# Python for Scientific Computing

http://bender.astro.sunysb.edu/classes/python-science

# Course Goals

- Simply: to learn how to use python to do
  - Numerical analysis
  - Data analysis
  - Plotting and visualizations
  - Symbol mathematics
  - Write applications
  - …

# Class Participation

- We'll learn by interactively trying out some ideas and looking at code
  - I want to learn from all of you—share you experiences and expertise
- We'll use slack to communicate out of class
  - Everyone should have received an invite to our slack: https://python-sbu.slack.com
- Try out ideas and report to the class what you've learned
  - I can set up an account for you on one of my Linux servers if you want a place to try things out (you would log in remotely)

# Slack

- Log onto our slack as soon as possible
  - If you didn't get an invite, e-mail me, and I'll add you
- Slack is a web-based team chat tool
  - I've setup a number of channels for us to focus our discussions
  - Everyone is expected to participate
- Your course grade is based on your participation
  - I have a simple script(https://github.com/zingale/slack_grader ) that I'll use for grading
    - Good contributions will get a comment on the slack, counting as "+1"
    - The script will record these points over the semester
    - Help, by using slack reactions for useful comments from your classmates
- In "free" mode, slack only keeps 10k messages—I don't think we'll go over that during the semester

# Why Slack?

- One of the goals of this class is to teach you tools that are used by computational science groups
- Slack has gained enormous adoption by research groups over the past few years
  - We'll see how to integrate github repos to it, so everyone can keep on top of code developments
  - It's easy to post code snippets in conversations
  - There are lots of integrations that are available to extend its usefulness

# Why Python?

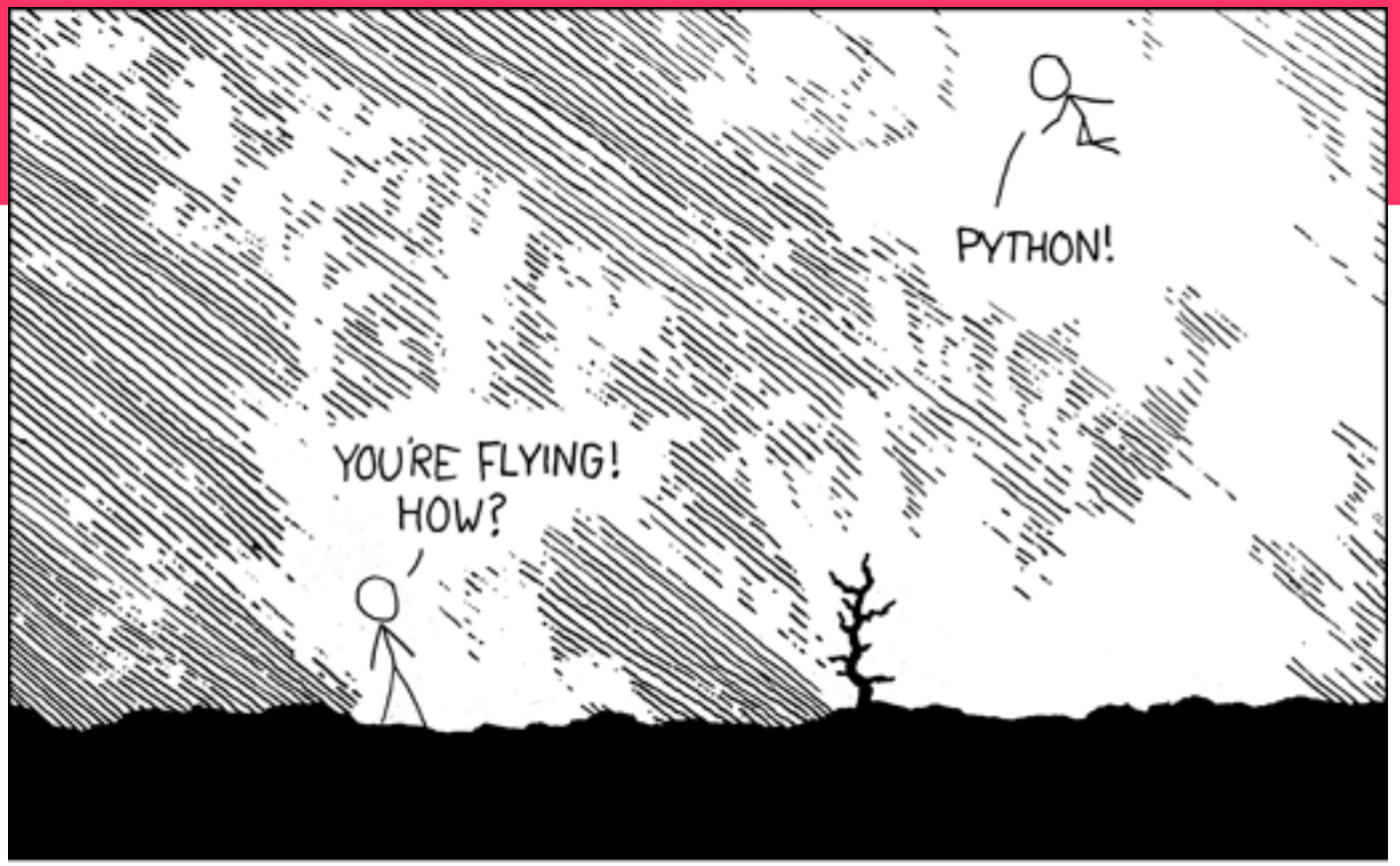
- Very high-level language
  - Provides many complex data-structures (lists, dictionaries, ...)
  - Your code is shorter than a comparable algorithm in a compiled language
- Many powerful libraries to perform complex tasks
  - Parse structured inputs files
  - send e-mail
  - interact with the operating system
  - make plots
  - make GUIs
  - do scientific computations
  - ...
- Easy to prototype new tools
- Cross-platform and Free

# Why Python?

- Dynamically-typed
- Object-oriented foundation
- Extensible (easy to call Fortran, C/C++, ...)
- Automatic memory management (garbage collection)
- Ease of readability (whitespace matters)

... and for this course ...

- Very widely adopted in the scientific community
  - Mostly due to the very powerful array library NumPy


PYTHON!
YOU'RE FLYING! HOW?


I LEARNED IT LAST NIGHT! EVERYTHING IS SO SIMPLE!
HELLO WORLD IS JUST print "Hello, world!"
I DUNNO... DYNAMIC TYPING? WHITESPACE?
COME JOIN US! PROGRAMMING IS FUN AGAIN! IT'S A WHOLE NEW WORLD UP HERE!
BUT HOW ARE YOU FLYING?
I JUST TYPED import antigravity
THAT'S IT?
... I ALSO SAMPLED EVERYTHING IN THE MEDICINE CABINET FOR COMPARISON.
BUT I THINK THIS IS THE PYTHON.

(xkcd)

# Installing Python

- Linux
  - Python is probably already installed
  - The dependencies we need for our class should be available through your package manager
- OS X / Windows
  - The easiest way to get everything we need for class is by installing Anaconda: https://www.continuum.io/downloads
    - You'll have a choice of python 2.x or 3.x—we'll try to write code compatible with both, but 3.x is the future
- If you run into problems ask on the discussion forum (I've already started a thread), or come by my office

# Hello, World!

- If you have python installed properly, you can start python simply by typing `python` at your command line prompt
  - The python shell will come up
  - Our hello world program is simply:

    ```
    print("hello, world")
    ```
  - Or, in python 2 (more on this later…):

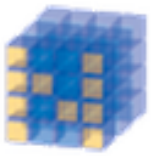
    ```
    print "hello, world"
    ```

# Communities

- Many scientific disciplines have their own python communities that
  - Provide tutorials
  - Cookbooks
  - Libraries to do standard analysis in the field
- For the most part, these build on the Open nature of python
- I've put links on our course page to some information on the python communities for:
  - Astronomy
  - Atmospheric Science
  - Biology
  - Cognitive Science
  - Psychology
  - Let me know of any others!

# Scientific Python Stack

- Most scientific libraries in python build on the Scientific Python stack:



**NumPy**
Base N-dimensional array package

**SciPy library**
Fundamental library for scientific computing

**Matplotlib**
Comprehensive 2D Plotting


**IPython**
Enhanced Interactive Console

**Sympy**
Symbolic mathematics

**pandas**
Data structures & analysis

(scipy.org)

# Basics of Computation

- Computers store information and allow us to operate on it.
  - That's basically it.
  - Computers have finite memory, so it is not possible to store the infinite range of numbers that exist in the real world, so approximations are made.
- You should have some familiarity with how computers store numbers
  - Great floating point reference
    - *What Every Computer Scientist Should Know About Floating-Point Arithmetic* by D. Goldberg

# Computer Languages

- You can write any algorithm in any programming language—they all provide the necessary logical constructs
  - However, some languages make things much easier than others
  - C
    - Excellent low-level machine access (operating systems are written in C)
    - Multidimensional arrays are “kludgy”
  - Fortran (Formula Translate)
    - One of the earliest complied languages
    - Large code base of legacy code
    - Modern Fortran offers many more conveniences than old Fortran
    - Great support for arrays
  - Python
    - Offers many high-level data-structures (lists, dictionaries, arrays)
    - Great for quick prototyping, analysis, experimentation
    - Increasingly popular in scientific computing

# Computer Languages

- IDL
  - Proprietary
  - Great array language
  - Modern (like object-oriented programming) features break the “clean-ness” of the language
- C++
- Others
  - Ruby, Perl, shell scripts, …

# Computer Languages

- Compiled languages (Fortran, C, C++, ...)
  - Compiled into machine code—machine specific
  - Produce faster code (no interpretation is needed)
  - Can offer lower level system access (especially C)
- Interpreted languages (python, IDL, perl, Java (kind-of) ...)
  - Not converted into machine code, but instead interpreted by the interpreter
  - Great for prototyping
  - Can modify itself while running
  - Platform independent
  - Often has dynamic typing and scoping
  - Many offer garbage collection

http://en.wikipedia.org/wiki/Interpreted_language

# Computer Languages

- Vector languages
  - Some languages are designed to operate on entire arrays at once (python + NumPy, many Fortran routines, IDL, ...)
    - For interpreted languages, getting reasonable performance requires operating on arrays instead of explicitly writing loops
      - Low level routines are written in compiled language and do the loop behind the scenes
    - We'll see this in some detail when we discuss python
  - Next-generation computing = GPUs ?
    - Hardware is designed to do the same operations on many pieces of data at the same time

# Object-Oriented Languages

- Python is an object-oriented language
- Think of an object as a container that holds both data and functions (methods) that know how to operate on that date.
  - Objects are build from a datatype called a class—you can create as many instances (objects) from a class as memory allows
    - Each object will have its own memory allocated
- Objects provide a convenient way to package up data
  - In Fortran, think of a derived type that also has it's own functions
  - In C, think of a struct that, again, also has it's own functions
- Everything, even integers, etc. is an object
  - `1 + 2` will be interpreted as `(1).__add__(2)` in python

# Programming Paradigms

| Paradigm | Description | Main characteristics | Related paradigm(s) | Critics | Examples |
|---|---|---|---|---|---|
| **Imperative** | Computation as statements that *directly* change a program state (datafields) | Direct assignments, common data structures, global variables | | Edsger W. Dijkstra, Michael A. Jackson | C, C++, Java, PHP, Python |
| **Structured** | A style of imperative programming with more logical program structure | Structograms, indentation, either no, or limited use of, goto statements | Imperative | | C, C++, Java |
| **Procedural** | Derived from structured programming, based on the concept of modular programming or the *procedure call* | Local variables, sequence, selection, iteration, and modularization | Structured, imperative | | C, C++, Lisp, PHP, Python |
| **Functional** | Treats computation as the evaluation of mathematical functions avoiding state and mutable data | Lambda calculus, compositionality, formula, recursion, referential transparency, no side effects | | | Erlang, Haskell, Lisp, Clojure, Scala, F# |
| **Event-driven including time driven** | Program flow is determined mainly by events, such as mouse clicks or interrupts including timer | Main loop, event handlers, asynchronous processes | Procedural, dataflow | | ActionScript |
| **Object-oriented** | Treats datafields as *objects* manipulated through pre-defined methods only | Objects, methods, message passing, information hiding, data abstraction, encapsulation, polymorphism, inheritance, serialization-marshalling | | See here and[1][2] | C++, C#, Java, PHP, Python, Ruby, Scala |
| **Declarative** | Defines computation logic without defining its detailed control flow | 4GLs, spreadsheets, report program generators | | | SQL, regular expressions, CSS |
| **Automata-based programming** | Treats programs as a model of a finite state machine or any other formal automata | State enumeration, control variable, state changes, isomorphism, state transition table | Imperative, event-driven | | |
| **Paradigm** | **Description** | **Main characteristics** | **Related paradigm(s)** | **Critics?** | **Examples** |

(Wikipedia)

# Potential Topics

- General python
- Advanced python / special modules
  - Regular expressions
  - Command line/input file parsing
  - Filesystem operations
- NumPy
- SciPy and numerical methods
  - Integration
  - ODEs
  - Curve fitting/optimization
  - Interpolation
  - Signal processing (FFT)
  - Linear algebra
- Plotting / visualization
  - matplotlib
  - MayaVi
- Workflow management with IPython
- Extending python w/ Fortran and C/C++
- Symbolic math with SymPy
- Writing python applications
- GUI programming
- Unit testing
- Git/github
- Others?

# Python Shell

- This is the standard (and most basic) interactive way to use python
  - Runs in a terminal window
  - Provides basic interactivity with the python language
- Simply type `python` (or `python3`) at your command prompt
  - You can scroll back through the history using the arrows

# IPython Shell

- Type `ipython` (or ipython3) at your prompt
- Like the standard shell, this runs in a terminal, but provides many conveniences (type `%quickref` to see an overview)
  - Scrollback history preserved between sessions
  - Built-in help with ?
    - function-name?
    - object?
  - Magics (`%lsmagic` lists all the magic functions)
    - `%run script`: runs a script
    - `%timeit`: times a command
    - Lots of magics to deal with command history (including `%history`)
  - Tab completion
  - Run system commands (prefix with a !)
  - Last 3 output objects are referred to via _, __, ___

# Jupyter Notebooks

- A web-based environment that combines code and output, plots, plain text/stylized headings, LaTeX, ...
  - Notebooks can be saved and shared
  - Viewable on the web via: http://nbviewer.ipython.org/
  - Provides a complete view of your entire workflow
- Start with `ipython notebook`
- I'll provide notebooks for a lot of the lectures to follow so you can play along on your own
  - The best way to learn is to experiment—download the notebooks and play around
  - Discuss anything you don't understand in the discussion forum

# Python Scripts

- Scripts are a non-interactive means of writing python code
  - `filename.py`
  - Can be executable by adding:

    ```
    #!/usr/bin/env python
    ```

    as the first line and setting the executable bit for the file
- This is also the way that you write python modules that can be `import`-ed into other python code (more on that later...)

# Python 2.x vs. Python 3

- See https://wiki.python.org/moin/Python2orPython3
- Mostly about cleaning up the language and making things consistent
  - e.g. `print` is a statement in python 2.x but a function in 3.x
- Some trivial differences
- `.pyc` are now stored in a `__pycache__` directory
- Some gotyas:
  - `1/2` will give different results between python 2 and 3
- It's possible to write code that works with both python 2 and 3—often we will do so by `importing` from `__future__`

# Python 2.x vs. Python 3

- Write for both
  - In python 2.6+, do

    ```
    from __future__ import print_function
    ```

    and then use the new `print()` style
  - `exec cmd` becomes `exec(cmd)`
  - Some small changes to how `__init__.py` are done (more on this later)
- One some systems, you can have python 2.x and 3.x installed side by side
  - May need to install packages twice, e.g. `python-numpy` and `python3-numpy`

# Class Organization

- We'll work mostly with Jupyter notebooks from now one (with a few exceptions)
- Each week, I'll ask you to work through some notebooks on your own, outside of class
  - These will always be posted on the class website
  - Great opportunity to ask questions on slack
- The hope is that we'll get a lot of the basic concepts for the week covered by working through the notebooks
- In class, we'll work on some exercises together
- We'll fine-tune some of this as we go through the semester

# Let's Play

- There are a number of notebooks on our website to demonstrate some core ideas
  - Data types
  - Advanced data types
  - Control flow
  - Functions
  - Classes
  - Modules