# Introduction to Scientific Python

Blake Fleischer, PhD

Research Scientist

Partnership for an Advanced Computing Environment (PACE)

# Objectives:

- Showcase Python as a viable and free alternative to scientific packages like R, MatLab
- Overview of some of Python's scientific functions



# Why Python for Science?

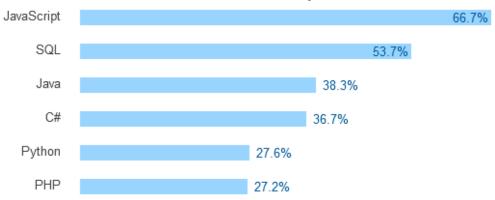
- Easy to learn
- Well Supported
- Useful after graduation (free and open source)
- Extremely popular outside of academia





# People use Python

#### 2017 StackOverflow Survey



#### Google searches for language + 'tutorial' (PYPL)

Worldwide, Aug 2017 compared to a year ago:

Rank	Change	Language	Share	Trend
1		Java	22.7 %	-0.7 %
2		Python	16.3 %	+3.7 %
3		PHP	8.9 %	-1.1 %
4		C#	8.3 %	-0.5 %

# Python Packages

 Extending beyond simple programming, additional functionality comes from packages



- Package discovery:
  - Finding the packages that suit your needs













### Tools of the Trade: Git

- "Version control is a system that records changes to a file or set of files over time so that you can recall specific versions later." https://git-scm.com
- Backbone of the developer world
- Git incorporates free web hosting for publicly visible files
- GT supports private repositories <a href="https://support.cc.gatech.edu/support-tools/faq/what-gt-github-enterprise">https://support.cc.gatech.edu/support-tools/faq/what-gt-github-enterprise</a>
- <a href="https://try.github.io/levels/1/challenges/1">https://try.github.io/levels/1/challenges/1</a>
- http://rogerdudler.github.io/git-guide/
- How to undo things:
  - https://github.com/blog/2019-how-to-undo-almost-anything-with-git

### Tools of the Trade: Anaconda

- Package manager for python useful for managing Python!
- From the author of Python's numpy and scipy packages

- To set up:
  - Download anaconda from <a href="https://www.continuum.io/downloads">https://www.continuum.io/downloads</a>
  - Install packages for this course:
  - conda install python=3 scipy numpy matplotlib jupyter notebook pandas pytables hdf5



# Tools of the Trade: Jupyter

Framework for interactive programming

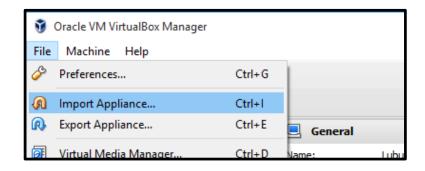
- Jupyter Notebook: a web interface to interactive programming
  - Interface for coding, viewing data, and plotting
  - Reproducible science

- Uses IPython
  - Access docstrings (help on commands)
  - Tab completion



### Materials for this Course:

- Download VirtualBox (free)
  - https://www.virtualbox.org/wiki/Downloads
- Download the .ovf image for the course (2 GB compressed, + ~5GB when added to virtualbox)
  - http://pace.gatech.edu/sites/default/files/Lubuntu32.ova





- Alternatively, install anaconda on your local machine and pull the materials from:
  - <a href="https://github.com/blakeflei/IntroScientificPythonWithJupyter">https://github.com/blakeflei/IntroScientificPythonWithJupyter</a>

### Overview

#### • Part I:

- Jupyter Notebook Overview
- Input/Output in Python
- Basic Math
- Indexing/Array Operations
- Plotting
- Fitting Plots

#### • Part II:

- Some Basic Statistics
- Signal Processing
- Ordinary Differential Equations
- Pandas
- Gotchas and Optmization

