



**OpenDreamKit**

**Computational environments  
for research and education**

**Min Ragan-Kelley**

**Simula Research Lab**

# OpenDreamKit

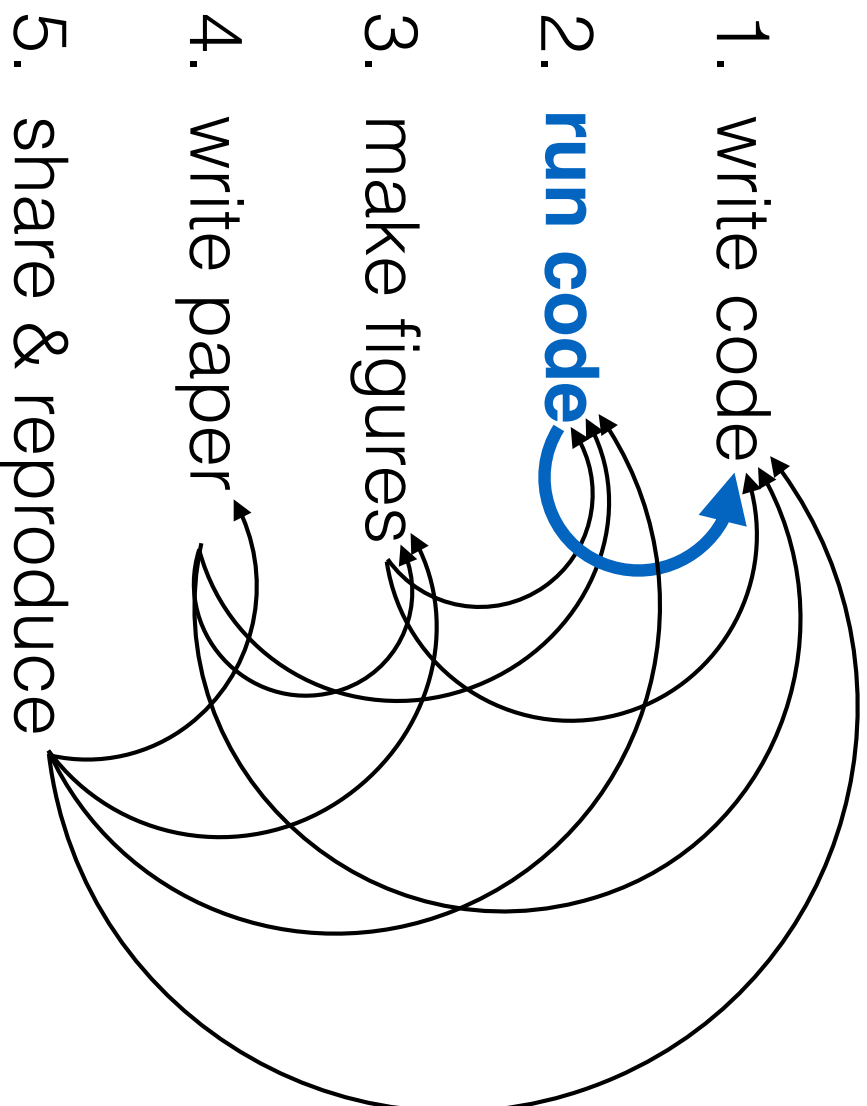
- H2020 project
- 16 Institutions
- 4 Years (2015-2019)

## Virtual Research Environments

- Generic (Jupyter, SageMath)
- Domain-specific (OOMMF micromagnetics)



# How do we do computational research?



**Python**



# IPython Interactive Python

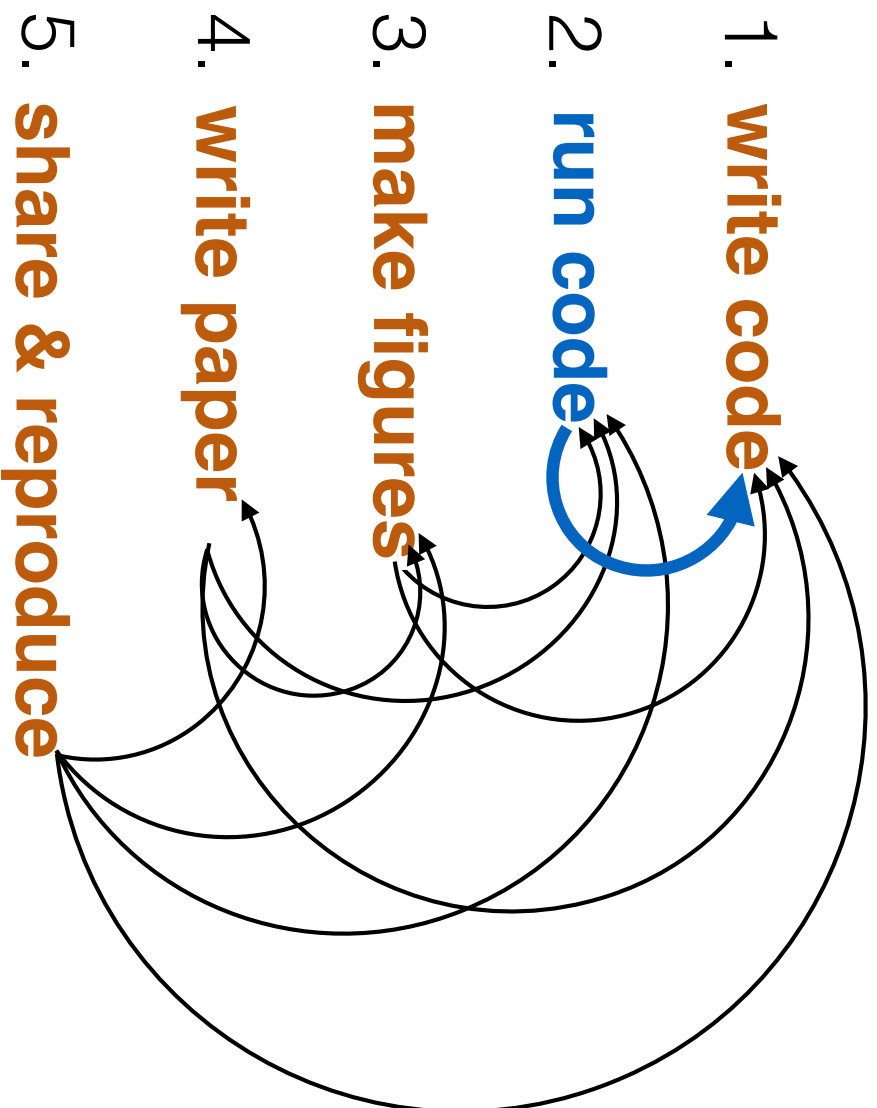
helps run code

- tab completion
- introspection
- %magics

```
minrk[02:13] ~/Documents/Jupyter/pres/AGU-2014 $ !python
```

A terminal window with a white background and a thin grey border. The prompt is "minrk[02:13] ~/Documents/Jupyter/pres/AGU-2014 \$". The command "!python" has been entered and executed, resulting in a blank terminal area below the prompt.

# What about Jupyter?





# What is Jupyter?

## Network Protocol



## ØMQ + JSON

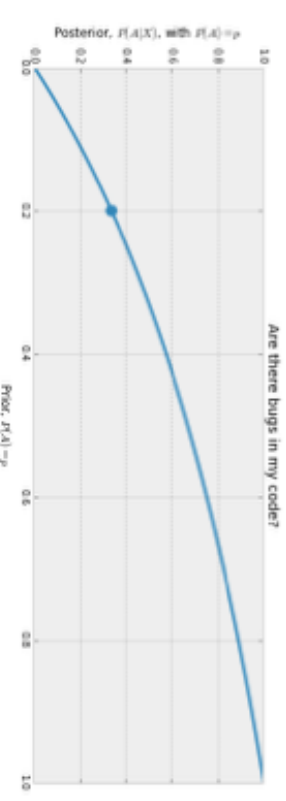
## Document Format

We have already computed  $P(X|A)$  above. On the other hand,  $P(X|1 - A)$  is subjective: our code can pass tests but still have a bug in it, though the probability there is a bug present is reduced. Note this is dependent on the number of tests performed, the degree of complication in the tests, etc. Let's be conservative and assign  $P(X|1 - A) = 0.5$ . Then

$$P(A|X) = \frac{1 \cdot p}{1 \cdot p + 0.5(1 - p)}$$
$$= \frac{1 + p}{2p}$$

This is the posterior probability. What does it look like as a function of our prior  $p \in [0, 1]$ ?

```
figsize(12.5, 4)
p = np.linspace(0, 1, 50)
plt.plot(p, 2 * p / (1 + p), color="#348AB0", lw=3)
# plt.fill_between(p, 2*p/(1+p), alpha=.5, facecolor="#A66020")
plt.scatter(0.2, 2 * (0.2) / 1.2, s=140, c="#348AB0")
plt.xlim(0, 1)
plt.ylim(0, 1)
plt.xlabel("Prior, $P(A) = p$")
plt.ylabel("Posterior, $P(A|X)$, with $P(A) = p$")
plt.title("Are there bugs in my code?")
matplotlib.text.Text at 0x1051de650
```





# Jupyter Protocol


## supercharge the P in REPR\*L

any mime-type output

- text
- svg, png, jpeg
- latex, pdf
- html, javascript
- interactive widgets

The screenshot shows a Jupyter notebook interface with several code cells and their outputs:

- Cell 5:** `print(df.head())` outputs a table with columns: date, cake, lies, pie.
- Cell 14:** `Math(r''',f(x) = \int_{-\infty}^{\infty} \hat{f}(\xi) e^{i2 \pi i \xi x} d\xi` outputs a mathematical formula.
- Cell 15:** `@interact def factor_xn(n=5): display(Eq(x**n-1, factor(x**n-1)))` outputs an interactive widget for a polynomial factorization.
- Cell 16:** A calendar widget showing months from Jan 2013 to Oct 2014.

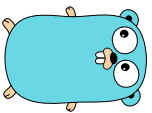
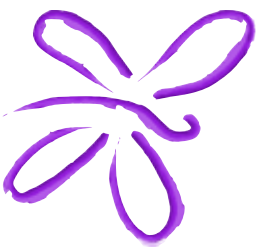


# Jupyter Protocol is language agnostic

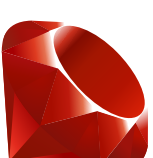
 **Scala**




**Julia**



 **python**<sup>TM</sup>

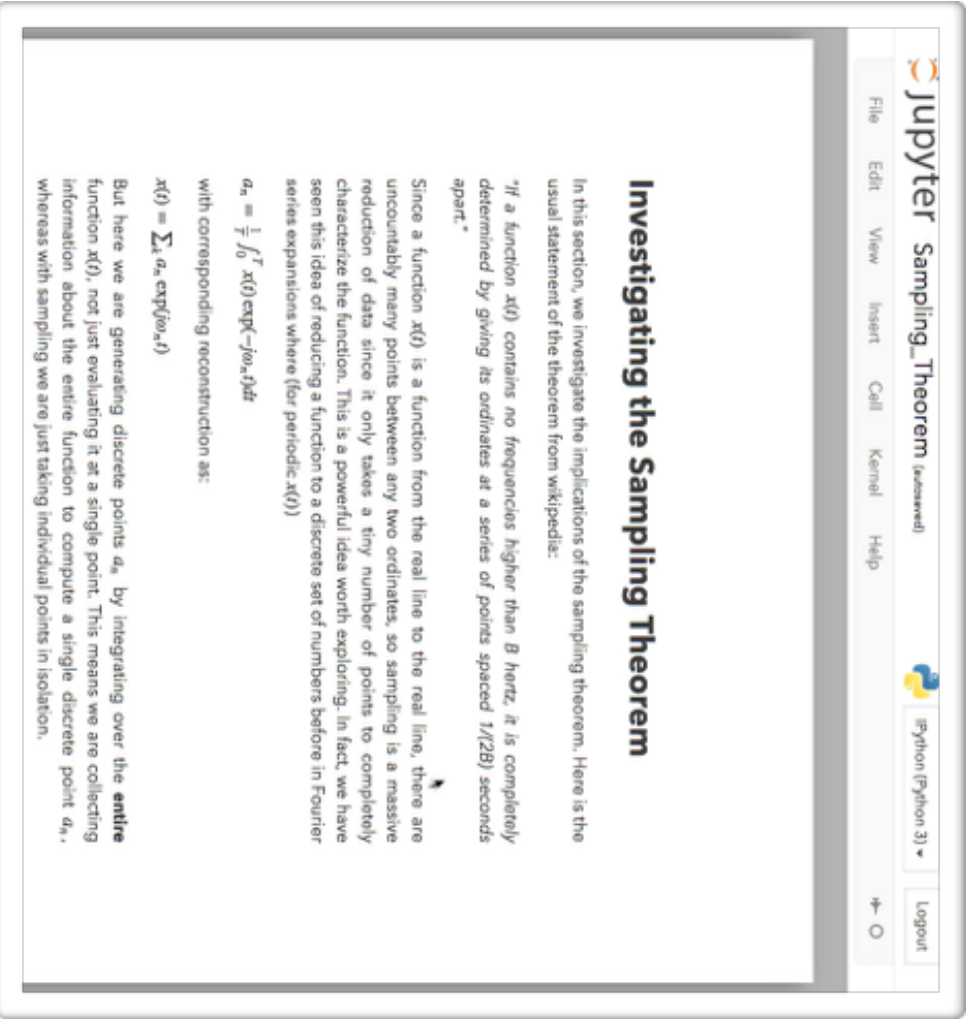






# Jupyter Notebooks

- notebook = sequence of cells
- text cell = markdown + latex)
- code cell = REEP (input + output)
- metadata everywhere



The screenshot shows a Jupyter Notebook window titled "Jupyter Sampling\_Theorem (unsaved)". The interface includes a top menu bar with "File", "Edit", "View", "Insert", "Cell", "Kernel", and "Help". On the right side, there are buttons for "Python (Python 3)", "Logout", and a refresh icon. The main content area contains a text cell with the following text:

### Investigating the Sampling Theorem

In this section, we investigate the implications of the sampling theorem. Here is the usual statement of the theorem from wikipedia:

*"If a function  $x(t)$  contains no frequencies higher than  $B$  hertz, it is completely determined by giving its ordinates at a series of points spaced  $1/(2B)$  seconds apart."*


Since a function  $x(t)$  is a function from the real line to the real line, there are uncountably many points between any two ordinates, so sampling is a massive reduction of data since it only takes a tiny number of points to completely characterize the function. This is a powerful idea worth exploring. In fact, we have seen this idea of reducing a function to a discrete set of numbers before in Fourier series expansions where (for periodic  $x(t)$ )

$$a_n = \frac{1}{T} \int_0^T x(t) \exp(-j\omega_n t) dt$$

with corresponding reconstruction as:

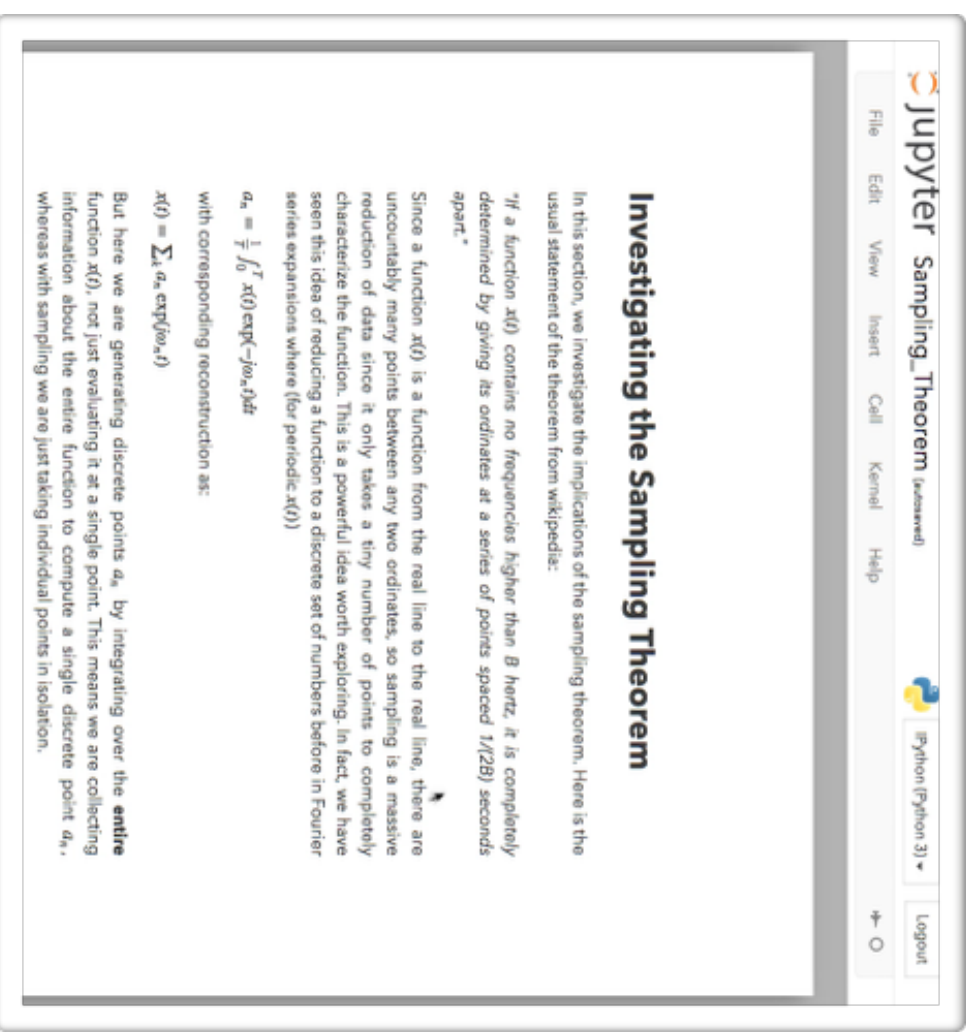
$$x(t) = \sum_k a_n \exp(j\omega_n t)$$

But here we are generating discrete points  $a_n$  by integrating over the **entire** function  $x(t)$ , not just evaluating it at a single point. This means we are collecting information about the entire function to compute a single discrete point  $a_n$ , whereas with sampling we are just taking individual points in isolation.



# Jupyter Notebooks

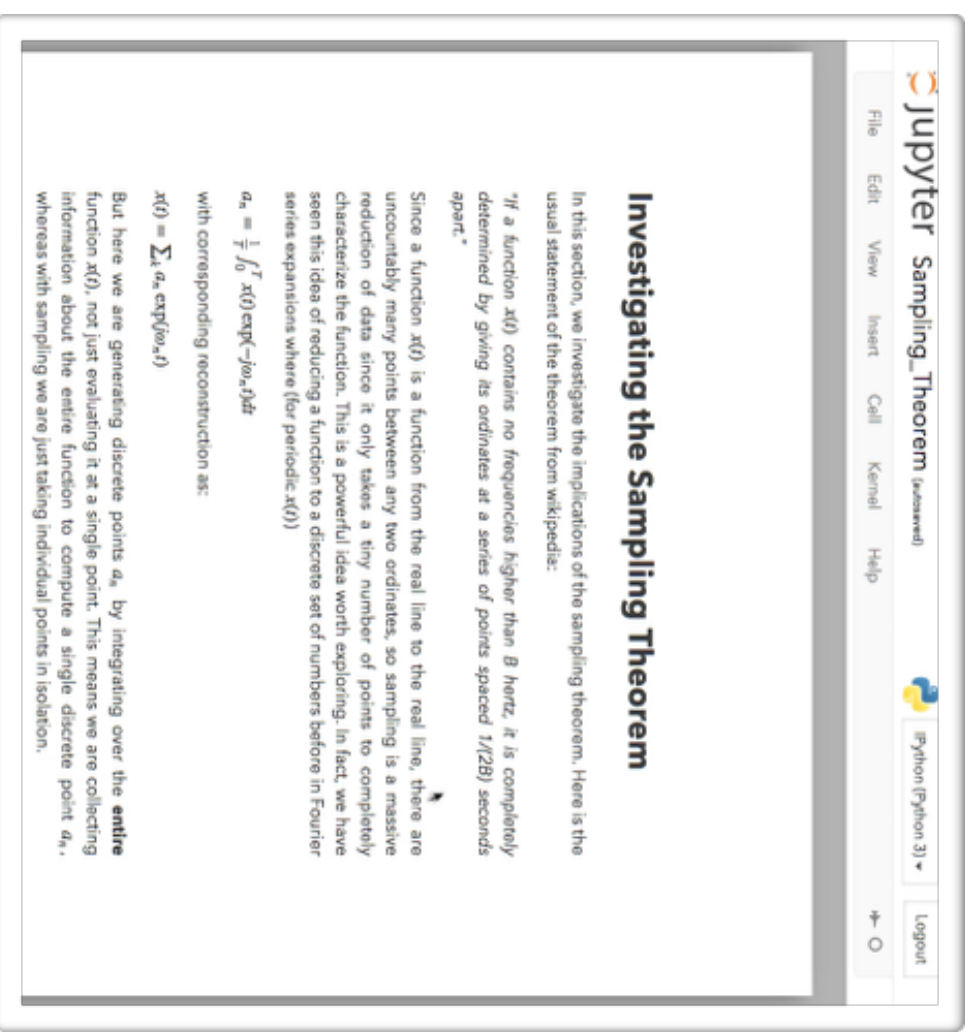
- Plain Text (JSON)
- Publicly documented schema
- Machine readable, easy to understand
- Transformable (nbconvert)





# Jupyter Notebooks

- interactive environment
- input format
- output format





# Lifecycle of a Computational Idea

1. Explore an idea interactively in a Notebook
2. *Build/add to a library based on what you learn*
3. Record and collaborate on analyses in Notebooks
4. Document, demonstrate, and share in Notebooks
5. Computational companions, reproducible papers



# Applications of Jupyter Notebooks

- **nbconvert** - convert notebooks to other formats (rst, html, latex/pdf, markdown, script, reveal.js slides)
- **nbviewer** - nbconvert to html on the web
- **nbgrader** - automated grading of notebooks
- **tmpnb** - containerized (docker) transient deployments of notebooks
- **thebe** - transient kernels on the web, without notebooks
- **dexy** - reproducible document-based workflows
- **jupyterhub** - multi-user notebook server for classes, groups
- **binder** - online notebooks populated from GitHub repos



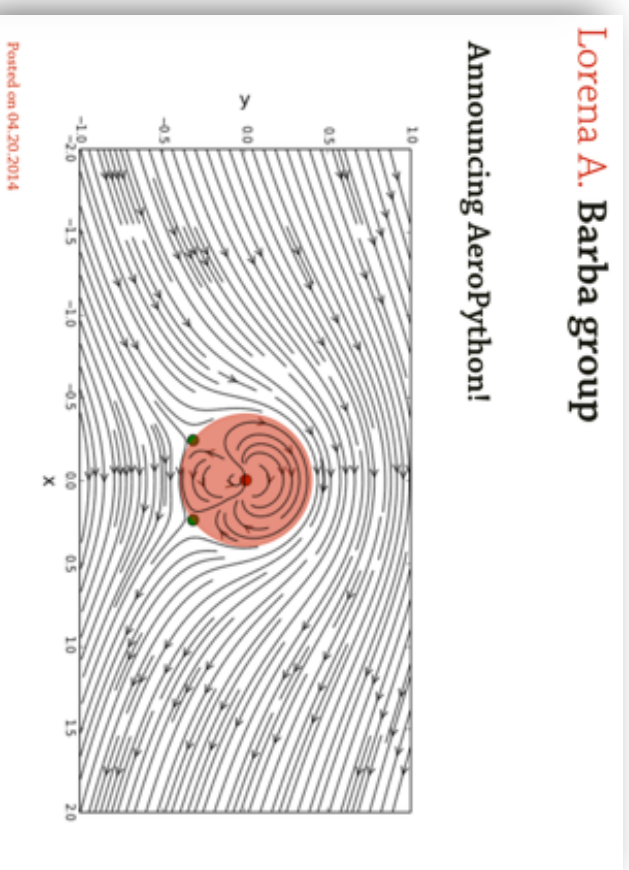
# Jupyter in the Classroom

Lorena Barba

AeroPython

Aerodynamics, George Washington U

Flipped Classroom



<http://lorenabarba.com/blog/announcing-aeropython>

# Jupyter in the Classroom



The screenshot shows a Jupyter notebook interface. At the top, there is a header with the Jupyter logo and the text "Jupyter at Bryn Mawr College". Below this, a "Public notebooks:" section lists several notebooks, including the one currently open: "Jupyter/hub/dblank/public / CS110 Intro to Computing / 2015-Fall".

The main content of the cell is a code execution block labeled "In [3]:". The code is:

```
fill(255, 0, 128);
beginShape();
vertex(10, 10);
vertex(70, 10);
vertex(80, 80);
vertex(40, 80);
vertex(5, 50);
vertex(10, 10);
endShape();
```

Below the code, the output is displayed as "Sketch #3:" followed by a small image of a pink polygon. The status of the sketch is shown as "Sketch #3 state: Done."

Doug Blank  
CS, Brynmawr

Calysto (Multiple languages, not Python)

JupyterHub

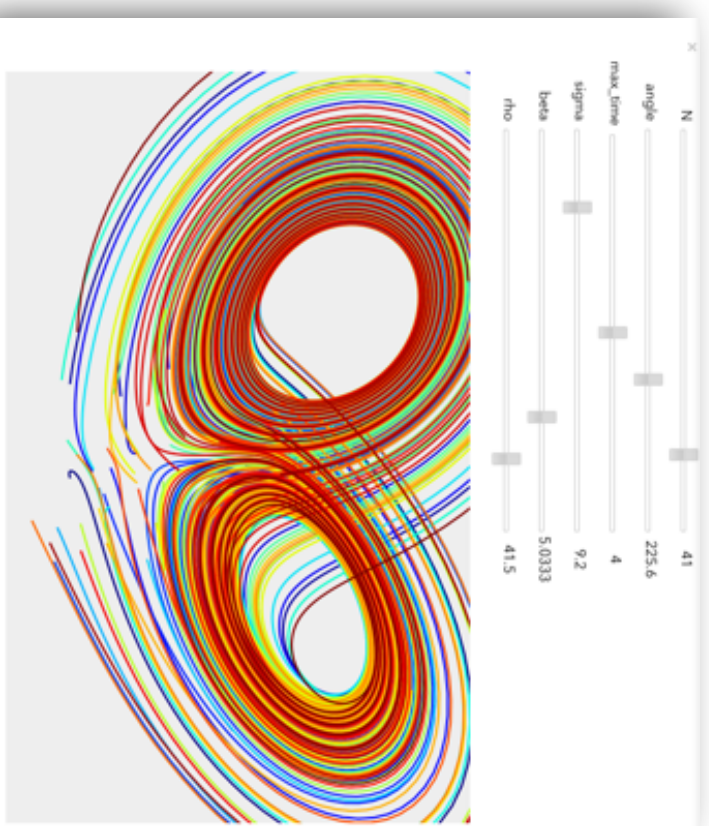


# Jupyter in the Classroom


Brian Granger

Computational Physics, Cal Poly

JupyterHub



<https://github.com/ellisonbg/phys202-2015>



# Jupyter in the Classroom

Eric Matthes

## High School Programming Alaska, USA


### How IPython Notebook and Github have changed the way I teach Python

Posted on [September 22, 2013](#)

I teach in a small high school in southeast Alaska, and each year I teach an Introduction to Programming class. I recently learned how to use [IPython Notebook](#), and it has completely [changed the way I teach my classes](#). There is much to improve about CS education at the K-12 level in the United States, and sharing our stories and our resources will go a long way towards improving what we offer to students.

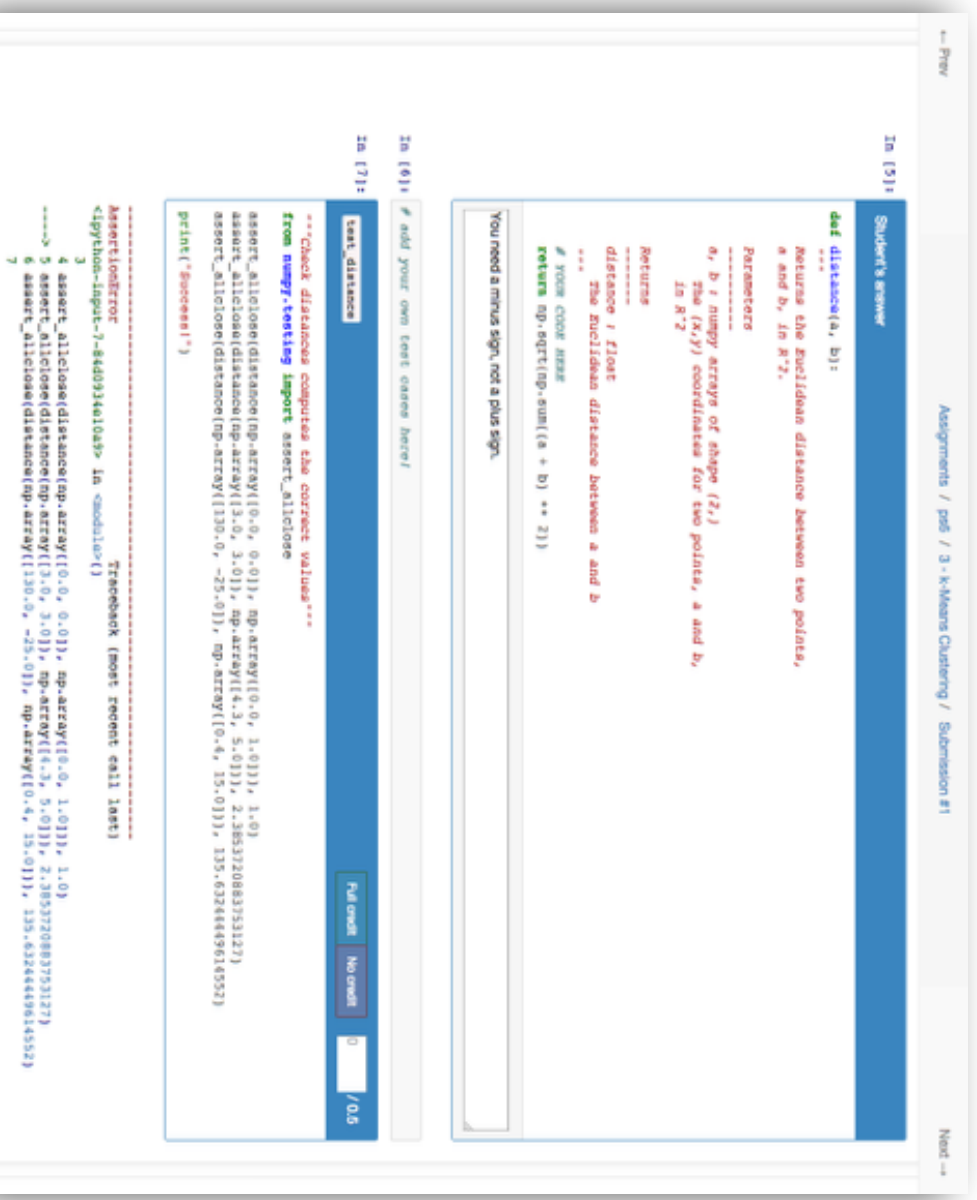


<https://peak5390.wordpress.com/2013/09/22/how-ipython-notebook-and-github-have-changed-the-way-i-teach-python/>



# Jupyter in the Classroom

Jessica Hamrick  
Computational Models of  
Cognition  
Psychology, UC Berkeley  
220 students  
JupyterHub  
NBGrader



The screenshot shows a Jupyter Notebook interface with the following content:

```
In [5]: Student's answer

def distance(a, b):
    """
    Returns the Euclidean distance between two points,
    a and b, in R^2.

    Parameters
    -----
    a, b : numpy arrays of shape (2,)
           The (x,y) coordinates for two points, a and b,
           in R^2

    Returns
    -----
    distance : float
    """
    # YOUR CODE HERE
    return np.sqrt(np.sum((a - b) ** 2))

You need a minus sign, not a plus sign.
```

In [6]: add your own test cases here!

```
In [7]: test_distance

***Check distance computes the correct values***
from numpy.testing import assert_allclose

assert_allclose(distance(np.array([0,0], 0,0)), np.array([0,0, 1,0]), 1,0)
assert_allclose(distance(np.array([3,0], 3,0)), np.array([4,3, 5,0]), 2.3853720883753127)
assert_allclose(distance(np.array([130,0], -25,0)), np.array([0,-4, 15,0]), 135.6326649614552)
print("Success!")
```

AssertionError: <ipython-input-7-84d034e10a3> In <module>:1  
Traceback (most recent call last):  
3 assert\_allclose(distance(np.array([0,0], 0,0)), np.array([0,0, 1,0]), 1,0)  
----> 5 assert\_allclose(distance(np.array([3,0], 3,0)), np.array([4,3, 5,0]), 2.3853720883753127)  
6 assert\_allclose(distance(np.array([130,0], -25,0)), np.array([0,-4, 15,0]), 135.6326649614552)  
7

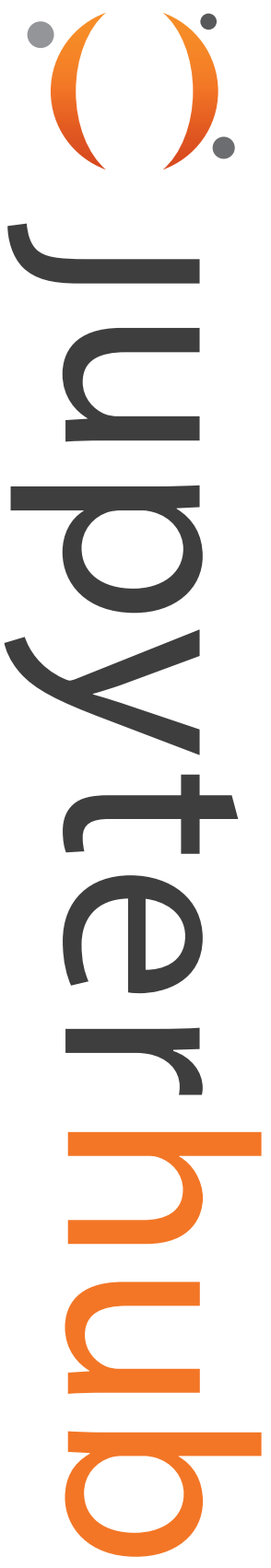
Full credit No credit 0 / 0.0



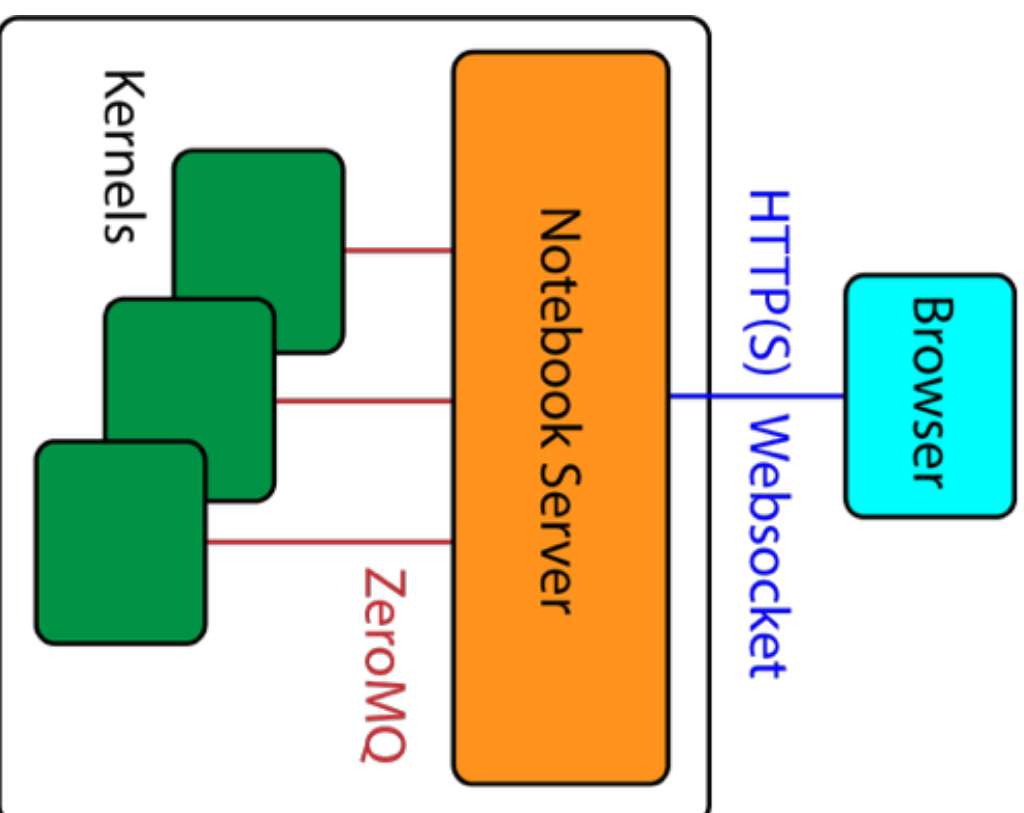
# NBGrader

Notebooks as assignments

- distributed to students via JupyterHub
- turned in online
- Test-based auto-grading
- Manual grading of prose assignments



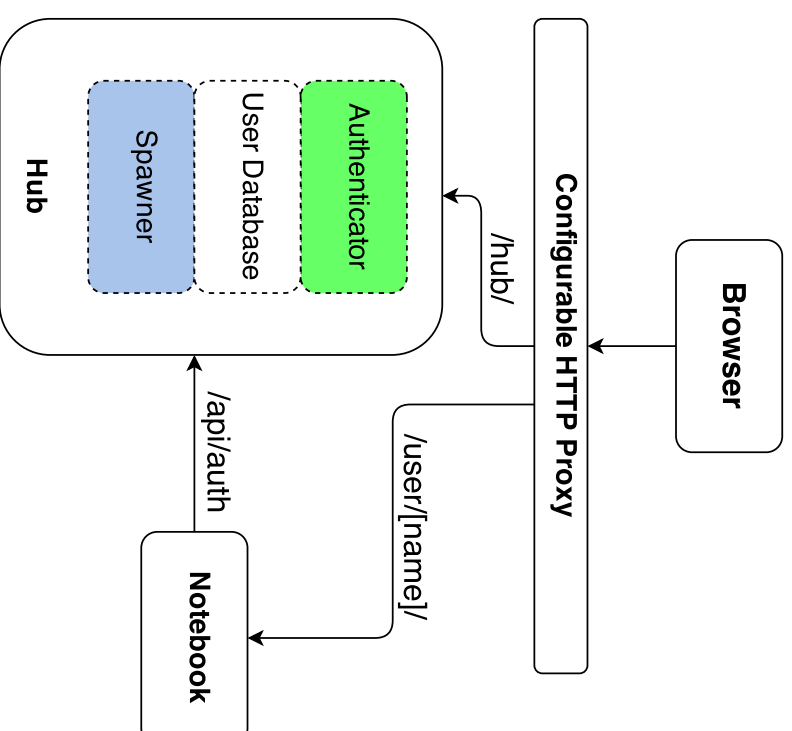
multi-user notebook server



Notebook Application

# Jupyter hub

- Manages authentication
- Spawns single-user servers on-demand
- Resume from db without restarting other components



# Jupyter hub

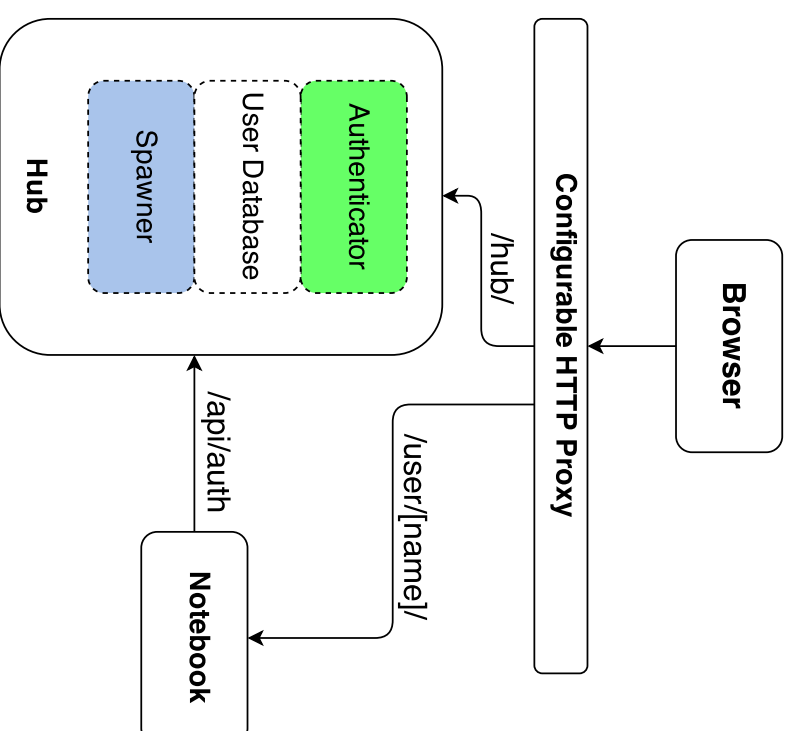
- Initial request is handled by Hub
- User authenticates via form / OAuth
- Spawner starts single-user server
- Hub notifies Proxy
- Redirects user to /user/[name]
- Single-user Server verifies auth with Hub





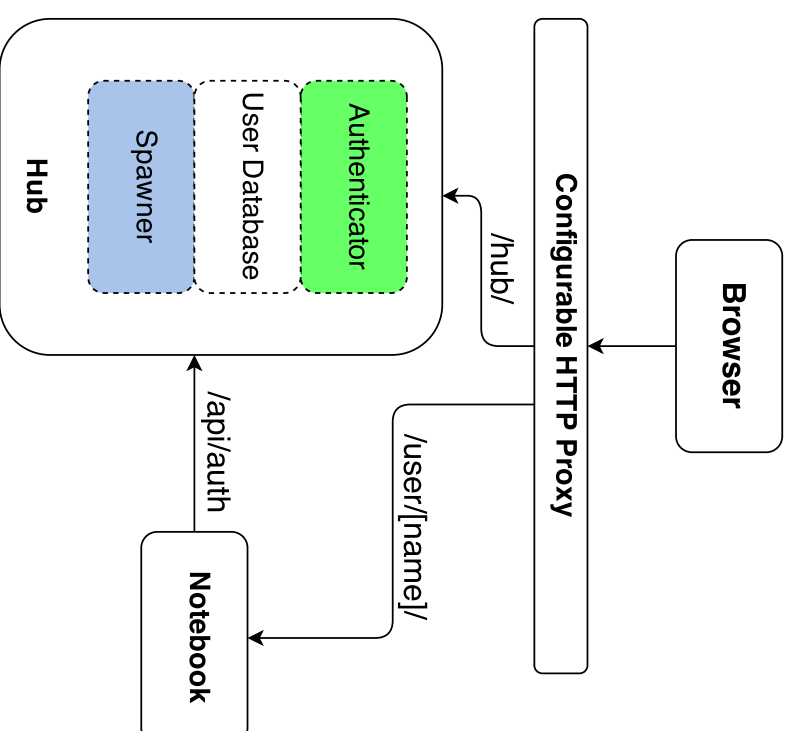
# Jupyterhub

- Pluggable Authentication
  - PAM, OAuth, SSO, etc.
- Pluggable Spawning
  - Popen, Docker, PBS, EC2, etc.



# Jupyter hub

- User-controls
- specify resources ✓
- multiple servers per user
- Sharing
- publishing notebooks for other users
- long-term: live collaboration






The  
University  
Of  
Sheffield.



BRYN  
MAWR  
COLLEGE

 Jupyterhub



WIKIMEDIA  
FOUNDATION



XSEDE

Extreme Science and Engineering  
Discovery Environment

 BROOKHAVEN  
NATIONAL LABORATORY

