Computational Physics

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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

http://hadron.physics.fsu.edu/~eugenio/comphy/
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 Programming
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%)**
  - Programming 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.
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
- Programming tools
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 programming/shell language

Programs (& Commands)
- Unix provides several hundred utility programs
- shell scripts also provide utility
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

Directories and Files

Tree Structure

Path Names

Absolute:
  - /home/sue/Pictures/pets/fido.jpg
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.
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