

Introduction to Computational Physics

PHYS 250 (Autumn 2018) – Lecture 2

David Miller

Department of Physics and the Enrico Fermi Institute
University of Chicago

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Outline

Computational Physics (PHYS 250)

Course Description PHYS 250 ([link to Course Catalog](#))

This course introduces the use of computers in the physical sciences. After an introduction to programming basics, we cover numerical solutions to fundamental types of problems, including cellular automata, artificial neural networks, computer simulations of complex systems, and finite element analysis. Additional topics may include an introduction to graphical programming, with applications to data acquisition and device control.

There are an infinite number of paths that we might follow and still not deviate from this description. I therefore would like to lay out some of the principles that will guide me, and us, in how we navigate through those many possibilities.

Outline

Version control

- The most important message of this slide is simple...**Use a software version control system for all of your code**
 - And that means now...not tomorrow or next week
 - Because if you wait until you need it, it will be too late

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/Users/fizisist/Pictures/Random/Git-Logo-2Color.png
/Users/fizisist/Pictures/Ra

A brief history of version control

- **The first version control systems were designed to be used on large systems where everyone logged into the same machine**
 - They tracked code on the same filesystem where it lived (e.g., in a subdirectory)
 - SCCS and RCS are examples
- **Then client-server systems were developed, so that developers could work on their own machines**
 - Checking code into a central server to share and collaborate
 - CVS and SVN are examples
- **More recently distributed version control systems have arisen**
 - These are decentralised, so everyone has a complete copy of the repository
 - Gives a lot of freedom to developers to share and merge as they like, so liked very much by the open source community
 - git, mercurial and bit keeper are examples

git, GitHub, & GitLab

<https://git-scm.com>, <https://github.com>, <https://about.gitlab.com>

- **git is the most popular open source version control system**
 - can host huge projects (Linux Kernel, LHC experiment software, etc)
 - scales very well and it's extremely fast and powerful
 - very flexible (= complex)
- **Distributed version control systems (`git`) are great, but they're made even better by using a social coding site (`GitHub` or `GitLab`)**
- **These sites allow developers:**
 - browse code easily
 - compare different versions
 - take copies (a.k.a. fork)
 - offer patches back to upstream repositories
 - And discuss and review these patches before acceptance
 - even build websites
- **The best known social coding site is GitHub, but there are others, e.g. BitBucket and GitLab**
 - Familiarity with `git/GitHub/GitLab` will serve you well, trust me

GitHub & GitLab resources

GitHub is a free resource as long as your code remains public (you can pay for private repositories). The Physical Sciences Division (PSD) at UChicago hosts a **private GitLab** repository.

- <https://psdcomputing.uchicago.edu/page/psd-repo>



PSD Repo



PSD Repo is a software source code repository managed by the PSD Computing office

UC LDAP	Standard
UC LDAP Username	
<input type="text" value="johndoe"/>	
Password	
<input type="password" value="*****"/>	
<input type="checkbox"/> Remember me	
Sign in	

PHYS 250 GitHub

<https://github.com/UChicagoPhysics/PHYS250>

Course materials are hosted in the **GitHub** UChicagoPhysics repository

The screenshot shows the GitHub repository page for 'UChicagoPhysics / PHYS250'. At the top, there are buttons for 'Watch' (0), 'Star' (0), and 'Fork' (0). Below that is a navigation bar with links for 'Code', 'Issues 0', 'Pull requests 0', 'Projects 0', 'Wiki', 'Insights', and 'Settings'. The main content area is titled 'University of Chicago PHYS 250 Computational Physics software repository' and includes a 'Manage topics' link and an 'Edit' button. Below this, it displays statistics: '15 commits', '1 branch', '0 releases', and '1 contributor'. A 'Branch: master' dropdown and a 'New pull request' button are also present. The commit history table lists the following changes:

File	Description	Time
fizist	Update example	Latest commit efe9be5 25 minutes ago
Examples	Update example	25 minutes ago
LearningGoals	UPdate Learning Goals	22 hours ago
Slides	Update Lecture 1 Slides	an hour ago
Syllabus	Updates to syllabus	22 hours ago
.gitignore	Update slides for day 1	3 days ago
README.md	Update README.md	3 days ago

- Slides (e.g. *these!*), syllabi, learning goals, and code examples
- Stable versions will be cross-posted to **Canvas** as well.
- Homework submission will be done via **GitHub** (*instructions to come*)

Linux “shell”

- We will be using an interface to Linux called a “shell”
- It is a command-line interpreter : you type, it executes
- Two major options are bash (as in, smash) and csh (like “sea shell”, modern version is “tcsh”, “tea sea shell”)
 - Only real difference: environment variables syntax
 - bash: `export X=value`
 - csh: `setenv X value`

Shell basics

Listing directory contents : `ls`, like “list”

Copy: `cp`

Where am I?: `pwd`, `cd`

Hello world!

Interactive in the python interpreter

From a script (containing the above print line):

Self-running script:

Lists (I)

In my opinion, python's great advantage is **list comprehension**.

List basics

Append elements

Concatenation

Removal of elements

Lists (II)

Element acces read/write

Test if an element is in a list (or not)

for and while loops

The `for` statement iterates through a collection, iterable object or generator function.

The `while` statement merely loops until a condition is `False`.

Iterate over list

Iterate using built-in `range` function

Iterate until a condition is met

Putting lists and loops together is amazing (and complex)

Filter one list into another (the “old” way)

List comprehension (the “pythonic” way)

where `filter` and `function` just perform “some” operation on the list elements. Basically, the syntax is:

and this replaces:

Useful list comprehension

Filter one list into another (the “old” way)

List comprehension (the “pythonic” way)

where `filter` and `function` just perform “some” operation on the list elements. Basically, the syntax is:

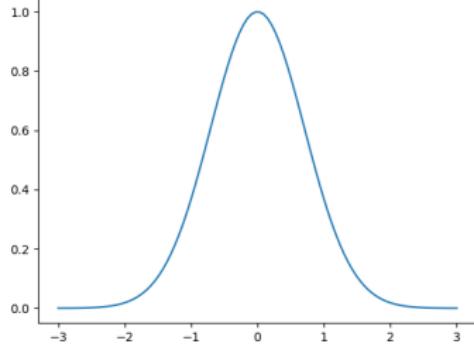
and this replaces:

Hello Gaussian!

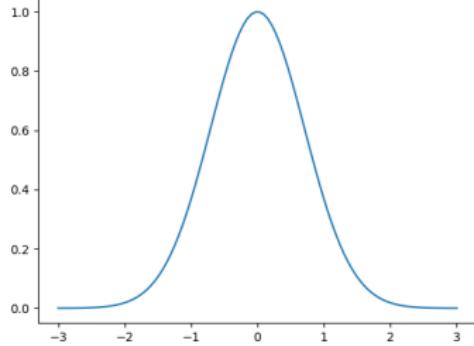
Basic but useful code example

Hello Gaussian!

Basic but useful code example



Hello Gaussian!



Basic but useful code example

But what about that `linspace` thingy? Google it! ([numpy docs](#))

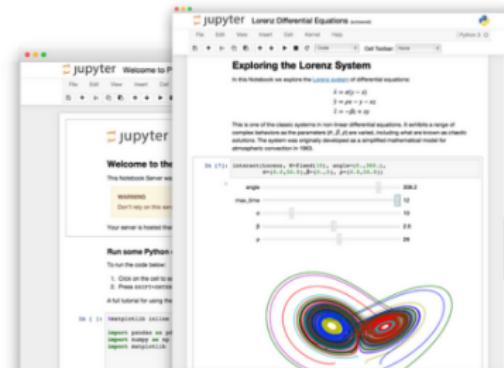
```
numpy.linspace(start, stop, num=50, endpoint=True,  
retstep=False, dtype=None)
```

“Returns num evenly spaced samples, calculated over the interval [start, stop].”

Jupyter notebooks

Interactive, web-based, integrated code and documentation environment

We will be following-up with more technical practice with python, but I want to introduce you to the resources that we'll be using this quarter for many of our examples and projects: **Jupyter notebooks**.



The Jupyter Notebook

The Jupyter Notebook is an open-source web application that allows you to create and share documents that contain live code, equations, visualizations and narrative text. Uses include: data cleaning and transformation, numerical simulation, statistical modeling, data visualization, machine learning, and much more.

[Try it in your browser](#)

[Install the Notebook](#)



Language of choice



Share notebooks



Interactive output



Big data integration

Jupyter notebooks on the PHYS 250 computing platform

Built for machine learning applications running mostly in Jupyter.

The screenshot shows a web browser window with the URL <https://ml.maniac.uchicago.edu>. The main content area displays a large photograph of the ATLAS particle detector at the Large Hadron Collider. Overlaid on this image is a dark blue banner containing the text "PHYS 250 FALL 2018 COMPUTING PLATFORM" in white, bold, sans-serif font. Below the main title, a smaller line of text reads "JupyterLab-based infrastructure for Computational Physics". To the right of the banner is a white 3D cube icon featuring a wrench and a vertical bar with three horizontal lines. The top navigation bar of the browser includes links for "Home", "About", "Services", and "Login". A sidebar on the left contains a link to "External resources" which lists "Intro to Linux (UChicago CSIL)", "Intro to Git (UChicago CSIL)", "PICUP (Partnership for Integration of Computation into Undergraduate Physics)", and "Computational Physics text from".

Purpose

A computational platform that supports on-demand JupyterLab instances for interactive python development as well as advanced computational resources such as those required for high-level, compute-intensive machine learning applications.

Elements

The platform provides hosted JupyterLab instances for the students in PHYS 250 (Autumn 2018) on GPU resources hosted by the computing center for the ATLAS Experiment

<input checked="" type="checkbox"/> External resources
Intro to Linux (UChicago CSIL)
Intro to Git (UChicago CSIL)
PICUP (Partnership for Integration of Computation into Undergraduate Physics)
Computational Physics text from

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The screenshot shows a web browser window with the URL <https://auth.globus.org/p/login?scope=um%3Aglobus%3A>. The title bar says "Log in using Globus". The page itself is titled "Globus Account Log In" and features a "Log in to use ml front" section. It prompts the user to "Use your existing organizational login" and provides a dropdown menu currently set to "University of Chicago". Below this, a note says "Didn't find your organization? Then use Globus ID to sign in. (What's this?)". A blue "Continue" button is visible. A callout box explains that "Globus uses CILogon to enable you to Log in from this organization. By clicking Continue, you agree to the CILogon privacy policy and you agree to share your username, email address, and affiliation with CILogon and Globus. You also agree for CILogon to issue a certificate that allows Globus to act on your behalf." At the bottom, there are two other sign-in options: "Sign in with Google" and "Sign in with ORCID ID".

Jupyter notebooks on the PHYS 250 computing platform

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The screenshot shows a web browser window for the PHYS 250 Computational Physics course. The URL is <https://ml.maniac.uchicago.edu/index.html>. The page features a large banner image of the ATLAS particle detector at CERN. Overlaid on the banner is the text "PHYS 250 FALL 2018 COMPUTING PLATFORM" in large white letters, with "JupyterLab-based infrastructure for Computational Physics" in smaller text below it. To the right of the text is a white cube icon with a wrench and a gear inside. Below the banner, the page content includes sections for "Purpose" and "Elements", and a sidebar with links to external resources and partners.

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The screenshot shows a web browser window with the title "PHYS 250 Computational Physic X". The URL in the address bar is <https://ml.maniac.uchicago.edu/profile.html>. The page content is for "PHYS 250 Autumn 2018". On the left, there is a large, semi-transparent watermark of a three-dimensional cube. On the right, there is a "Profile Information" box containing the following details:

Name:	David Miller
Email:	davemilr@uchicago.edu
Organization:	

Below the profile information is a blue "Logout" button. At the bottom of the page, there is a copyright notice and logos for NSF and the U.S. Department of Energy.

© 2018 University of Chicago. This platform is supported by National Science Foundation grants: NSF OAC-1724821 "CIF21 DIBBs: El: SLATE and the Mobility of Capability", NSF CNS-1730158 "CI-New: Cognitive Hardware and Software Ecosystem Community Infrastructure (CHASE-CI)", NSF OAC-1541349 "OC*ONI DIBBs: The Pacific Research Platform", NSF PHY-1624739 "U.S. ATLAS Operations: Discovery and Measurement at the Energy Frontier", NSF PHY-1148698 "The Open Science Grid, The Next Five Years: Distributed High Throughput Computing for the Nation's Scientists, Researchers, Educators, and Students", the Department of Energy ASCR/NGNs DORM project "Virtual Clusters for Community Computation (VC3)", and by the Enrico Fermi Institute at the University of Chicago.

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© 2018 University of Chicago. This platform is supported by National Science Foundation grants: NSF OAC-1724821 "CIF21 DIBBs: El: SLATE and the Mobility of Capability", NSF CNS-1730158 "El-New: Cognitive Hardware and Software Ecosystem Community Infrastructure [CHASE-El]", NSF OAC-1541349 "CC'DNI DIBBs: The Pacific Research Platform", NSF PHY-1624739 "U.S. ATLAS Operations: Discovery and Measurement at the Energy Frontier", NSF PHY-1148698 "The Open Science Grid, The Next Five Years: Distributed High Throughput Computing for the Nation's Scientists, Researchers, Educators, and Students", the Department of Energy ASCR/NGNs DDHM project "Virtual Clusters for Community Computation (VC3)", and by the Enrico Fermi Institute at the University of Chicago.

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<https://ml.maniac.uchicago.edu/services.html>

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Service	Name	Started at	Ending at	GPUs	Cores	Memory	Link	Status	Command
No data available in table									

Showing 0 to 0 of 0 entries

Service	Name	Started at	Ending at	GPUs	Cores	Memory	Link	Status	Command
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The screenshot shows a web browser window with the title "PHYS 250 Computational Physicist". The URL is <https://ml.merac.uchicago.edu/PrivateJupyter.html>. The page is titled "PHYS 250 Autumn 2018" and includes links for "Home", "About", "Services", and "Profile".

Private JupyterLab

Use this for private code development or if you need dedicated resources.

Instructions (read first)

- Fill out the form to the right.
- Upon submission a dedicated JupyterLab instance will be spawned in the background
- You'll receive a JupyterLab link to be used once the notebook has been scheduled (this can take several minutes, or longer if the resources are busy)
- We suggest organizing your notebook in GitHub and cloning it manually once your notebook starts up. Remember to push any changes before the notebook expires.

Configure your JupyterLab instance

Please only select what you actually need.

Name *

Password *

Expiration of your JupyterLab [days] *

GPUs

CPUs

Memory [GB]

Check out a GitHub repo (use full URL including ".git")

START

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Service	Name	Started at	Ending at	GPUs	Cores	Memory	Link	Status	Command
Private JupyterLab	lecture-1	Tue, 02 Oct 2018 14:31:14 GMT	Wed, 03 Oct 2018 14:31:14 GMT	0	1	8Gi	http://mi.usatlas.org:31155	Running	Delete

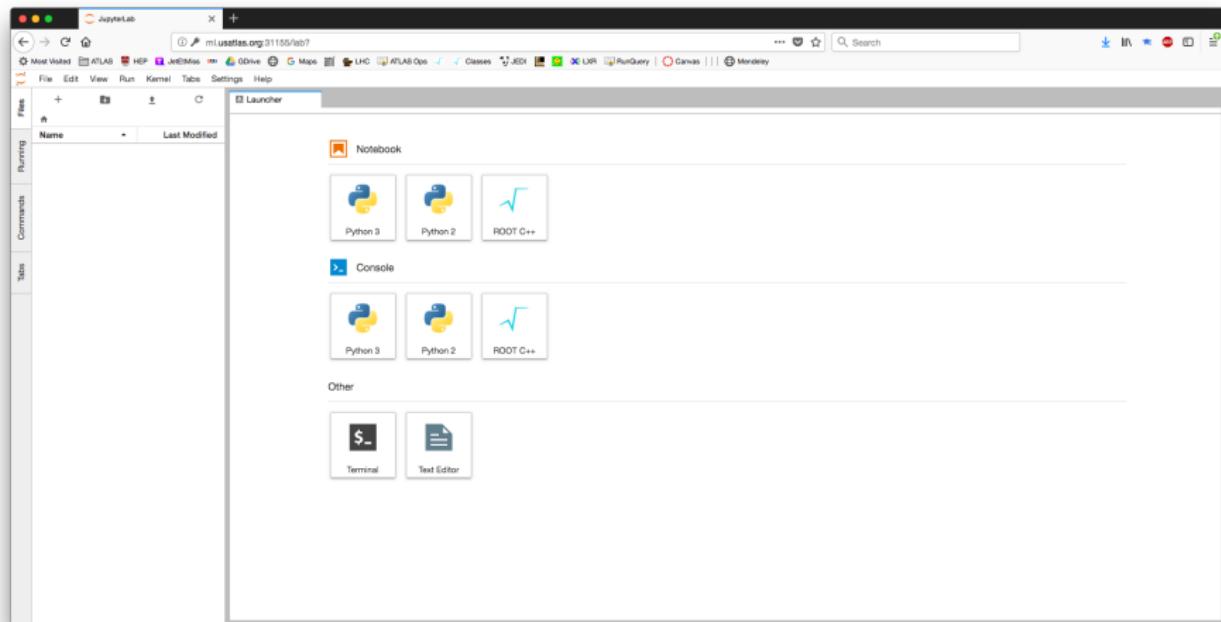
Below this, a message says "Showing 1 to 1 of 1 entries".

Further down, there's a section titled "All Services" with another table showing five entries:

Service	Name	Started at	Ending at	GPUs	Cores	Memory
Private JupyterLab	lecture-1	Tue, 02 Oct 2018 14:31:14 GMT	Wed, 03 Oct 2018 14:31:14 GMT	0	1	8
Private JupyterLab	instructor-lab	Mon, 01 Oct 2018 18:40:41 GMT	Tue, 02 Oct 2018 18:40:41 GMT	0	1	8
Private JupyterLab	test-3	Fri, 28 Sep 2018 20:07:37 GMT	Sat, 29 Sep 2018 20:07:37 GMT	0	1	8
Private JupyterLab	my-lab 2	Fri, 28 Sep 2018 19:59:02 GMT	Sat, 29 Sep 2018 19:59:02 GMT	0	1	8
Private JupyterLab	my-lab 2	Fri, 28 Sep 2018 19:58:19 GMT	Sat, 29 Sep 2018 19:58:19 GMT	0	1	8

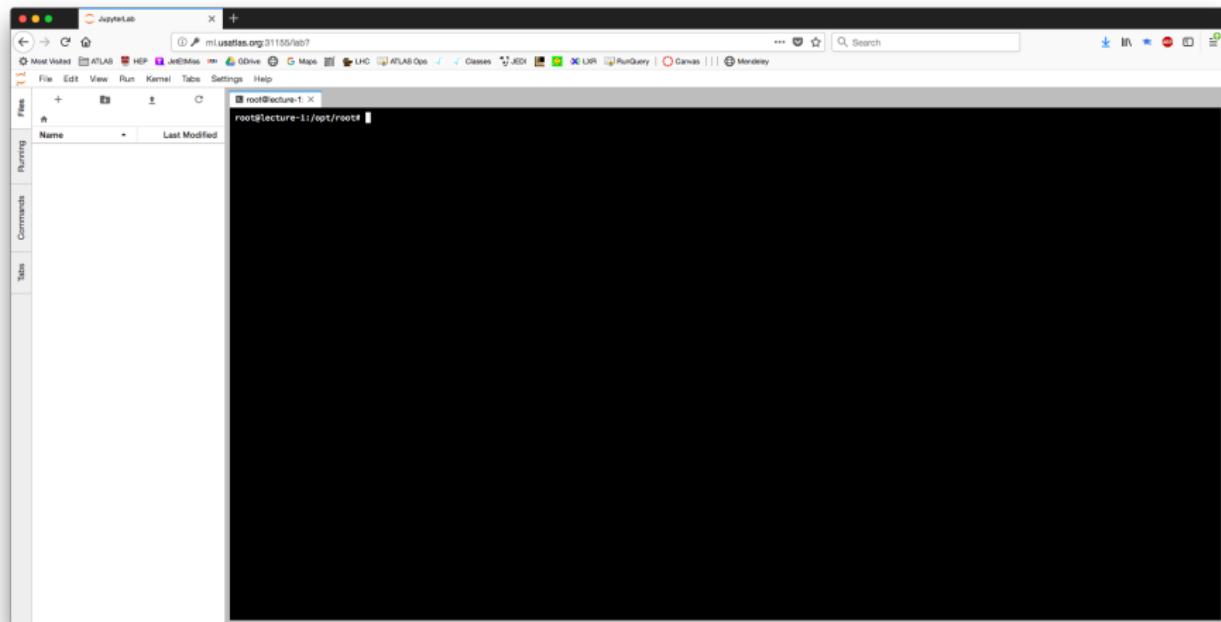
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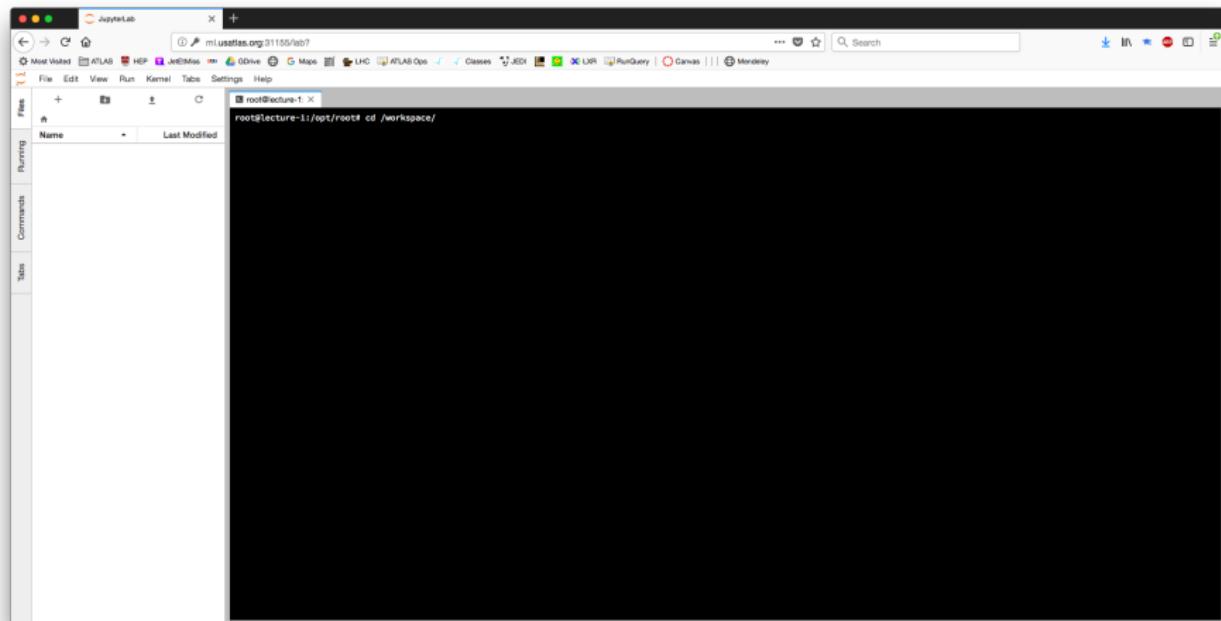
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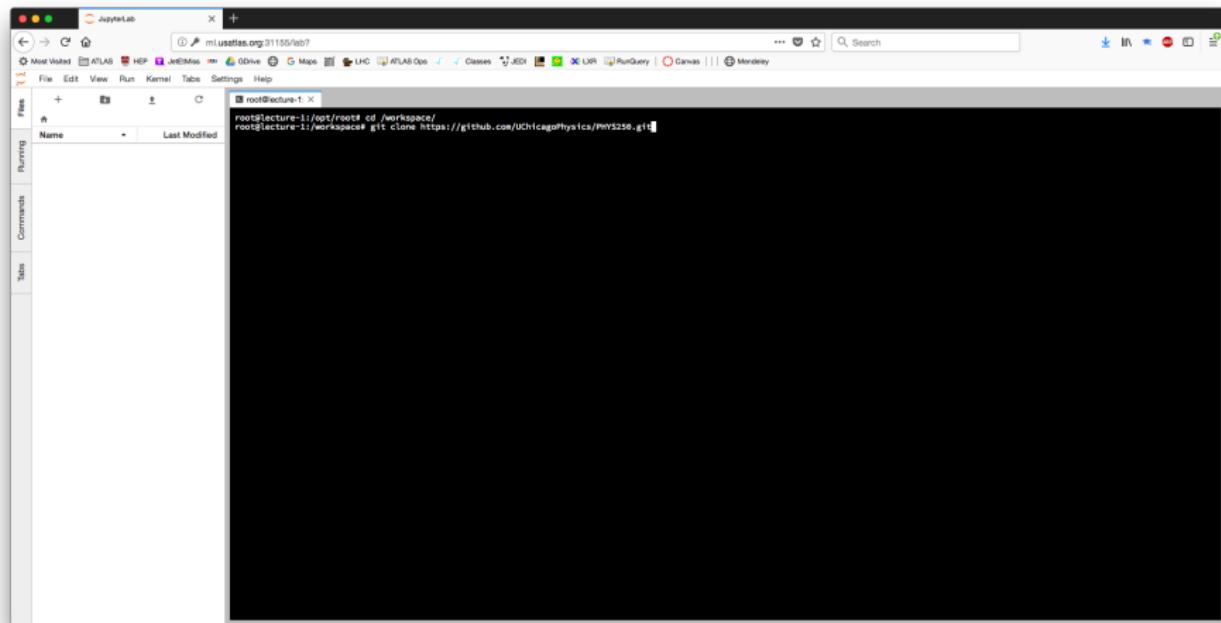
PHYS 250: Computational Physics

Welcome to the University of Chicago PHYS 250 Computational Physics repository!

This repository will hold the Syllabus, Learning Goals, Code Examples, and Lecture Notes for the course. Periodically, some of these materials will be moved to the [Course page for the course](#), which for the Autumn 2018 Academic Quarter is:

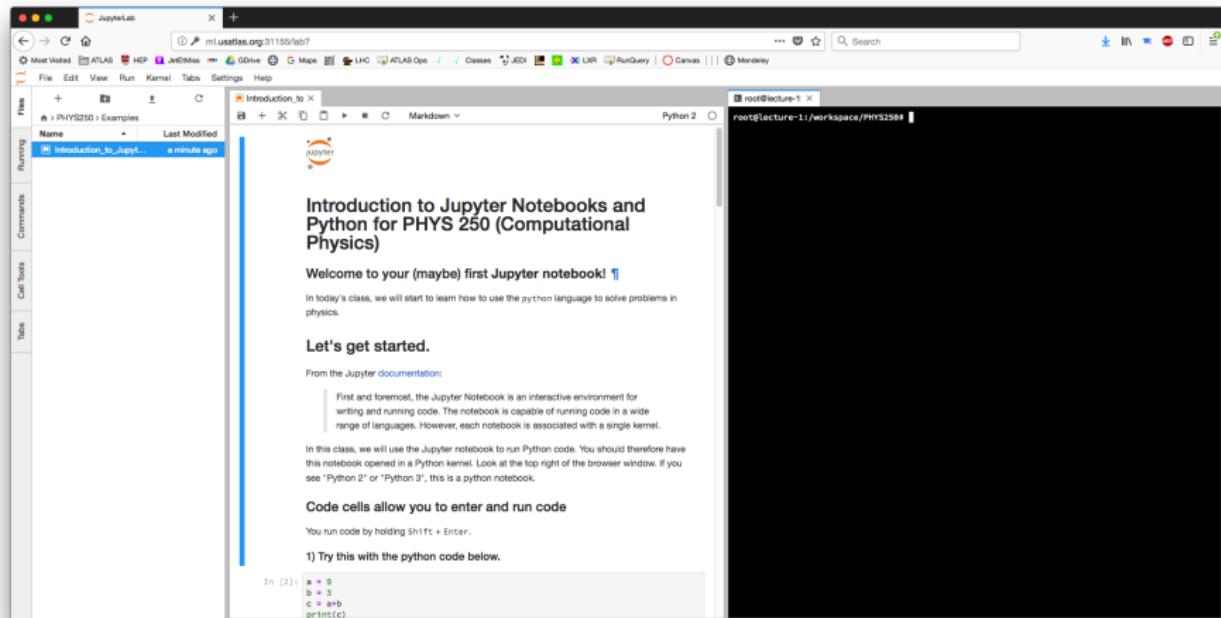
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Outline

Random Numbers

Random numbers may seem innocuous, but they underlie nearly everything you do electronically, rely on for security, or employ in the context of simulations and evaluation of models.

- **cryptography**
- **computer simulation**
 - the most well version of which is named after the gambling town, **Monte Carlo**
- **sampling**

As such, their use, their control, and the evaluation of just how random they are, is of paramount importance for computational physics.

And you thought lava lamps were a thing of the past



Cryptography relies on the ability to generate random numbers that are both unpredictable and secret. But **random** is a very malleable term.

True vs. Pseudo: it's more than semantics

The computers of today are, by design and by implementation, **deterministic**. That means that an **algorithm cannot**, on its own and without input from an external source, provide a stream of 100% uncorrelated random sequences. Hence the division:

- **TRNGs: True** random number generators
 - generally use some physical process that is unpredictable, but often slow and requires specialized hardware
 - possibly combined with some compensation mechanism that might remove any bias in the process
 - examples include: lava lamps, quantum processes, radioactive decays, thermal noise
- **PRNGs: Pseudo-random** number generators
 - based on algorithms and, therefore, not truly *random*
 - do not require special hardware and therefore are very portable and fast
 - can be reproduced given initial conditions

We will, perhaps obviously, focus on PRNGs.

(but if you want to build a wall of lava lamps in KPTC, I will cheer you on)

Pseudo-random number generators (PRNGs)

The idea behind an algorithmic PRNG is to generate a sequence of numbers, $x_1, x_2, x_3 \dots$ using a recurrence of the form

$$x_i = f(x_{i-1}, x_{i-2}, \dots, x_{i-n}), \quad (1)$$

where n initial numbers (“seeds”) are needed to begin the recurrence. The magic lies in the function, f , used, and the resulting *uniformity* and *correlation length* across some sequence of numbers.

Linear congruential generators (LCGs) are one of the oldest PRNGs and have the form

$$x_{i+1} = (ax_i + c) \mod m \quad (2)$$

IBM mainframes in the 60s had $a = 65539$, $c = 0$, and $m = 2^{31}$. This leads to

$$x_{i+2} = 6x_{i+1} - 9x_i \quad (3)$$

which, maybe you can tell, isn’t great.

Python random number generator: Mersenne Twister

Python comes with a built-in (`stdlib`) random number generator that can be accessed with:

In addition, the `numpy` package provides an even more developed set of tools with `numpy.random`.

Both of these use the Mersenne Twister algorithm, which was developed in 1997 by Matsumoto and Nishimura and is a version of a generalized feedback shift register PRNG. The name comes from the fact that the period is given by a Mersenne prime

$$M_n = 2^n - 1, n \in \mathbb{N} \quad (4)$$

(In preparing this, I found out that the largest known prime number $2^{77,232,917} - 1$ is a Mersenne prime, found on December 26, 2017.)