Scientific Computing: Lecture 1

- Introduction to course, syllabus, software
- Getting started
  - Enthought Canopy, TextWrangler editor, python environment, ipython, unix shell
- Data structures in Python
  - Integers, floats, strings, lists, tuples, dictionaries, functions

CLASS NOTES

- Take a look at course website ASAP. Download class codes.
- Read Chap. 1 by Tuesday
- See me if you have concerns or questions.

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Course information

- Instructor: Dr. Gladden, VCRSP & Assoc. Prof. of Physics
- Office: Lyceum 313
- Email: jgladden@olemiss.edu
- Website: www.phy.olemiss.edu/~jgladden/sci_comp/
  (for example code, lecture slides, assignments)
- Syllabus and course description.
- Office hours: Please schedule with Ms. Sarah Krueger (skrueger@olemiss.edu)
- Textbook:
  A Primer on Scientific Programming with Python
  5^{th} edition, Hans Petter Langtangen
  This is a good resource which we will refer to regularly, but we will not be working through it chapter by chapter.

Course Goals

- The goal of this course is to provide you with both a general understanding of fundamental concepts in scientific computing and to teach you the skills to implement them to solve problems in your research.
- Scientific computing is a HUGE field with many specialized niches. We will focus on the fundamental concepts which form the basis for these specializations.
- We will be using the programming (scripting) language Python which has gained popularity in the scientific community (and many other areas!)
  - Scripted rather than compiled
  - Cross platform, even for GUIs (windows, menus, mouse, ...)
  - Easy to learn (as you will see)
  - Similar syntax as Matlab, but more flexible
  - Large and mature code base (libraries)
- This, however, is NOT intended to be a course in Python!

Course tools

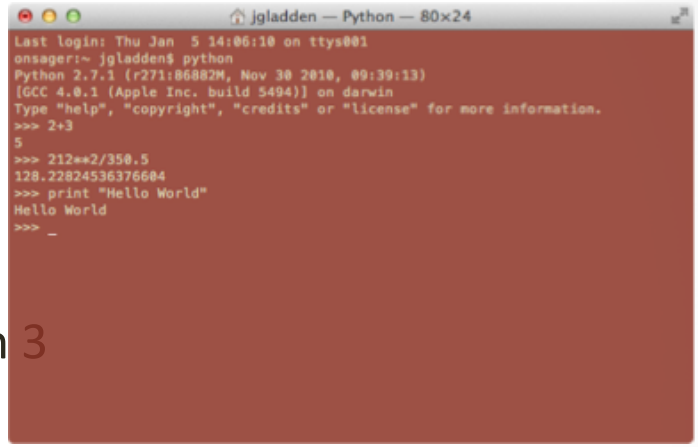
- All software we will use in class is freely available. Links to downloads are on the Resources page of the Course website.
- Python:
  - Recent major version change (2.7 to 3.4). For compatibility we will use 2.7.
  - Already installed on MacOSX and Linux. Can be downloaded for Windows.
  - Another option is a "kitchen sink" python distribution with most scientific libraries already included. A popular one is Enthought Canopy (free for basic sunscription)
  - Programs are just text files. Want a code editor that has "syntax highlighting" for python. Textwrangler is good on Mac, Notepad++ is common for Windows. Many options -> Google! Canopy has a decent built in editor.
- Saving your class work. Several options here:
  - You are encouraged to bring your own laptop!
  - Some classroom computers may be available.
    - A USB thumb drive (>2Gb) is probably easiest.
    - You can save files to a scratch directory on the desktop and upload them to a network drive (Box, Google Drive, DropBox, ftp server, …)
    - Do NOT expect all your work to be safe on these computers!

Topics for the semester

- Introduction to Python (4 weeks)
  - Data structures, flow control, conditionals, input/output, functions
  - Graphical representation of data
    - Plots with “matplotlib”, “publication quality”, multiple data sets and visualization.
  - Object oriented programming
- Linear and non-linear regression (1 week)
- Numeric differentiation and Symbolic Mathematics (2 weeks)
  - Numeric precision and discretization error issues & Sympy
- Numeric integration and systems of ODEs (2 weeks)
- Partial Differential Equations (1 week) – for graduate students only
- Roots of polynomials and other functions (1 week)
- Matrix algebra and manipulation (1 week)
- Parallel computing (1 week)
- Graphical User Interfaces (GUIs) [or other!] (1 week)

Getting started with python

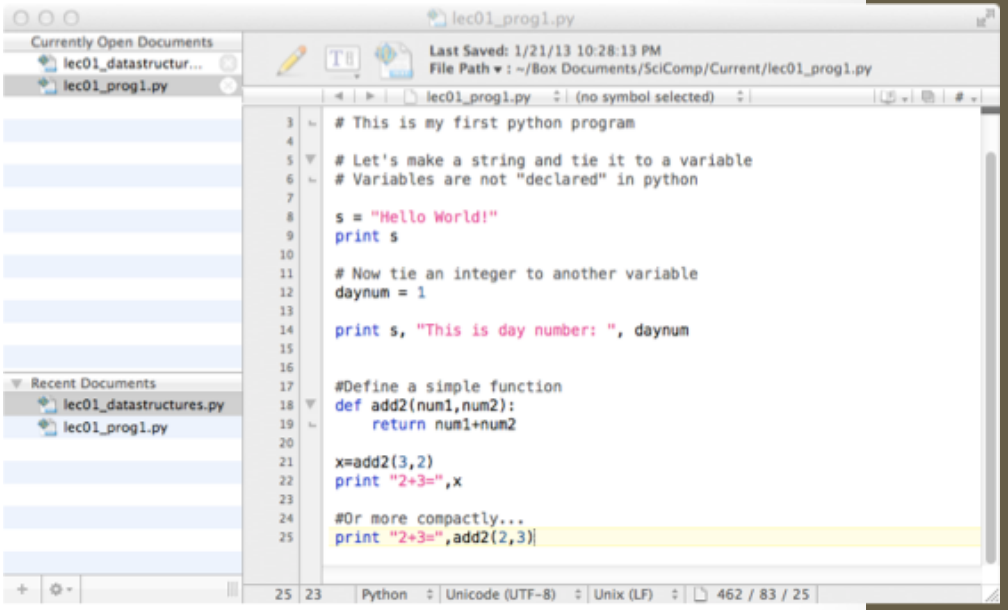
- Open a terminal window (Applications -> Utilities -> Terminal)
- Type `python`
- Type `2+3` and press enter
- Type `212**2/350.5`
- Type `print "Hello World"`
  - `print("Hello World")` in Python 3
- Press Control-D (or `exit()`)to exit.

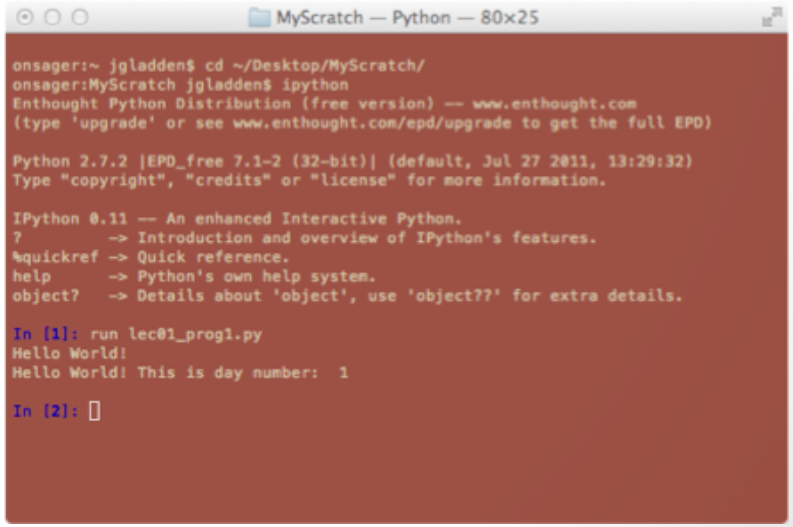


- Now repeat the above commands in ipython.
- These are called the "interpreters" which execute commands line by line. Useful for debugging or quick and dirty calculations you don't really need to save.
- Real work is done by typing these commands into a text file (with ".py" extension and then having the interpreter execute the commands line by line (or block by block)

Writing and running a program

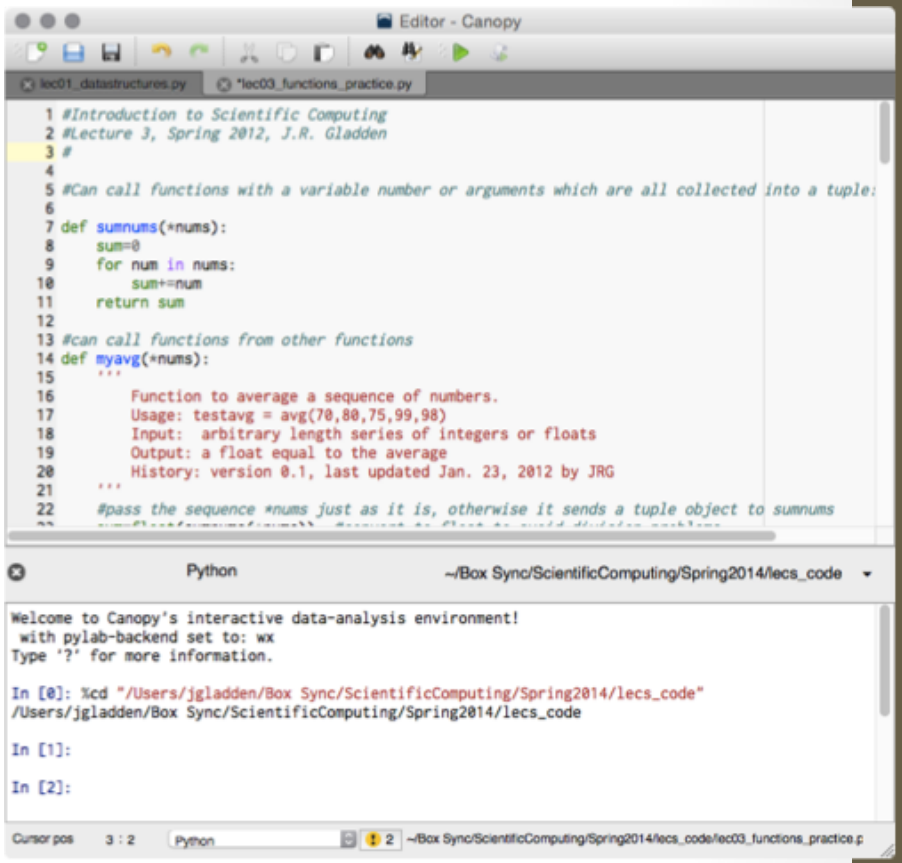
- Create a directory “MyScratch” on the Desktop.
- Open up TextWrangler, type the following commands in a new window.
- Save the file as “lec01_prog1.py” in your new directory.
- In your terminal window, type `cd ~/Desktop/MyScratch/` then `ipython`.
- Now execute the program with `run lec01_prog1.py`
- Note the syntax highlighting and other features of Textwrangler and Canopy.
- Try same program in regular python interpreter with `python lec01_prog1.py`.





Enthought Canopy

- Canopy is a python integrated development environment for scientists.
- Commercial, but freely available to academics. Need to create an account.
- Convenient editor and interpreter and module management (installation and updates)
- Not the best editor and can crash on more complex programs.
- https://www.enthought.com/product/canopy/



Python Notebooks

- Interesting option for interactive work, especially for display to an audience.
- Similar to Mathematica Notebooks – mix of code and descriptive text.
- Run through a browser!
- ”Sessions” with formatted text, graphics, media, and live code can be easily shared.
- Sessions can be run on remote machines through the browser
  - Code is actually executed in the remote machine which could be a large parallel machine.

Data structures in python

- All programming languages have various types of data structures.
- Common to all are:
  - Strings: `s="Hello World"`, or `s='Hello World'`
  - Integers (no decimal): `n=10`
  - Floating point numbers or floats (decimal): `mass=10.0`
- Specific to python are:
  - Lists: `grades = [95,"Bobby",97.5,"Sue",82,"Sarah"]`
  - Tuples: `temperatures = (22.3, 23.1, 24.3)`
  - Dictionaries: `rgbcolors={'red':(1,0,0),'green':(0,1,0),'blue':(0,0,1)}`
- These are all "built in" data types in all python distributions
- Code examples …

Modules (Libraries)

- Much of python's power comes from external modules or libraries. There are literally thousands of them and counting.
- Some come with every python distribution (the standard library), some must be downloaded and installed.
- They are loaded with the `import` statement in a variety of ways.
  - `import math` or `import math as m`,
  - `from math import *` or `from math import sin`
  - Note: Trig functions are RADIAN based (not degrees).
- Each library includes a bunch of functions that will be available after importing.
- Code examples ….

Functions

- Functions are a way of performing a specific task that will need to be done repeatedly.
- Starts with `def` keyword.
- NOTE: indentation IS important in python! Each block of code must have the same indentation.
- Rule of thumb
  - After each ":", indentation must increase.
- Functions must be defined before they are called.
- Generally, define all functions in top of program OR in a separate file (called in with an import statement) if there are many functions.

```
def functname(arg1,arg2,…):
    # python statements
    # to process arguments
    return result

#Example: add 2 numbers
def add2(num1,num2):
    sum=num1+num2
    return sum

myresult = add2(3,4)
#myresult now has value of 7
```