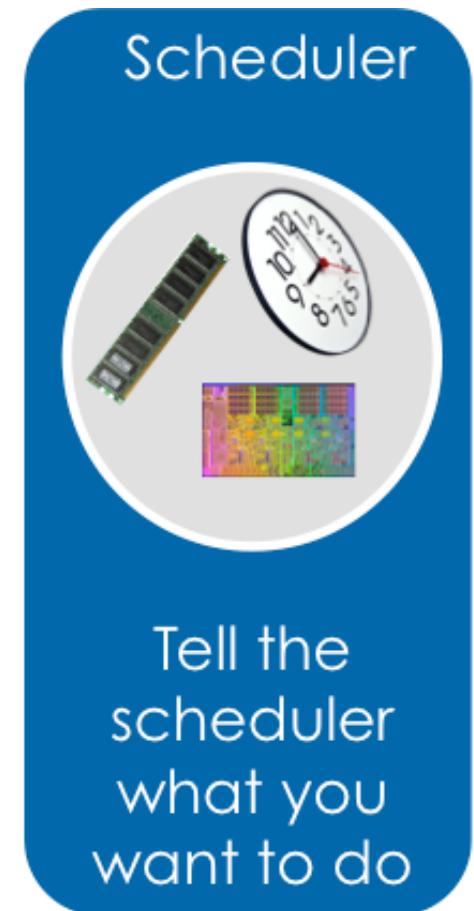


# Walltime

**#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



# UF Research Computing

## ▶ 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



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## **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>

## Training Resources [\[edit\]](#)

The most recent set of slides, handouts and recordings from training sessions are listed below.

- **UF Research Computing: An Introduction and Getting Started**

- Download the slides from the presentation.



- View a recording of the session

- **An Introduction to the Linux Command Line**

- Download the slides from the presentation.
    - Download the handout with the exercises
    - Download an example Linux cheat sheet.



- View a recording of the session

# 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

