Computational Physics

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Department of Physics
Florida State University
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http://hadron.physics.fsu.edu/~eugenio/comphy/

Syllabus

Also available on the course website

- Meeting Times:

Tues & Thur 315B MCH 2:00pm – 3:15pm
format: lecture + lab

- Office Hrs:

205 Keen Wednesday 2:30 – 4:30

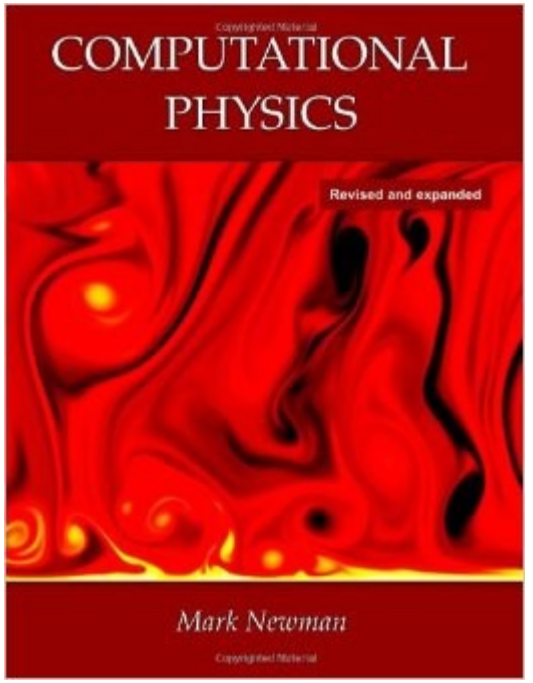
Additional times available upon request

Course Resources

- Books

Mark Newman *Computational Physics,*
Revised and expanded

COMPUTATIONAL PHYSICS
with Python



- Course Website

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Goals

- **Introduce Modern Scientific Programing**
  - This includes numerical analysis, object-oriented programing, scientific graphics, software engineering, and modeling advanced physical systems.

Course Overview

- Intro to Linux/Unix & Unix programing tools.
- Programing in Python and OOP
- Plotting & Visualization packages and Web Resources
- Numerical Limits in Computing
- Finding Roots of Equations
- Code Management Techniques
- Numerical Differentiation & Integration
- Multidimensional & Monte Carlo Integration
- Analyzing Data Sets
- Introduction to Batch & Parallel Programing

Grading

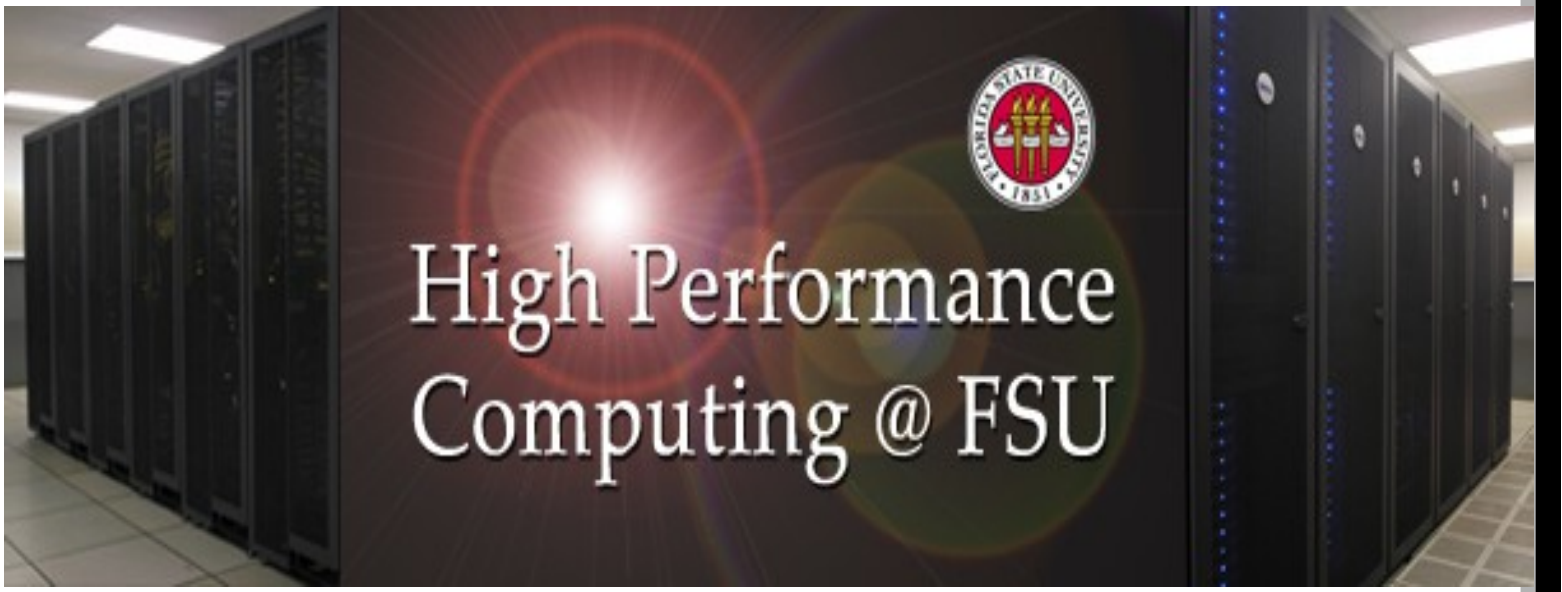
- Students will be graded based upon the successful completion of in-class participation, assigned in-class/homework exercises, & computational exams/projects.
  - Exercises (50%) & Participation (10%)
    - Exercise problems typically from the course text.
  - Take-home(or in class) project exams (40%)
    - Programing challenges where collaboration is not allowed.

There is no final exam in this course.

Programing Language

- The Programing Language for this course is Python.
  - ~1/3 of this course will focus on Python programing basics and following programming standards

Computing Resources



- FSU HPC
  High Performance Computing
  - hpc-login.rcc.fsu.edu
    - linux login server
    - Benchmarked at 265 teraflops

The FSU HPC system is comprised of 12,492 x86 64-bit compute cores linked together by low-latency infiniband networks for MPI communication.

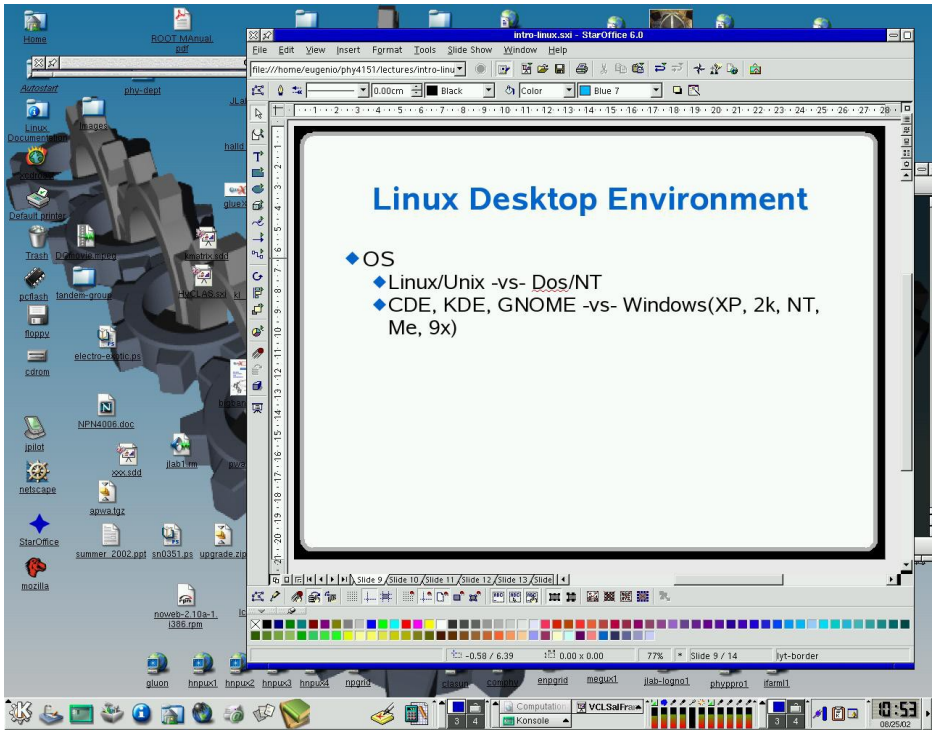
Any Questions so far?

Brief Introduction to Linux/Unix

- The Operating System
  - Kernel
  - Shell
  - Programs & Commands
- The File System
  - Paths
  - Tree Structure
  - Directories, Files, and Inodes
- Desktop Environments

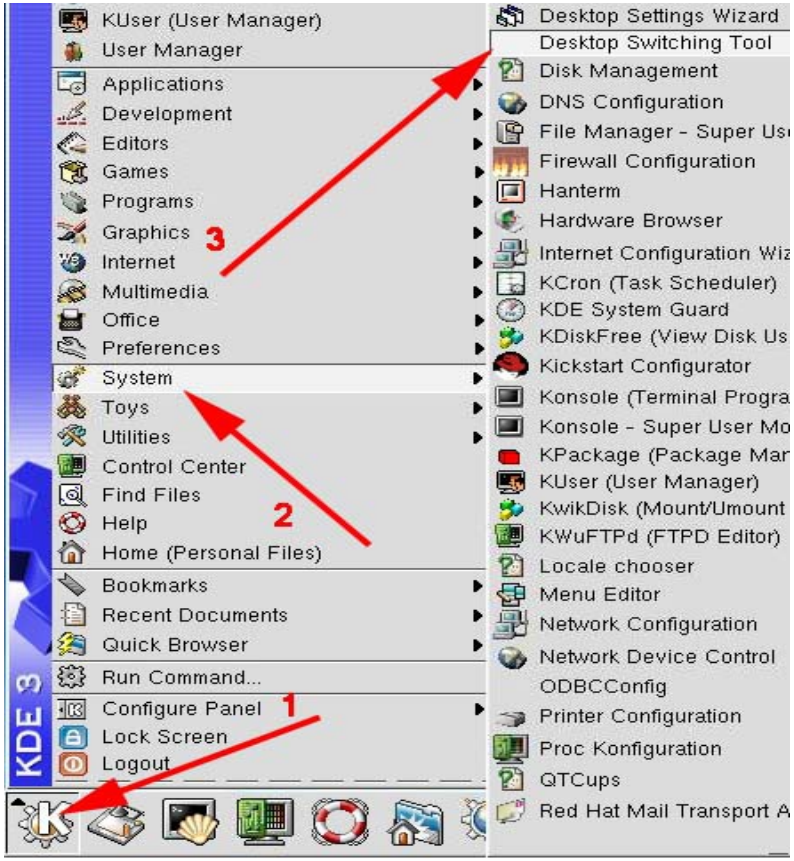
Unix Desktop Environment

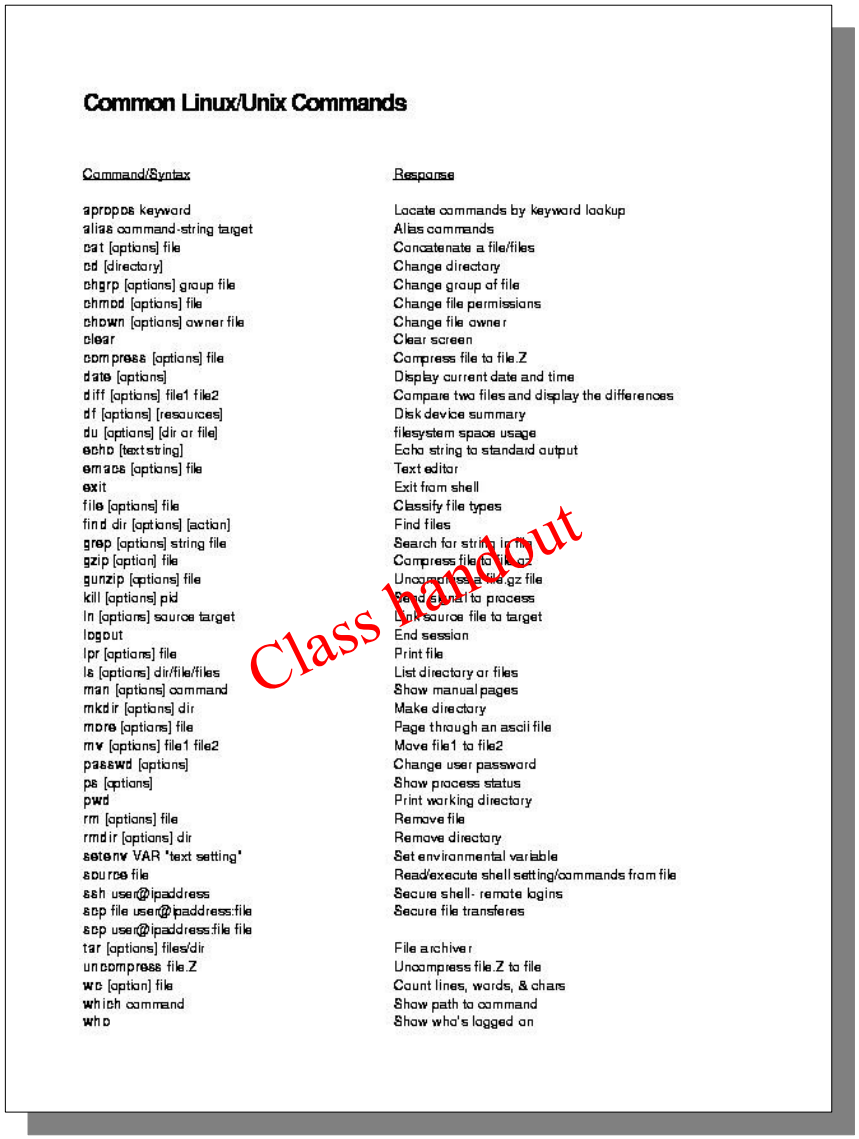
- OS
  - Linux/Unix ↔ DOS/Windows NT
- Desktop->Development Environments
  - KDE, GNOME ↔ Windows 10, macOS, iOS, Android



Programs & Shell Commands

- Common commands
- Programing tools





Common Linux/Unix Commands

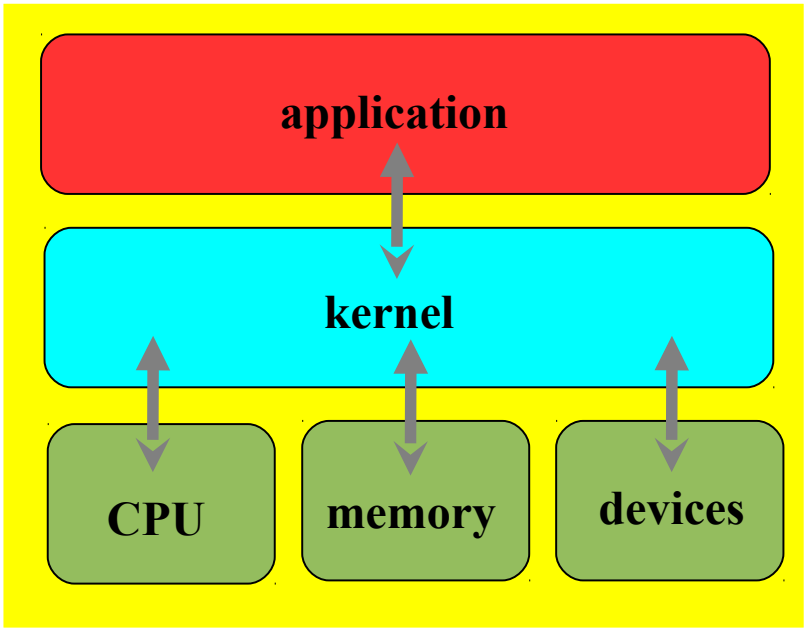
Command/Syntax	Response
apropos keyword	Locate commands by keyword lookup
alias command-string target	Alias commands
cat [options] file	Concatenate a file/files
cd [directory]	Change directory
chgrp [options] group file	Change group of file
chmod [options] file	Change file permissions
chown [options] owner file	Change file owner
clear	Clear screen
compress [options] file	Compress file to file.Z
date [options]	Display current date and time
diff [options] file1 file2	Compare two files and display the differences
df [options] [resources]	Disk device summary
du [options] [dir or file]	filesystem space usage
echo [text string]	Echo string to standard output
emacs [options] file	Text editor
exit	Exit from shell
file [options] file	Classify file types
find dir [options] [action]	Find files
grep [options] string file	Search for string in file
gzip [option] file	Compress file to file.gz
gunzip [options] file	Uncompress a file.gz file
kill [options] pid	Send signal to process
ln [options] source target	Link source file to target
logout	End session
lpr [options] file	Print file
ls [options] dir/file/files	List directory or files
man [options] command	Show manual pages
mkdir [options] dir	Make directory
more [options] file	Page through an ascii file
mv [options] file1 file2	Move file1 to file2
passwd [options]	Change user password
ps [options]	Show process status
pwd	Print working directory
rm [options] file	Remove file
rmdir [options] dir	Remove directory
setenv VAR "text setting"	Set environmental variable
source file	Read/execute shell setting/commands from file
ssh user@ipaddress	Secure shell- remote logins
scp file user@ipaddress:file	Secure file transferes
scp user@ipaddress:file file	
tar [options] files/dir	File archiver
uncompress file.Z	Uncompress file.Z to file
wc [option] file	Count lines, words, & chars
which command	Show path to command
who	Show who's logged on

Class handout

The Operating System

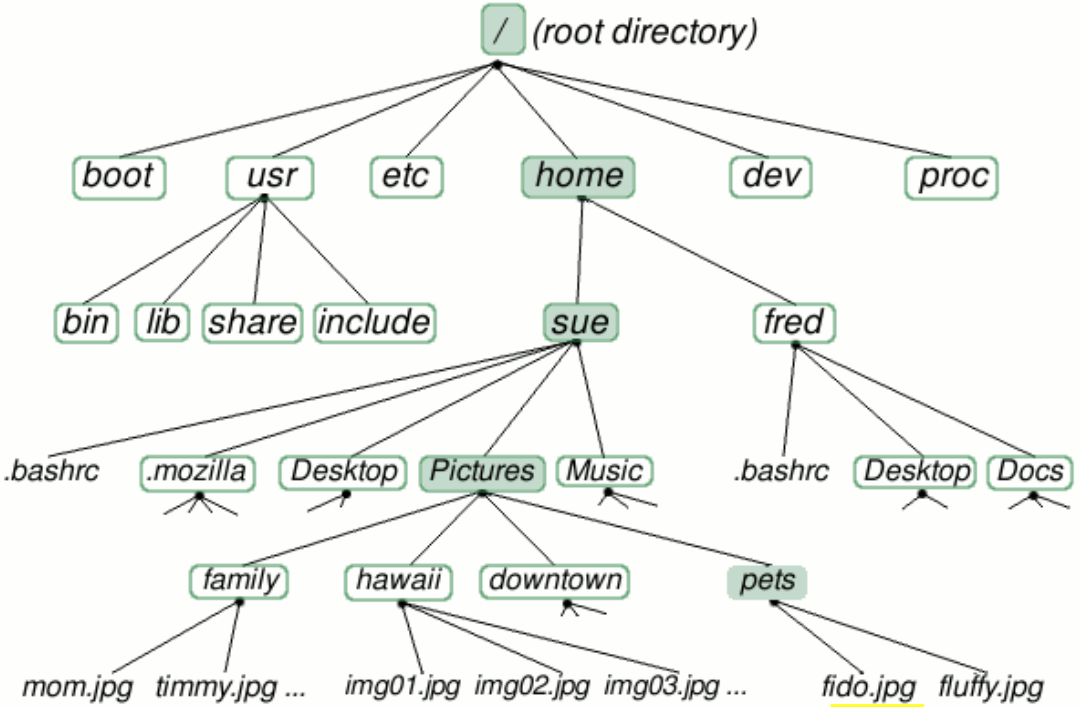
- Kernel
  - Interacts with hardware and provides user services
- Shell
  - Command interpreter providing a layer between the OS and the User
  - Several shells are available
    - sh, csh, ksh, tcsh, bash, ...
    - each shell includes a programing/shell language
- Programs (& Commands)
  - Unix provides several hundred utility programs
  - shell scripts also provide utility

A layered system provides functionality and hardware portability



The File System

- File System Components
  - Directories and Files
- Tree Structure
- Path Names
  - Relative (/home/sue):
    - Pictures/pets/fido.jpg
    - ./Pictures/pets/fido.jpg
    - ../sue/Pictures/pets/fido.jpg
- Absolute:
  - /home/sue/Pictures/pets/fido.jpg



current dir ./ upper level dir ../

Getting Started

- Today we will:
  - **Obtain an HPC Physics Computer Account**
  - **Use a classroom computer to connect to the HPC**
  - **Utilize basic unix commands and understand unix concepts**

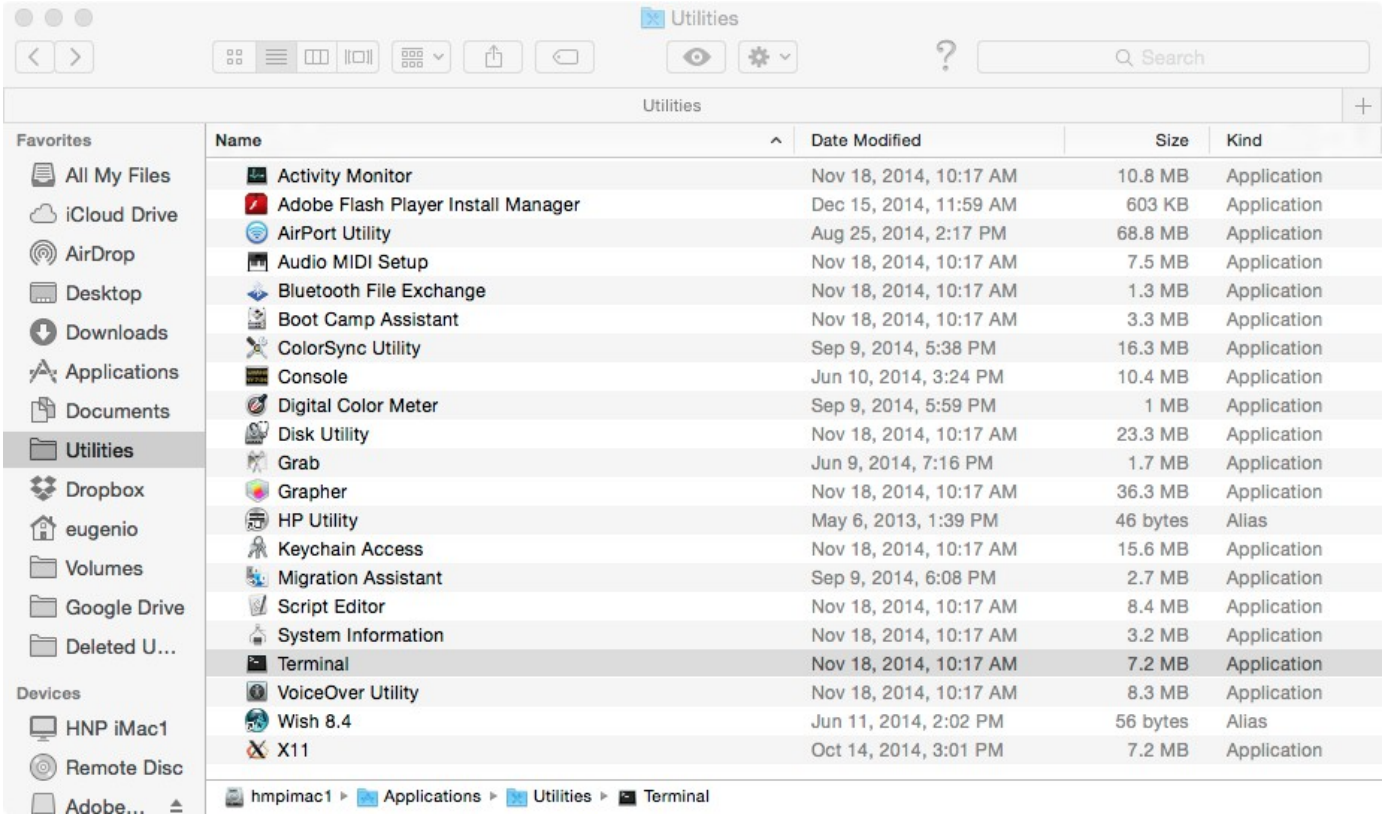
Obtain an HPC Physics Computer Account

- Go the FSU Research Computing Center website and request an account
  - https://rcc.fsu.edu
    - Select “MY RCC ACCOUNT” and then “Sign Up”
    - Follow the instructions completing the account request form
      - Select for Sponsor: **“Eugenio, Paul”**
      - Shell: select **“/bin/tcsh”**
    - After your account has been approved, you should receive an email notification.

Use a classroom computer to connect to the Physics HPC

- From the OSX Finder open the Terminal application
  - Finder->Applications->Utilities->Terminal
- Create a secure terminal shell connection to the HPC
  - In the Terminal window execute the command:
    - **ssh -Y <yourUserName>@hpc-login.rcc.fsu.edu**

      where <yourUserName> is replaced by your fsu user name.



OSX Finder

Terminal application

Utilize basic unix commands and understand unix concepts

- Read the Handout "*Basic Unix Commands and Concepts*" and explore unix via a terminal shell session on the Physics HPC.

  Get online: BasicUnixCommandsAndConcepts.pdf

  - Also explore the unix commands provided on the handout "Common Linux/Unix Commands"

    Get: unix_commands.pdf

If your Physics HPC account has not bee approved yet, then use the macOS/OSX terminal shell to explore unix.

Work through the Unix handout testing Unix commands on the HPC