

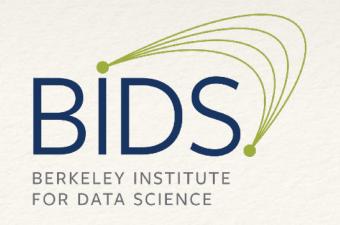


#### From Colombia to Jupyter:

an odd path through physics, open source software and data science

Fernando Pérez

fernando.perez@berkeley.edu

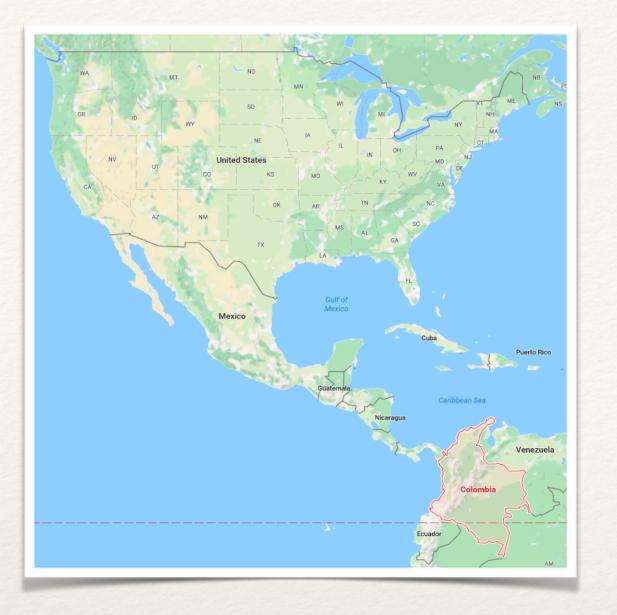






#### A bit about me...

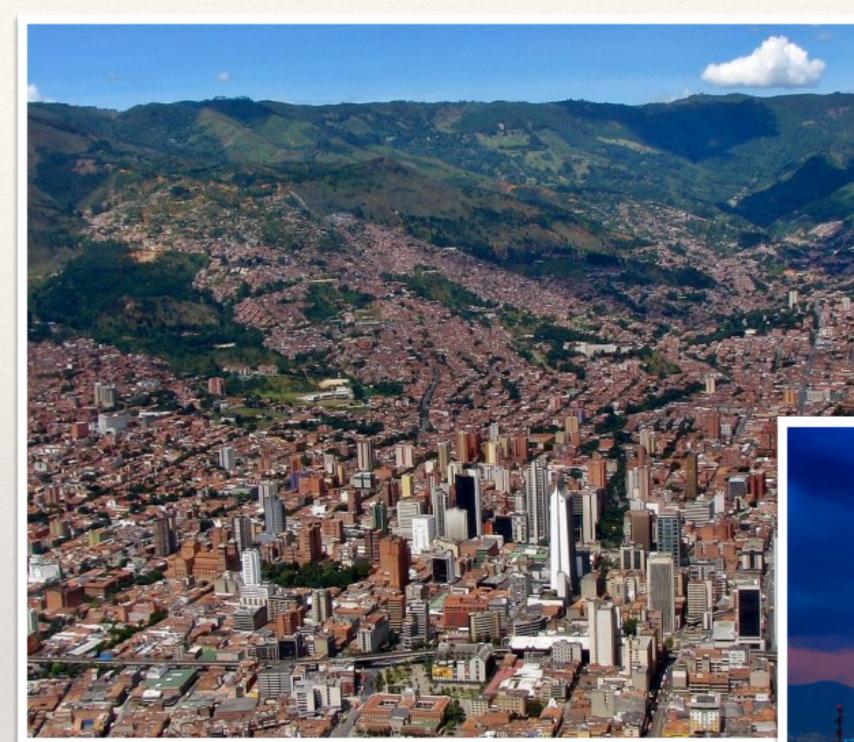








### Medellín, Colombia





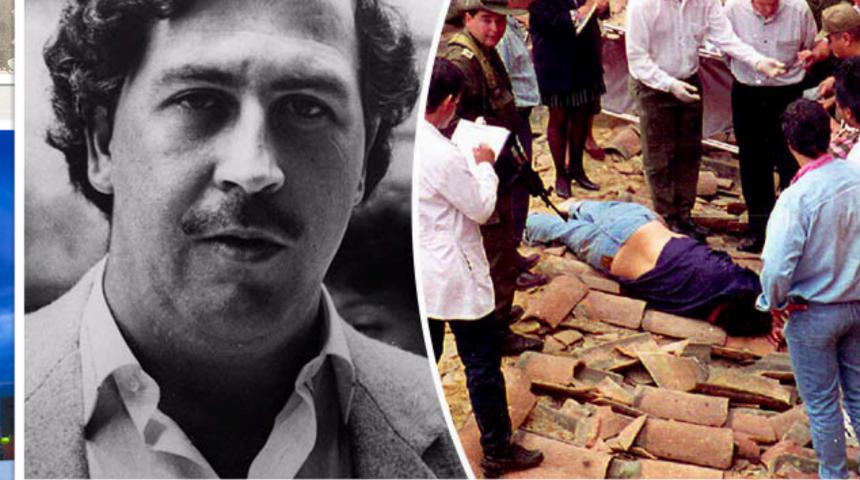
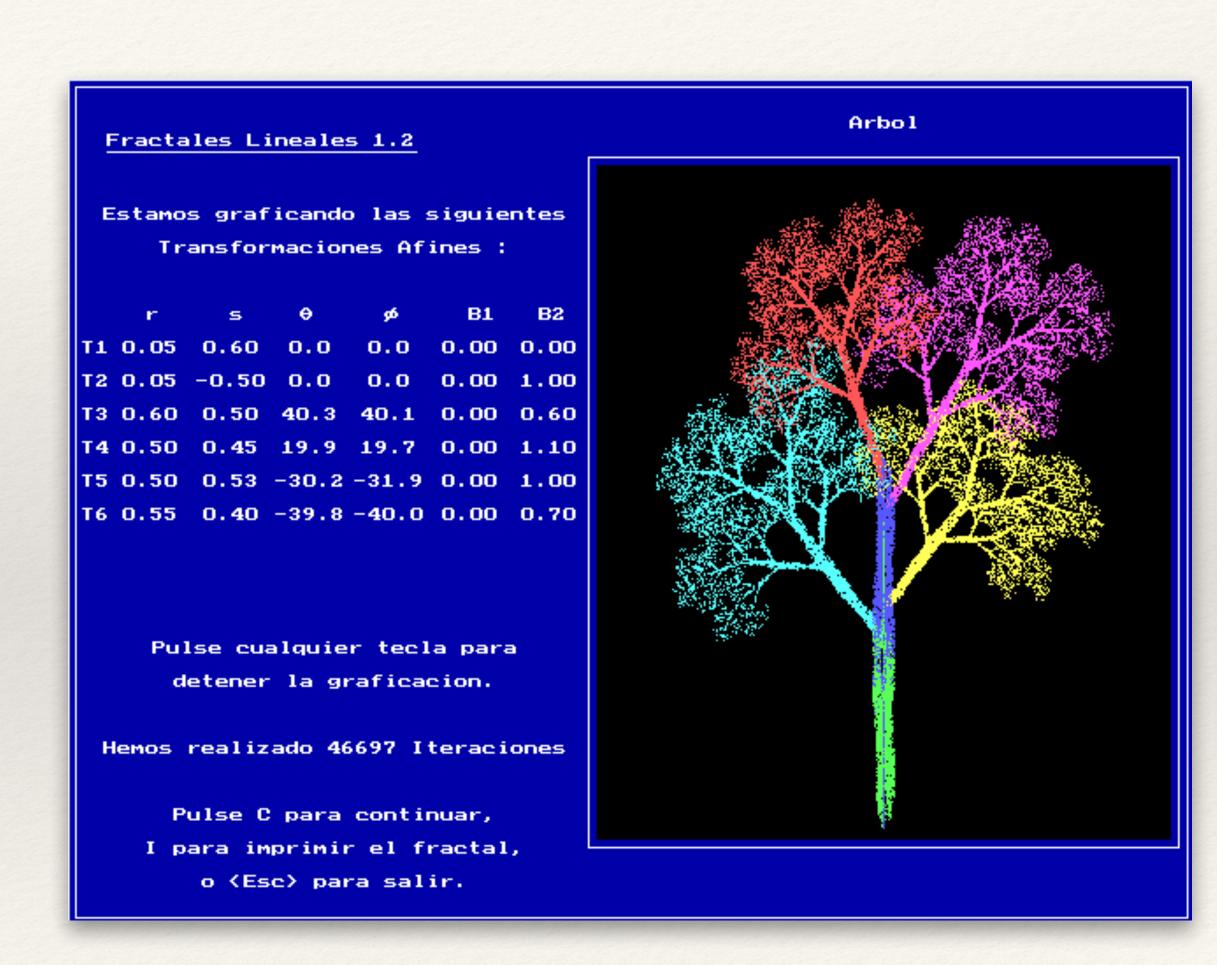


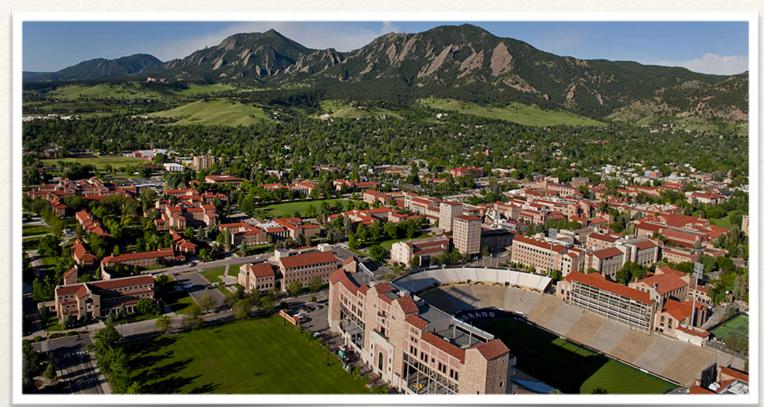
Image Credits:
latinorebels.com
totalspanishcolombia.com

#### My interest at the time: physics & computing

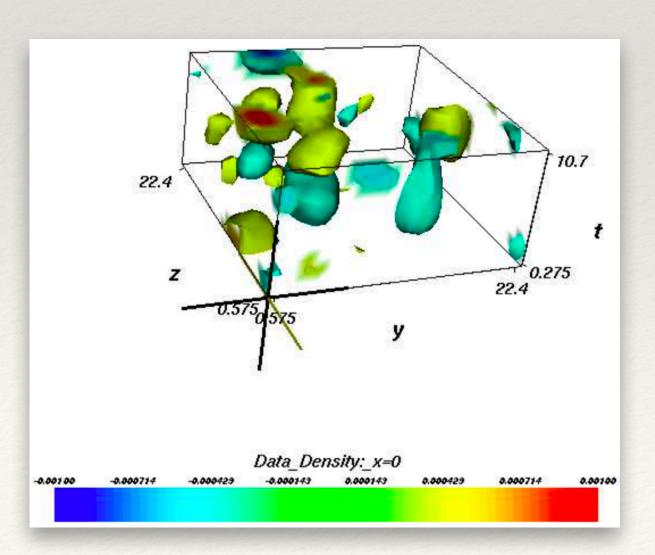
- Simulating fractals in TurboPascal
- Program on paper, use mom's office PC on weekends
- Debug on paper. Think a lot away from the screen

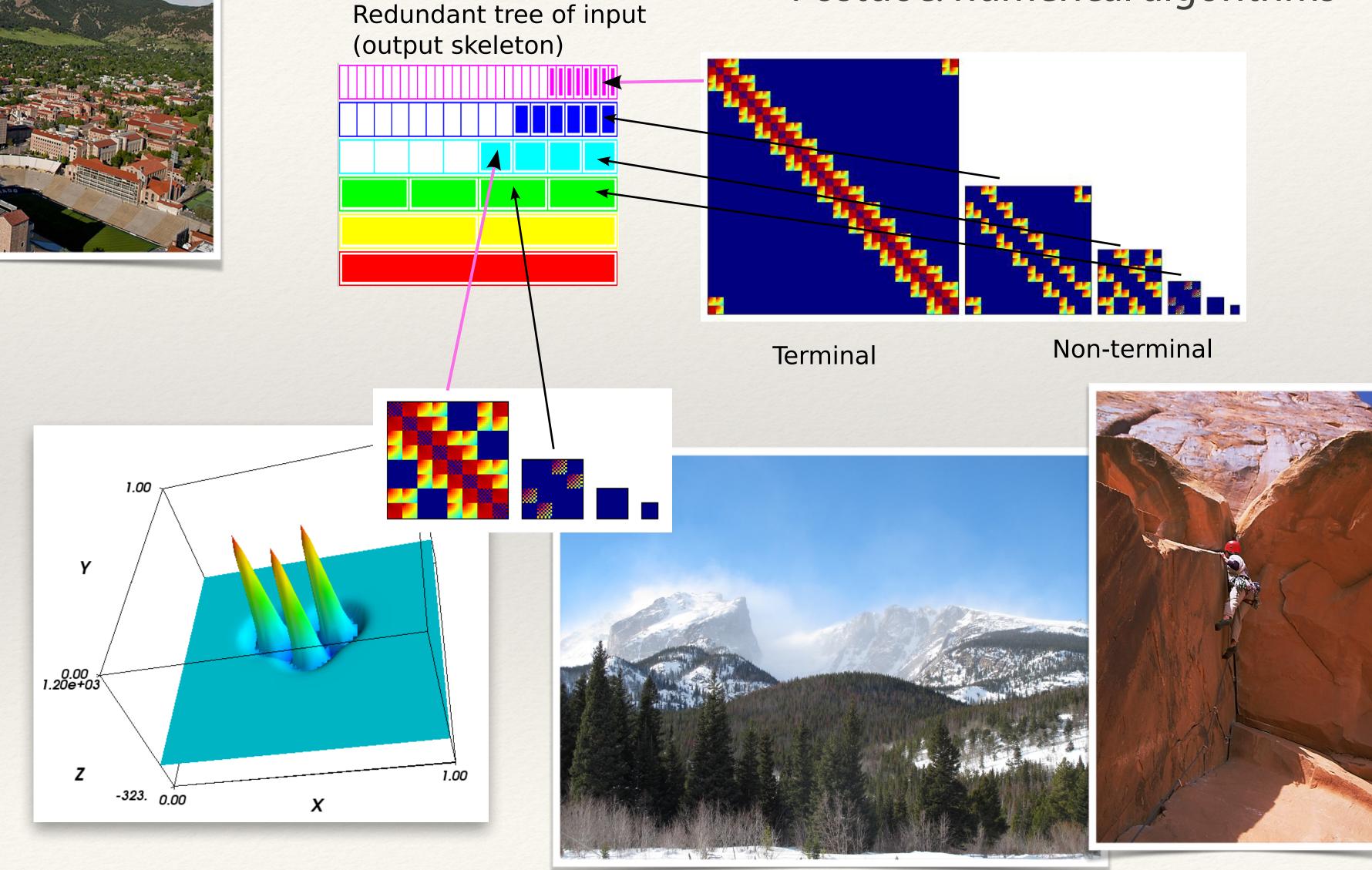


#### Physics and applied math at CU Boulder



PhD: Lattice QCD
Simulations





Postdoc: numerical algorithms

### Why do I do what I do?

#### Why?

- \* Ethical: openness as fairness
- \* Human/social: openness fosters collaboration.
- \* Epistemological: proprietary science is an oxymoron.
- \* Technical: Python was cool:)

#### Personal: crisis, motivation and support

- \* A PhD in crisis
- \* Support from
  - \* An incredible (second) advisor Anna Hasenfratz
  - \* My wife!!
  - \* A path forward from bad PhD to great Postdoc Gregory Beylkin.

#### What?

## "The purpose of computing is insight, not numbers"

-Hamming'62

## IPython: Interactive Python, 2001

A humble start: IPython 0.0.1, 259 LOC

"Just an afternoon hack"

```
ipython-0.0.1.py
ipython-0.0.1.py ×
   Globals for SI units (including g=9.8)
                                          : _load_units = %(_load_units)s
   Starting number for prompt counter
   Number of history items to store in cache : _cache_size = %(_cache_size)s
    load Numeric = 1
    _load_Gnuplot = 1
    load gracePlot = 1
    load_units = 1
    _cache_size
                = 1000
    _prompt_ini
   # *** Don't modify below unless you know what you're doing. ***
   # Crude first version, with minimal object structure. This could be done much
   # generators). But it seems to work ok. Haven't checked for memory circularity
   # problems, though.
   #**********************
           Copyright (C) 2001 Fernando P@rez. <fperez@pizero.colorado.edu>
      Distributed under the terms of the GNU General Public License.
       The full text of the GPL is available at:
    __author__ = 'Fernando P@rez. <fperez@pizero.colorado.edu>'
   __version__ = '0.1'
    #***********************
       """Simple interactive prompt like Mathematica's."""
       def __str__(self):
    return '\nIn['±_prompt_count`+']:= '
       """Simple interactive continuation prompt."""
                  ... '+' '*(len('In['+__prompt_count`+'_]:= ')-3)
   #***************************
   # Function definitions
   def _history_print(arg):
    """Printing with history cache management.
       This is invoked everytime the interpreter needs to print, and is activated by setting the variable sys.displayhook to it.""
             _p,_pp,_ppp,_cache,_prompt_count
```

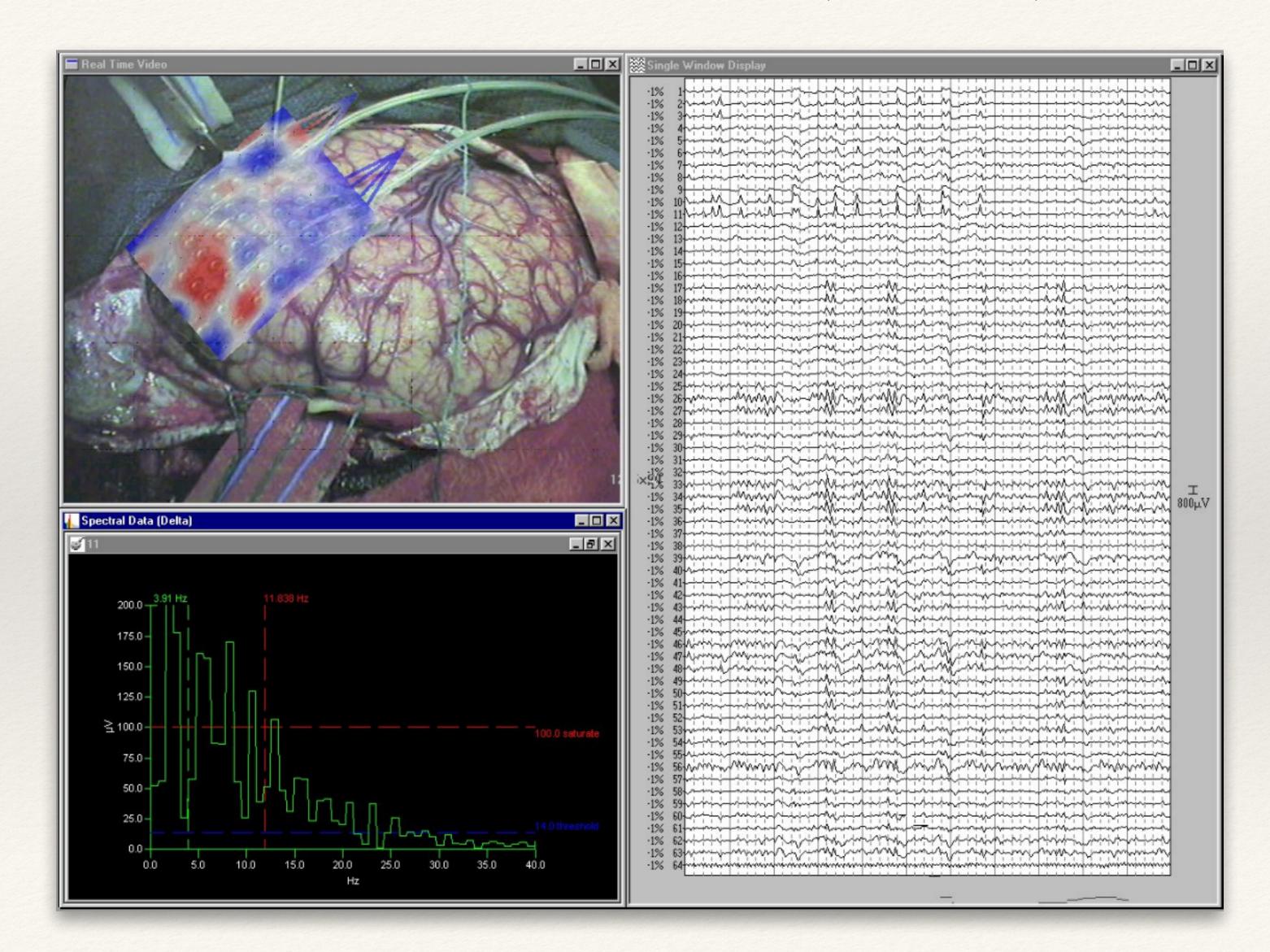
```
1. IPython: Users/fperez (python3.5)
 jlab) dreamweaver[~]> ipython
Python 3.5.2 |Continuum Analytics, Inc.| (default, Jul 2 2016, 17:52:12)
Type "copyright", "credits" or "license" for more information.
IPython 5.1.0 -- An enhanced Interactive Python.
          -> Introduction and overview of IPython's features.
%quickref -> Quick reference.
       -> Python's own help system.
object? -> Details about 'object', use 'object??' for extra details.
 n [1]: %pylab
Using matplotlib backend: MacOSX
Populating the interactive namespace from numpy and matplotlib
 n [2]: from IPython.display import display
   ...: from pandas datareader import data
   ...: from datetime import datetime
   ...: ticker = 'MSFT'
   stock = data.DataReader( ticker, 'yahoo', start=datetime(2012, 1, 1))
   ...: display(stock[:3])
   stock['Close'].plot(title='%s Closing Price' % ticker);
                                      Low Close Volume Adj Close
2012-01-03 26.549999 26.959999 26.389999 26.77 64731500 23.304317
2012-01-04 26.820000 27.469999 26.780001 27.40 80516100 23.852755
2012-01-05 27.379999 27.730000 27.290001 27.68 56081400 24.096507
In [3]:
Figure 1
                             MSFT Closing Price
      65
      60
      55
                                Aug 2014
                                      Feb 2015
                          Feb 2014
```

### First outcome: I was good for something

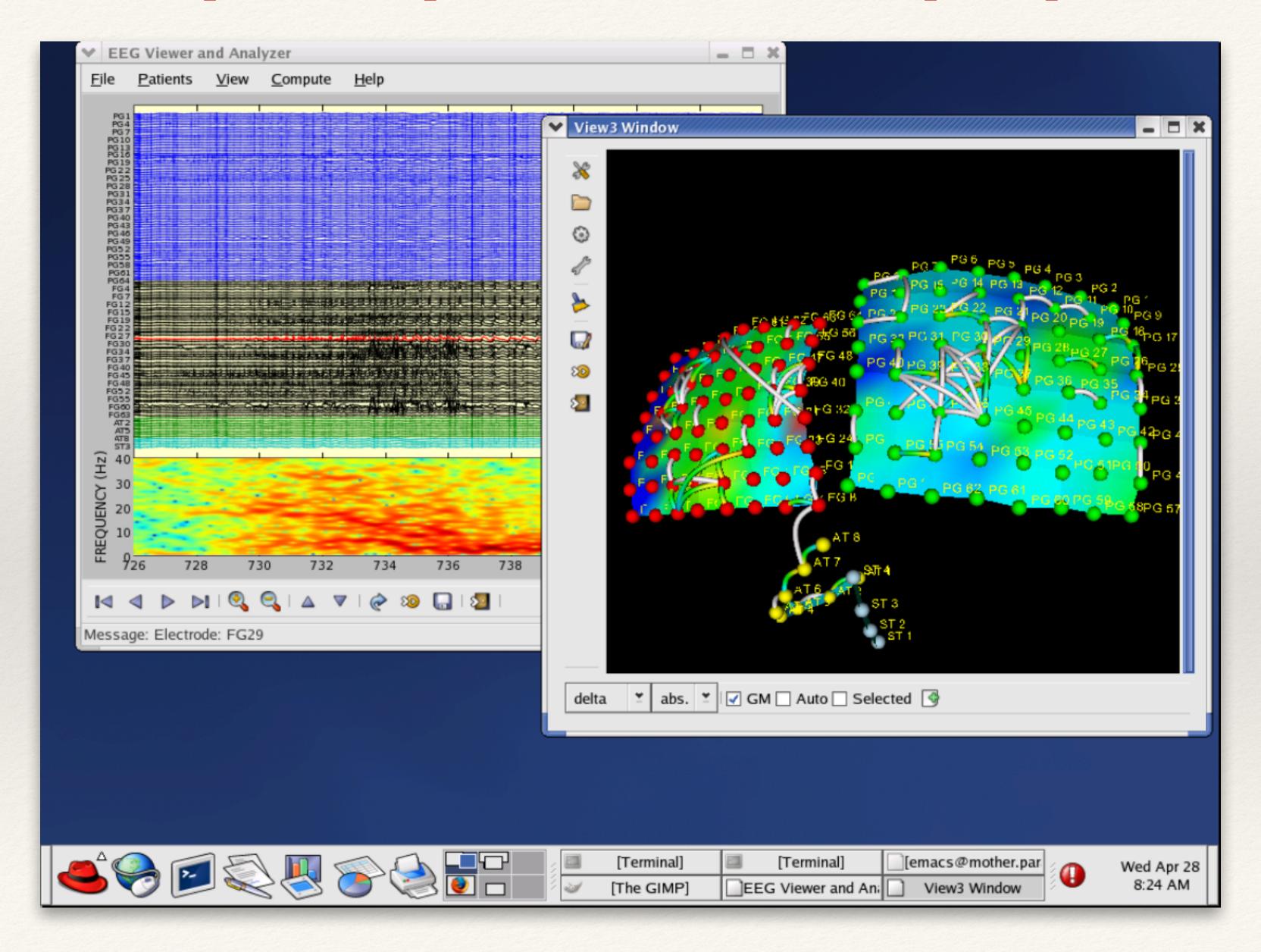
## Second outcome: finding a community

#### Built by regular individuals

John Hunter, Department of Pediatric Neurology, University of Chicago.



#### matplotlib: open replacement for proprietary tools



#### John D. Hunter, 1968-2012



#### Not just IPython: an entire ecosystem

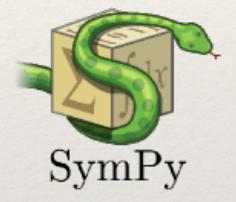






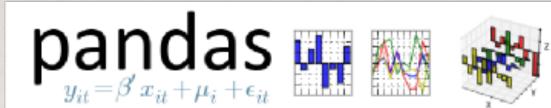




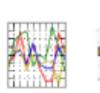


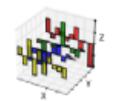










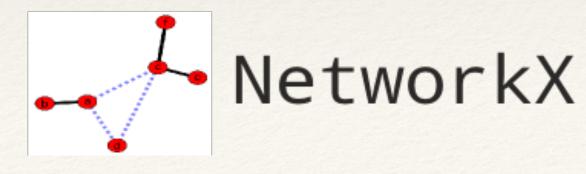












#### Having to justify our existence

SciComp Development Model Examples Wrapup

#### Outline

- Scientific Computing
  - Existing tools
  - Python?
- Development in Python
- OK, but does anyone use it?
  - EEG analysis for epilepsy
  - Multiwavelets for PDEs
  - JPL: Mars mission data visualization
  - PMV: structural bioinformatics
  - MayaVi: customizable data visualization
  - Sage
  - IPython

#### Jupyter team today: where all the credit goes

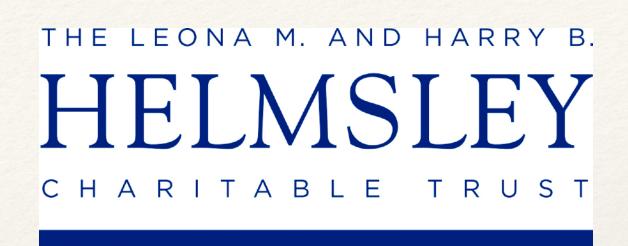




## Jupyter - funding and resources









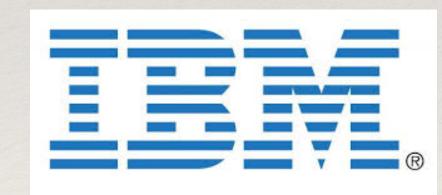














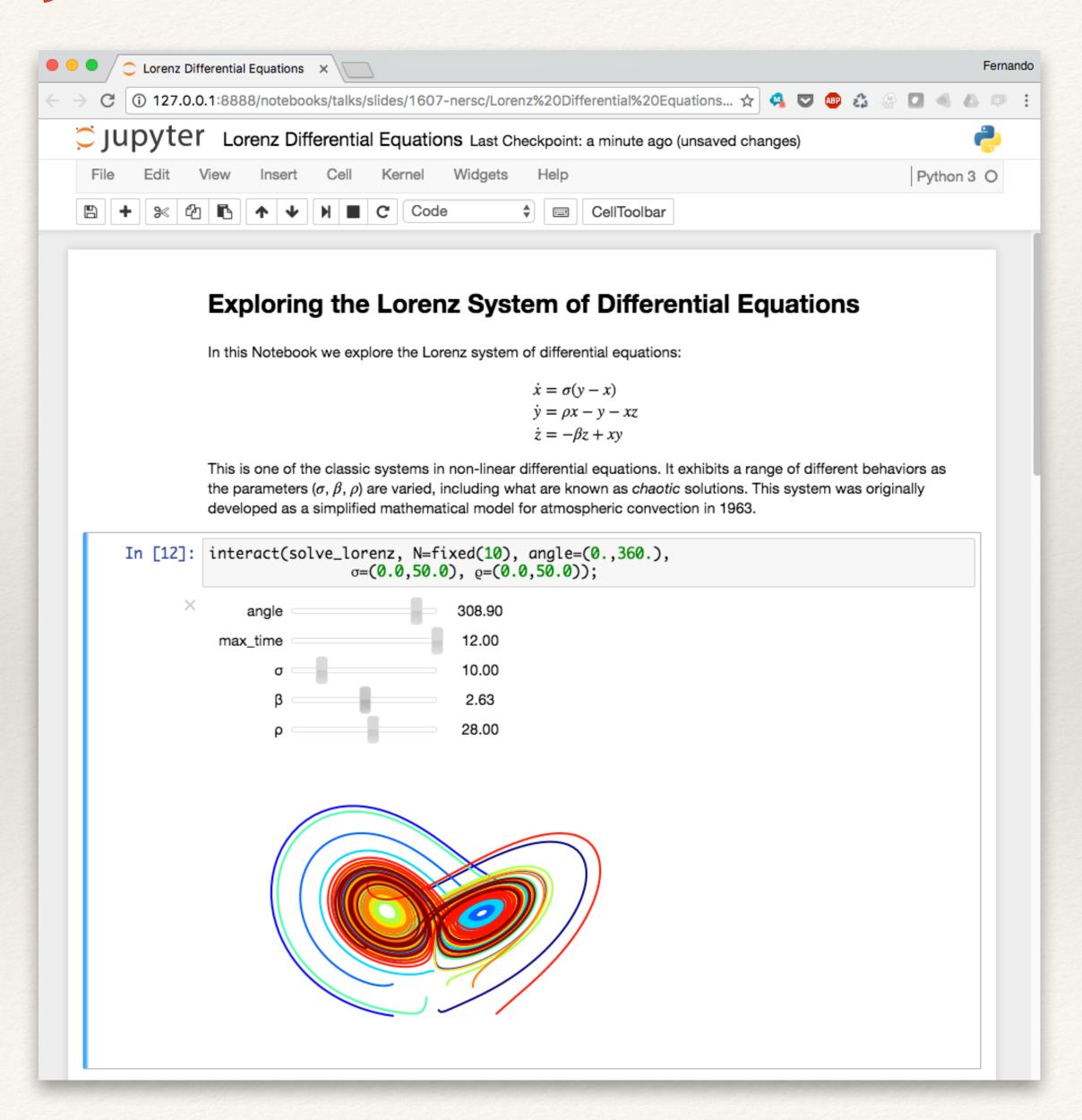






### The IPython/Jupyter Notebook

- \* Rich web client
- \* Text & math
- \* Code
- \* Results
- \* Share, reproduce.



## Jupyter Protocol is language agnostic





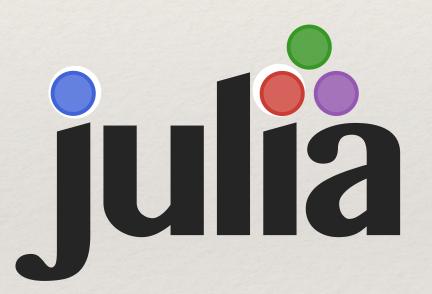
















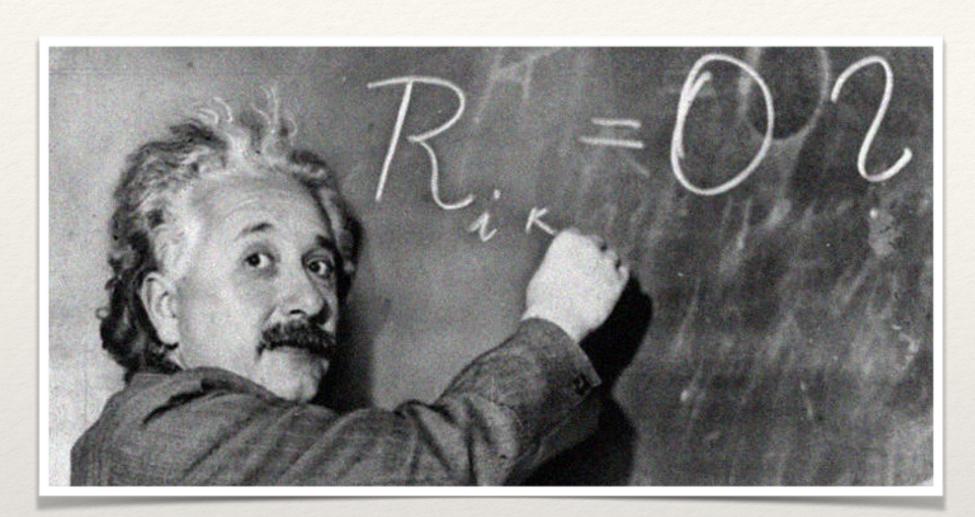






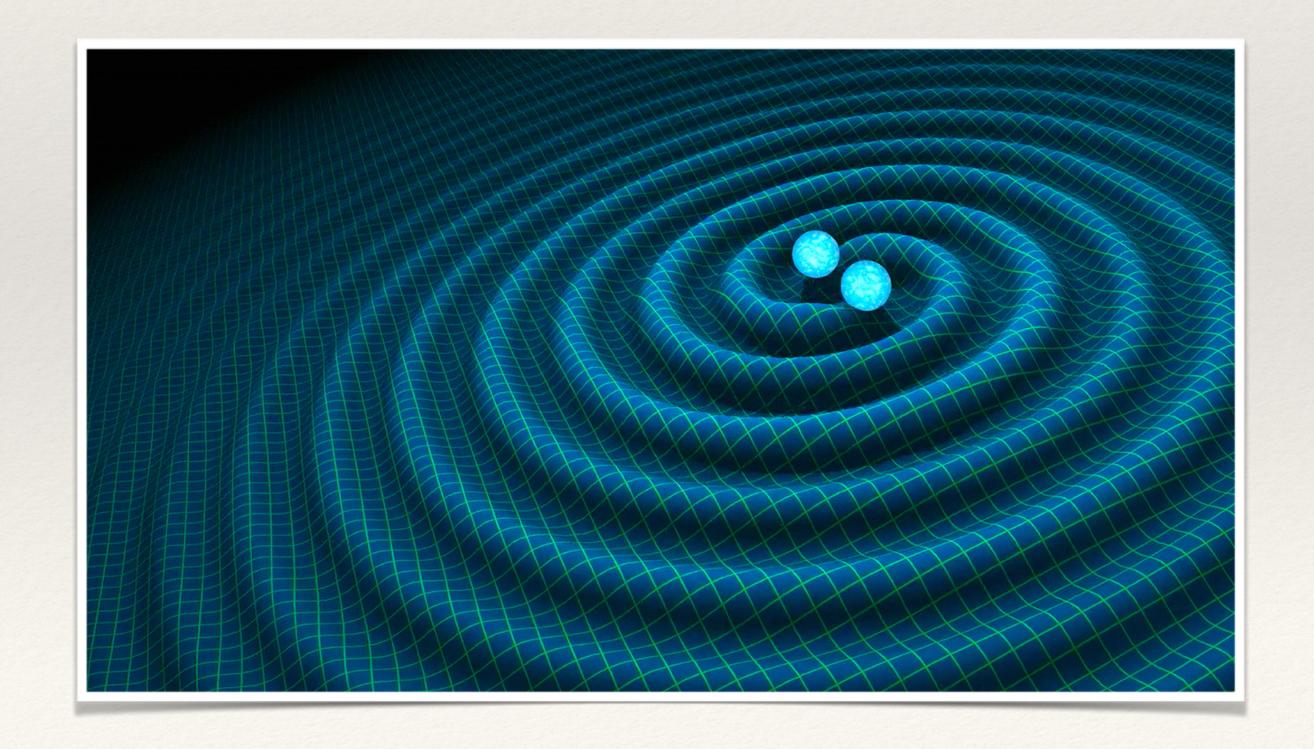
~100 different kernels: <a href="https://github.com/jupyter/jupyter/wiki/Jupyter-kernels">https://github.com/jupyter/jupyter/wiki/Jupyter-kernels</a>

#### A long time ago in a galaxy far, far away...



$$R_{\mu\nu} - \frac{1}{2} R g_{\mu\nu} + \Lambda g_{\mu\nu} = \frac{8\pi G}{c^4} T_{\mu\nu}$$

Einstein's Field Equations of General Relativity
Annalen der Physik, 1916



#### September 14, 2015





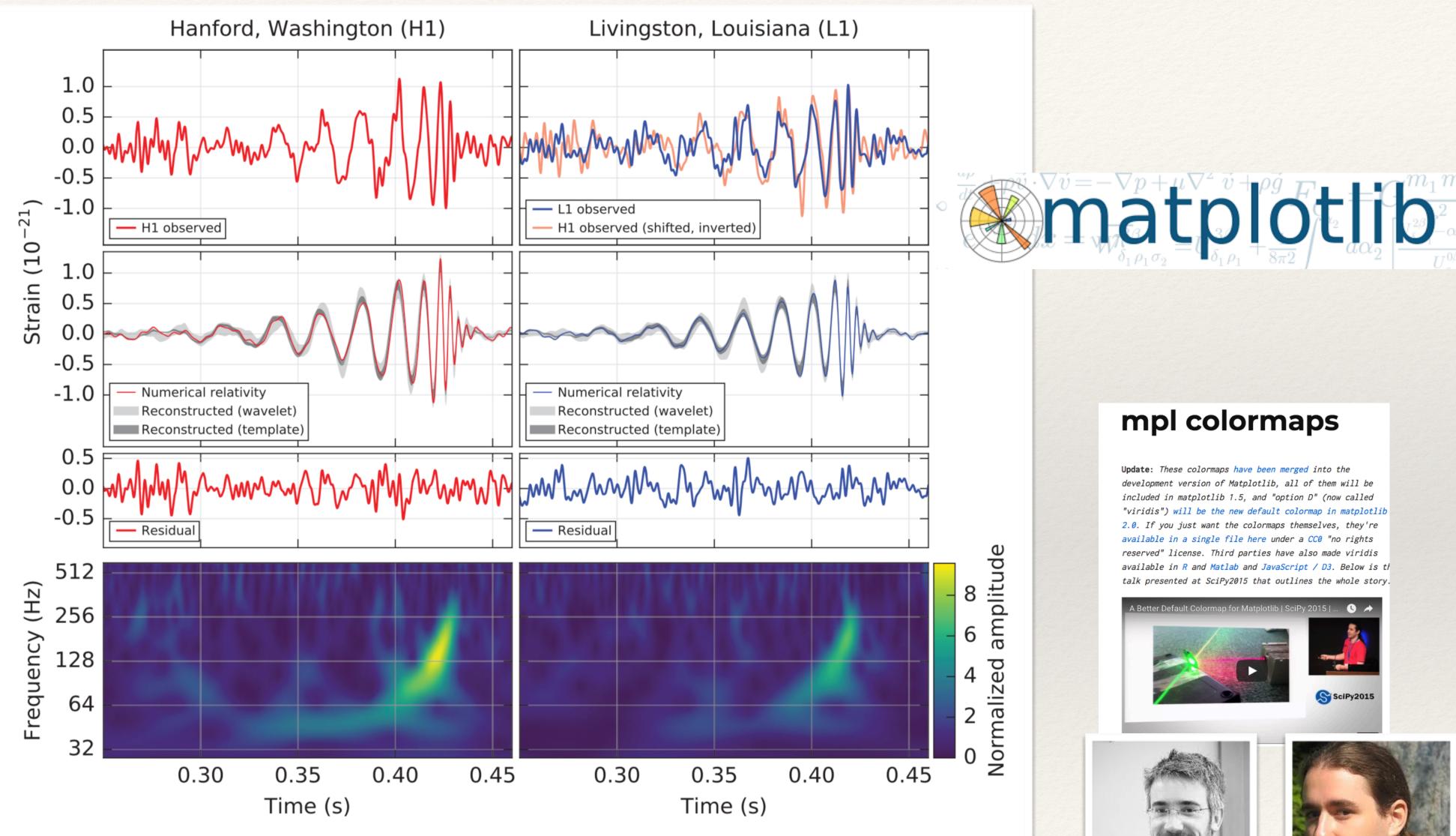
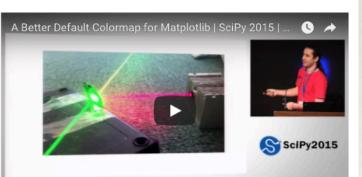


FIG. 1. The gravitational-wave event GW150914 observed by the LIGO Hanford (H1, left column panels) and Livingston (L1, right column panels) detectors. Times are shown relative to September 14, 2015 at 09:50:45 UTC. For visualization, all time series are filtered with a 35–350 Hz bandpass filter to suppress large fluctuations outside the detectors' most sensitive frequency band, and band-reject

#### mpl colormaps

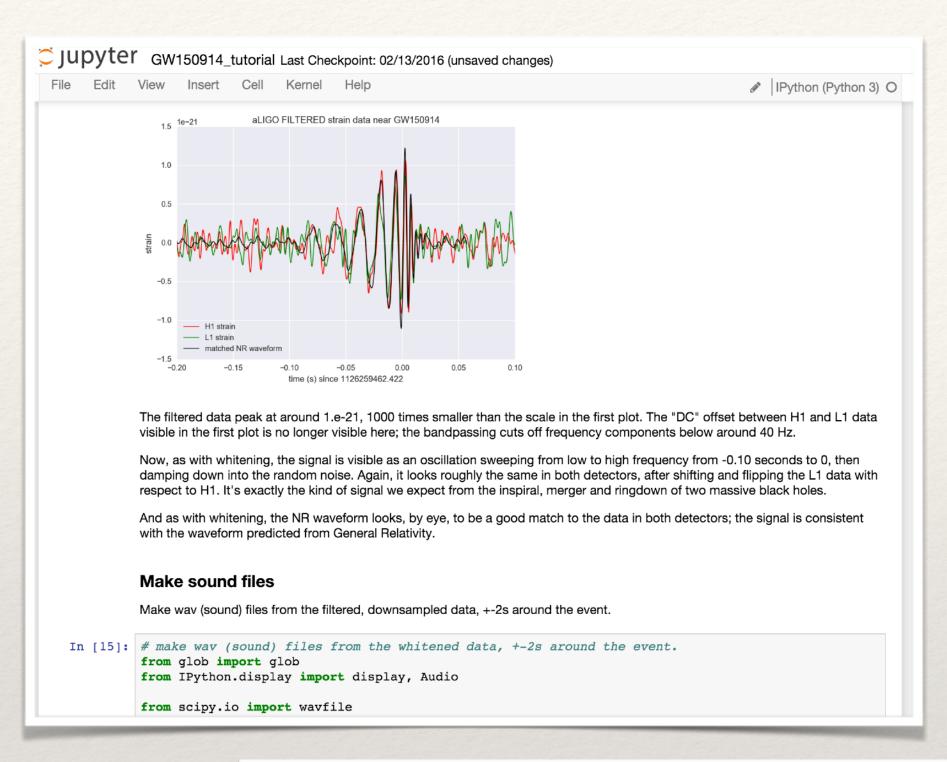
talk presented at SciPy2015 that outlines the whole story

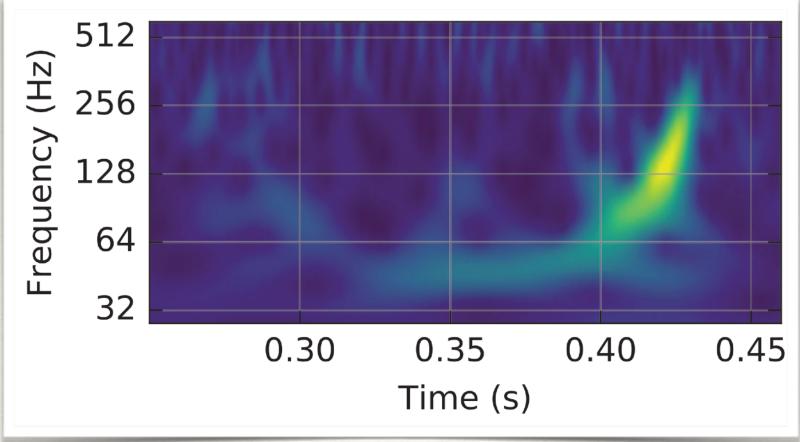






#### The song of the universe



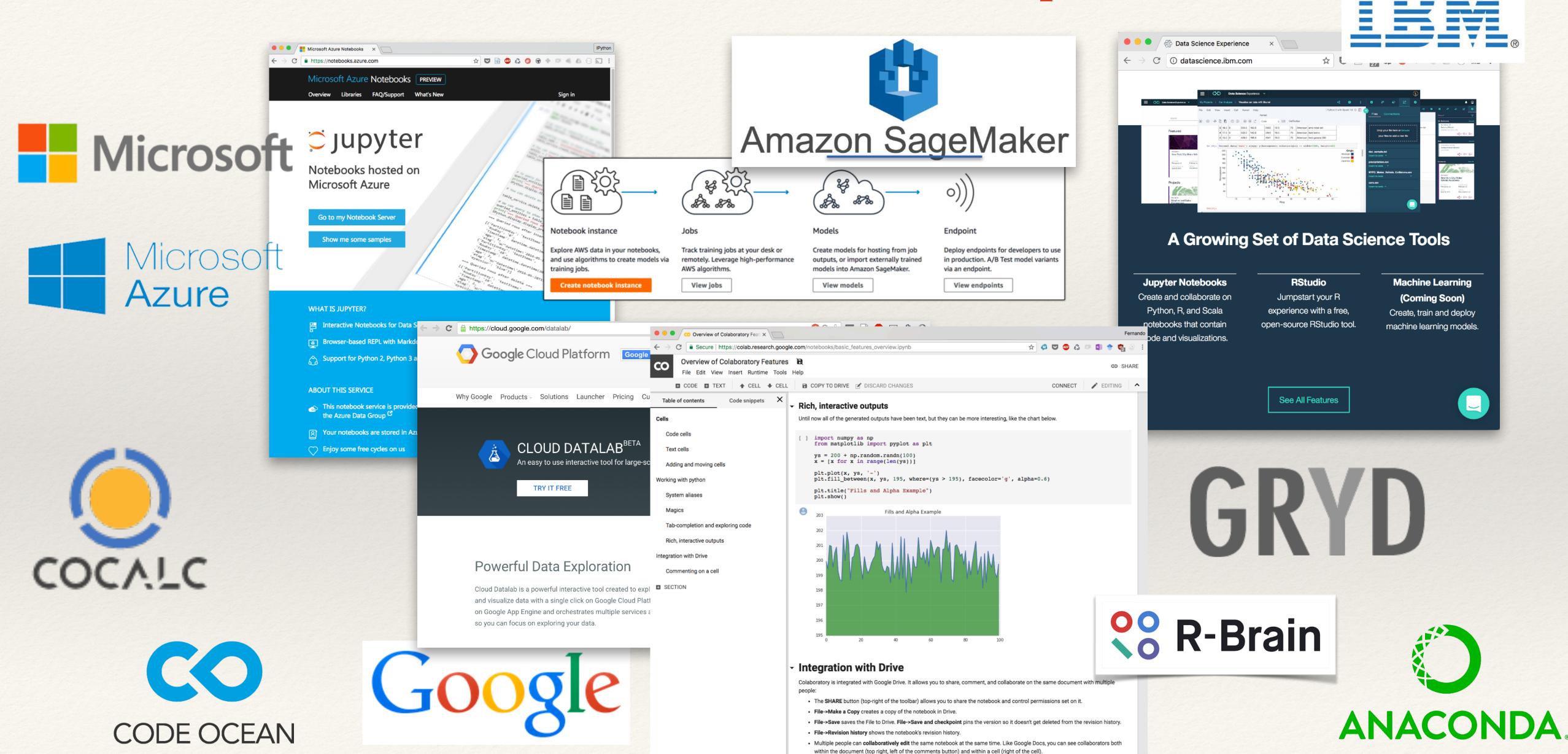


#### Make sound files

Make wav (sound) files from the filtered, downsampled data, +-2s around the event.

```
# make wav (sound) files from the whitened data, +-2s around the event.
from glob import glob
from IPython.display import display, Audio
from scipy.io import wavfile
# function to keep the data within integer limits, and write to wavfile:
def write wavfile(filename,fs,data):
    d = np.int16(data/np.max(np.abs(data)) * 32767 * 0.9)
    wavfile.write(filename,int(fs), d)
                                # Mon Sep 14 09:50:45 GMT 2015
tevent = 1126259462.422
                                # seconds around the event
deltat = 2.
# index into the strain time series for this time interval:
indxt = np.where((time >= tevent-deltat) & (time < tevent+deltat))</pre>
# write the files:
write_wavfile("GW150914_H1_whitenbp.wav",int(fs), strain_H1_whitenbp[indxt])
write_wavfile("GW150914_L1_whitenbp.wav",int(fs), strain_L1_whitenbp[indxt])
write wavfile("GW150914 NR whitenbp.wav", int(fs), NR H1 whitenbp)
for wav in glob('*whitenbp.wav'):
    display(wav)
    display(Audio(filename=wav))
'GW150914_H1_whitenbp.wav'
                     0:00 🦸
```

#### Wide industrial adoption





THE OFFICIAL JUPYTER CONFERENCE

AUG 21-22, 2018: TRAINING AUG 22-24, 2018: TUTORIALS & CONFERENCE NEW YORK, NY

Leverage the power of Jupyter for collaborative, extensible, scalable, and reproducible data science.









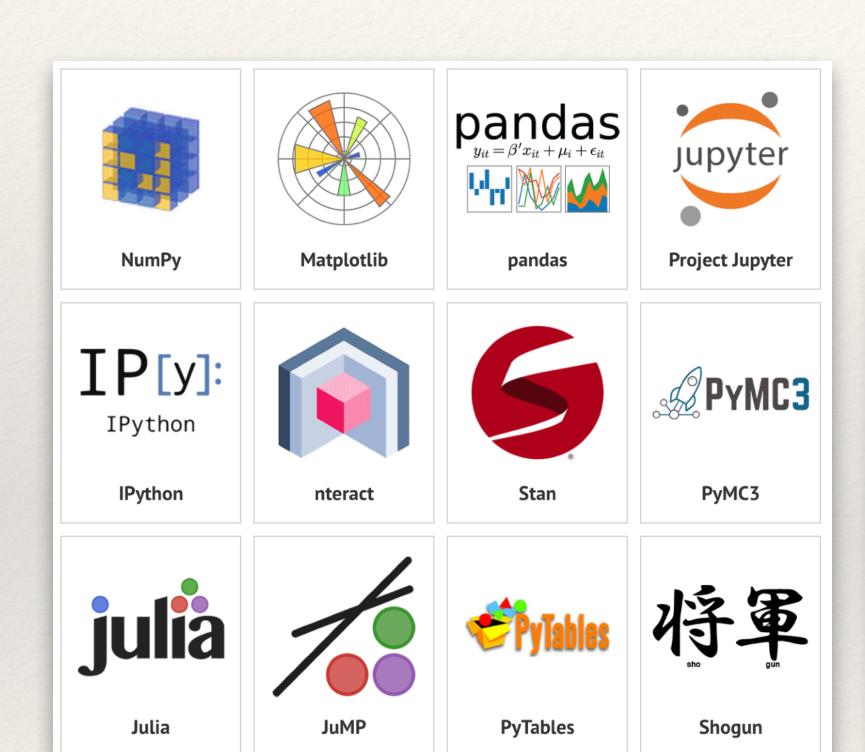
jupytercon.com @JupyterCon, photos by @triciaphoto

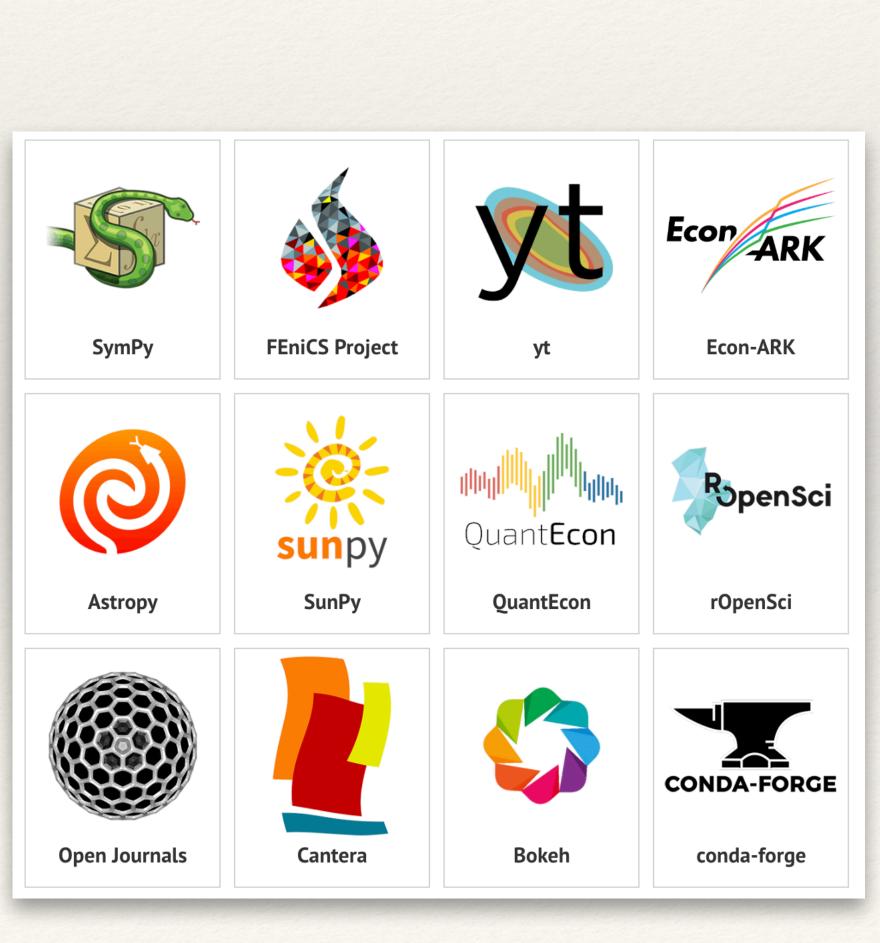
# If the world doesn't give you a space, you'll need to create it

#### 2012

# NUMF(G)CUS

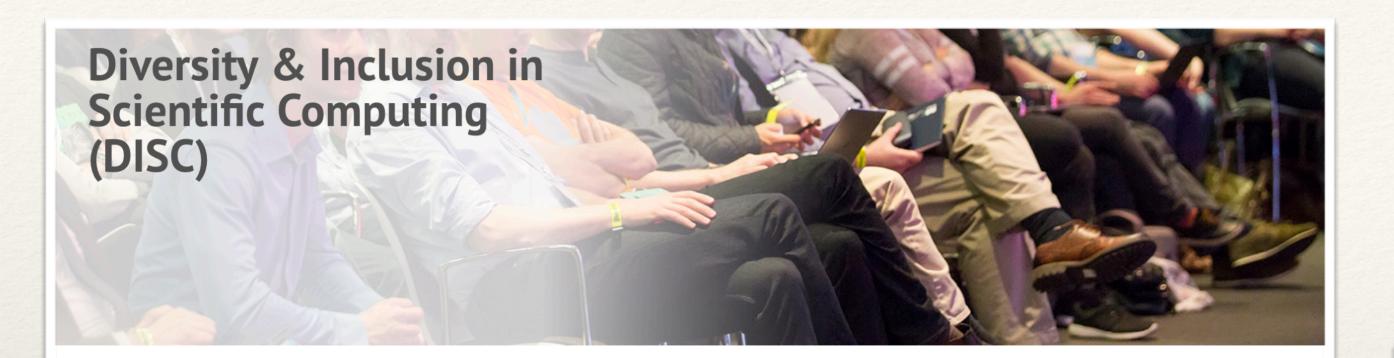
#### OPEN CODE = BETTER SCIENCE







#### NumFOCUS: beyond code, communities



#### **DISC Program Mission**

NumFOCUS recognizes that the open source data science community is currently highly homogenous. We believe that diverse contributors and community members produce better science and better projects. NumFOCUS strives to help create a more diverse community through initiatives and programming devoted to increasing participation by and inclusion of underrepresented people.

Join the DISC Mailing List

#### **NumFOCUS Diversity Statement**

NumFOCUS welcomes and encourages participation in our community by people of all backgrounds and identities. We are committed to promoting and sustaining a culture that values mutual respect, tolerance, and learning, and we work together as a community to help each other live out these values.

For a more detailed explication of NumFOCUS's position on diversity in the community, see the Diversity Appendix.



The John Hunter Matplotlib Summer Fellowship, named in memory of Matplotlib creator John Hunter, sponsors one to two students to work full-time for 3 months on Matplotlib during the summer (in the northern hemisphere), supervised and mentored by a senior contributor from the project. The fellowship is designed to help prepare recipients to become active contributors and core maintainers of Matplotlib.

Learn More About Matplotlib

Donate to Support the Fellowship



#### 2013: Berkeley Institute for Data Science















December 12, 2013, 11:00 - 3:00 pm Banatao Auditorium, Sutardja Dai Hall















# Creating good institutional spaces is hard, but critical!



#### Reproducible Research

An article about computational science in a scientific publication is **not** the scholarship itself, it is merely **advertising** of the scholarship. The actual scholarship is the complete software development environment and the complete set of instructions which generated the figures.

Buckheit and Donoho, WaveLab and Reproducible Research, 1995

### Collaborative and Reproducible Data Science

#### STAT 159 @ Berkeley, Fall 2017

- Version control: Git and GitHub
- \* Programming: Python
- \* Process automation: Make
- Data analysis: Numpy, Pandas, Matplotlib, NLTK, Scikit-Learn, ...
- \* Documentation: Sphinx
- Software testing: PyTest
- Continuous Integration: Travis
- \* Reproducible containers: Binder

Jupyter

http://bit.ly/stat159-f17

### Student feedback

Anyway, I would like to meet with you in the coming weeks to update you about the progress I've made in my jump into reproducibility, especially my experience with contributing to pandas and the few chapters of "The Practice of Reproducible Research" I got to read.

New open source contributor

assistance. I was mainly interested in having you as an advisor because I'm interested in the idea of responsible research practices in this type of setting where the data cannot be shared - what do responsible research practices look like for analysis like this? How do I present the results in a way that shows all the steps taken and all the analyses run without giving too much information about the data?

Undergraduate research project

Journalist who now is applying to Data Science graduate programs (admitted to Columbia, JH, ...)

Your class still exert a great influence on my current projects. I've been working on create detailed buyer personas since I came back to China and using the method you taught in class to develop pricing and operating algorithm with Python, establishing a price estimation model and optimizing the valuation system of Airbnb with modified AeroSolve Module.

To be honest, I was hesitating before whether I could do a good job in data analysis given that I originally majored in journalism. Thanks to your encourage, now I feel more confident and develop a clear career

### Data 8 & Data 100: massive uptake



D8: ~1,300 students

D100: ~800 students



### Data 8 & Data 100 Enrollment Data 8 Data 100 1200-1000 800 600 400 200-

http://data8.org - http://ds100.org

# Fastest growing courses in Berkeley history

#### Data 8 in Fall 2018

- \* ~ 1,300 enrolled students
- \* ~ 200 waitlisted

#### **Annual combined numbers**

- Data 8: ~ 3,000 students
- \* UC Berkeley: ~ 7,500

At steady state, will easily reach ~50% of campus!

## Last two points: representation...

### Fair participation of all, across

- \* Gender
- \* Ethnic
- Religious
- \* National
- \* Economic
- \* ... boundaries, with support, opportunity and respect.

### Representation does matter!

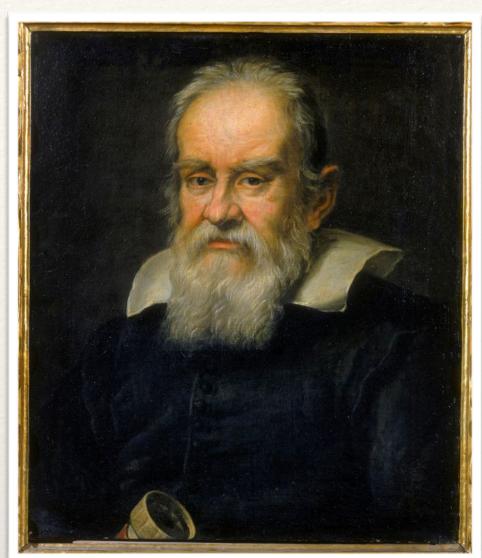




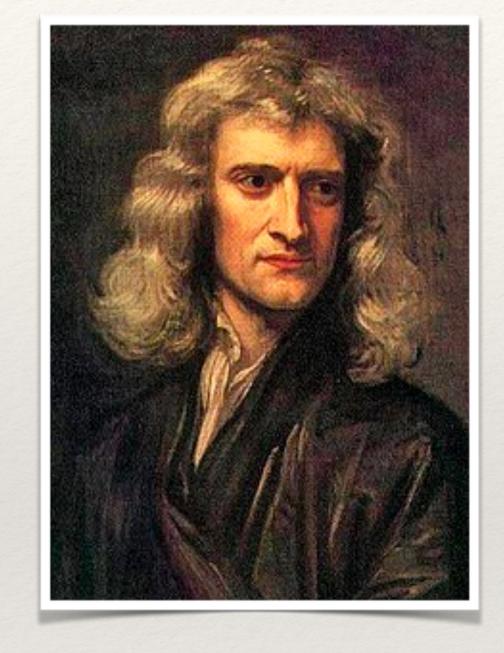
Williams [Venus/Serena's father] had created a plan to turn his daughters into champions

"The blueprint was already there," Francois [Naomi's father] told me. "I just had to follow it."

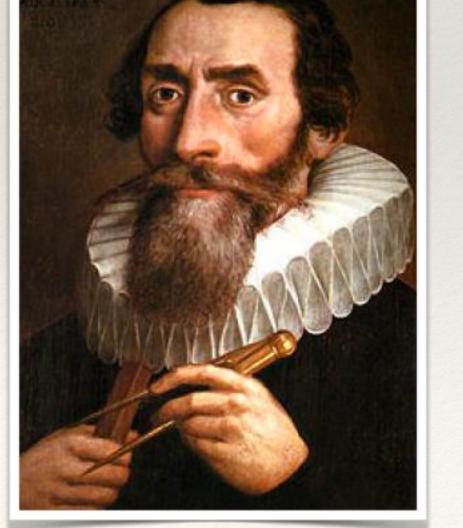
# But... a teenager in Colombia...



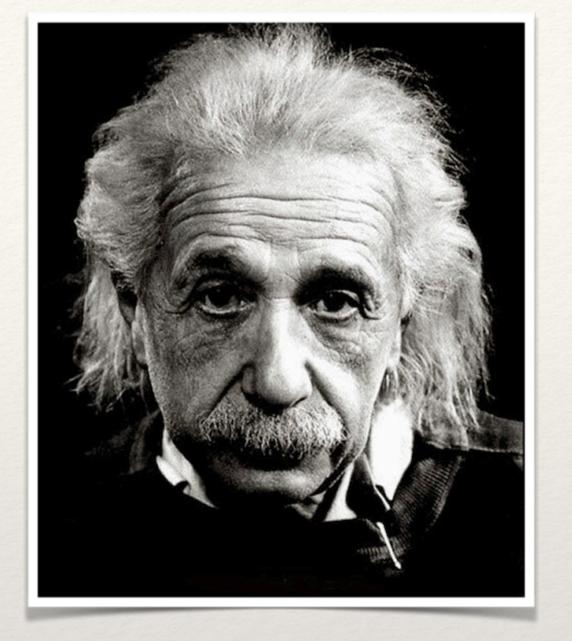
Galileo Galilei 1564-1642



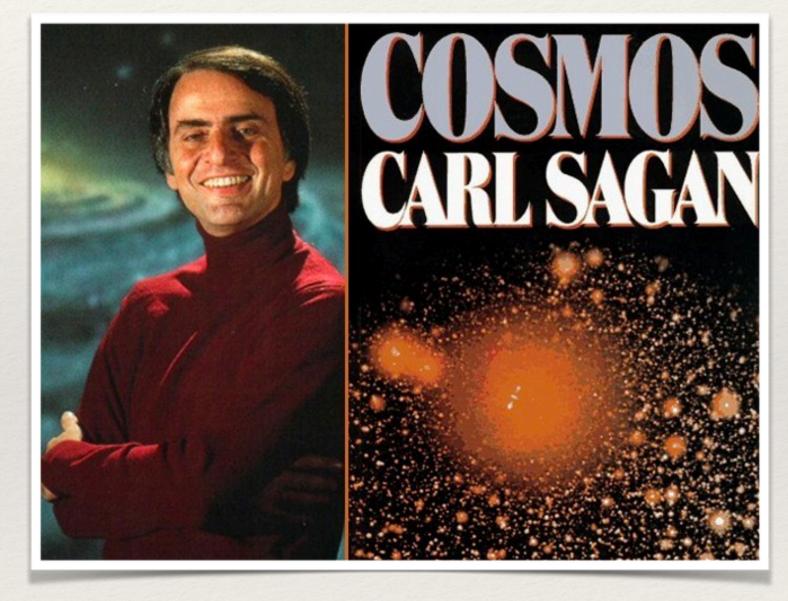
Isaac Newton 1643-1727



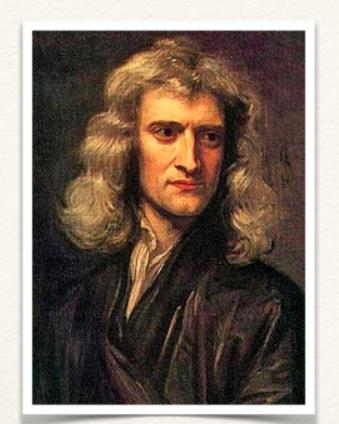
Johannes Kepler 1571-1630



Albert Einstein 1879-1955



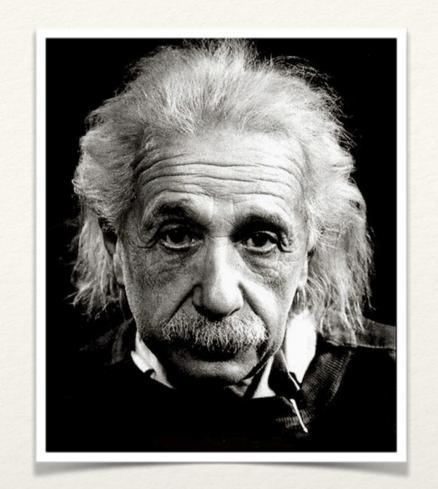
Carl Sagan 1934-1996

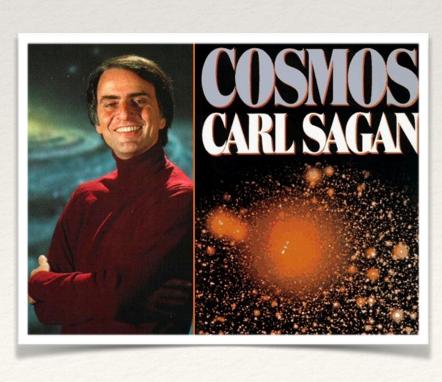




# humanity and ideas







### ... and careers

## Choose your mentors carefully

- PhD Advisor: one of the most important relationships in your life.
- \* Power dynamics is stacked against you.
- \* Personal qualities of mentor have to compensate for that...
  - And in many cases they do! There are amazing mentors out there:)
- \* Due diligence: ask hard questions of former students, postdocs and the mentor.
- \* A good mentor **pushes you hard** to do your best work, but always treats you first as a human being who merits **respect**.
- In a bad relationship, walk away! The earlier the better.

### Beyond Academia?

#### You can choose a different path!

- It does NOT mean you
  - are not smart/hard working enough,
  - are a sellout,
  - only care about \$\$\$,
  - don't care about the really hard/interesting problems,
  - wasted your time going to grad school,
  - \* are a failure as a person,

**\*** ...

# Beyond Academia...



#BPEP - connecting the #entrepreneurial #postdoc community at @UCBerkeley to #startup #founders who've been there!



7:45 PM - 20 Sep 2018



#### **Science Communication & Careers Beyond the Bench**



#### **Keynote Address**

5:00pm

Jamie Talan, MPH

Atlantic Fellow at Global Brain Health Institute,

UCSF Memory & Aging Center

#### **Panel Discussion with Science Communication Professionals**

6:00pm

#### Danielle Pasquel, PhD

Associate Scientific Director at Golin

#### Deb Aronson, PhD

VP, Medical Director at ghg

#### Lisa Brown, PhD

Medical Science Liason at Assurex Health

#### Elizabeth M. Vancza, PhD, DABT

Senior Toxicologist, Safebridge Consultants, Inc.

#### Travis J. Bernardo, PhD

Senior Medical Writer, BGB Group

#### **Networking Reception with Panelists**

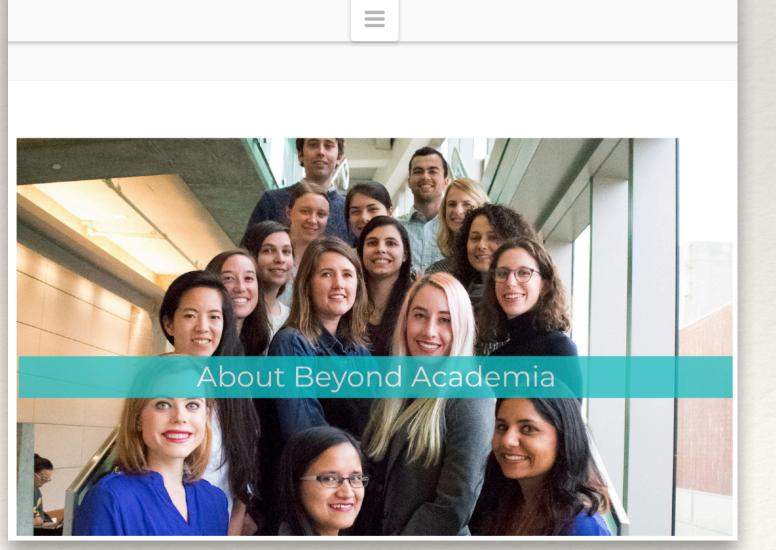
7:00 - 8:00pm

# Event Hosted By: Networking Canal NYCSciComm.Org Career & Professional Development Program for Graduate Students and Postdocs Graduate Division of Biomedical Sciences Belfer Institute for Advanced Biomedical Studies

EINSTEIN

Albert Einstein College of Medicine

DOI: 10.1126/science.1200613



Beyond Academia
Connecting PhDs with the World

### Thank You!