OpenDreamKit

Computational environments
for research and education

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Simula Research Lab

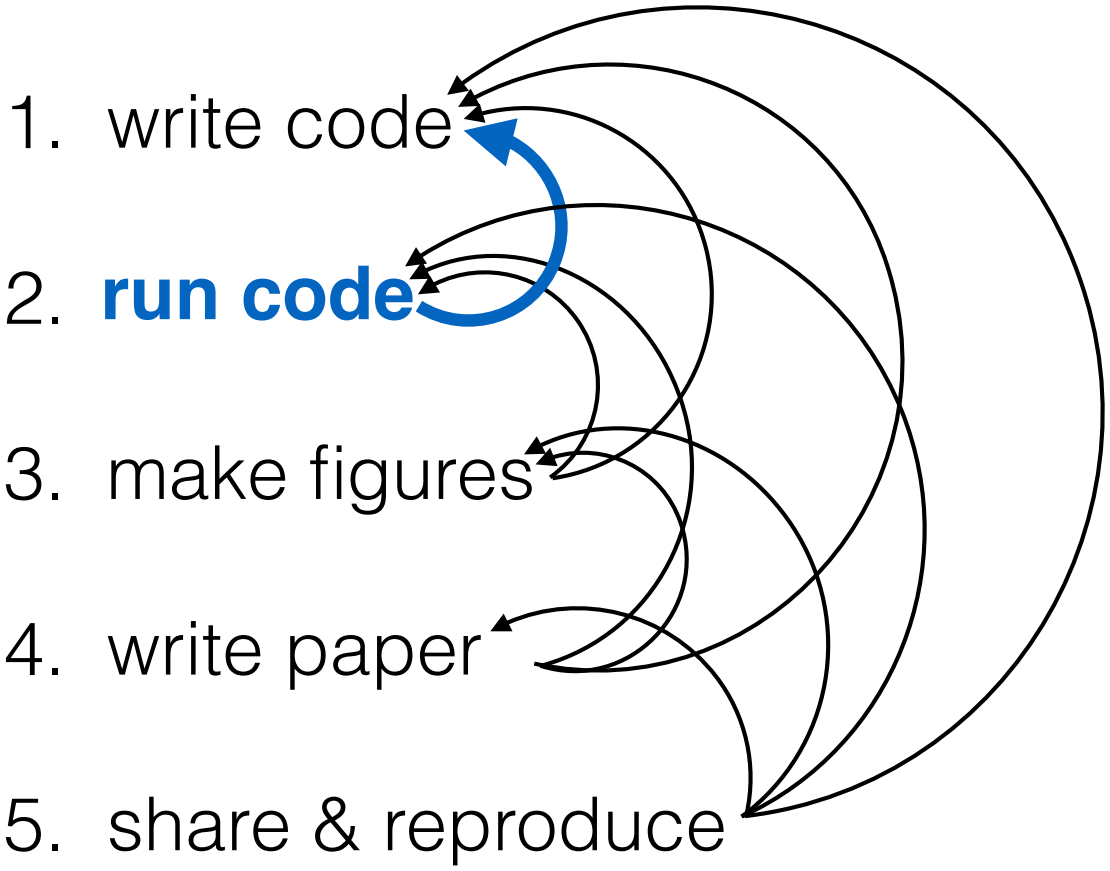
OpenDreamKit

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

Virtual Research Environments

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

How do we do computational research?

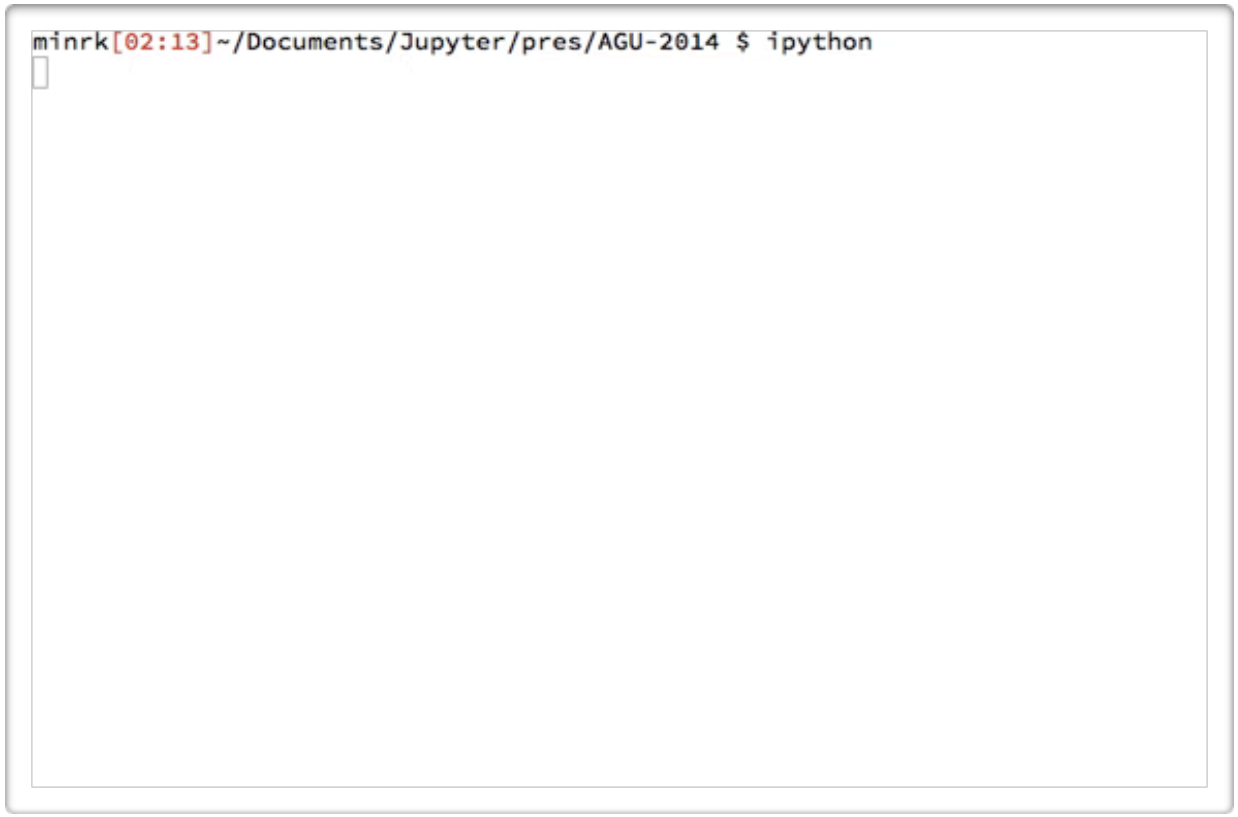


IPython

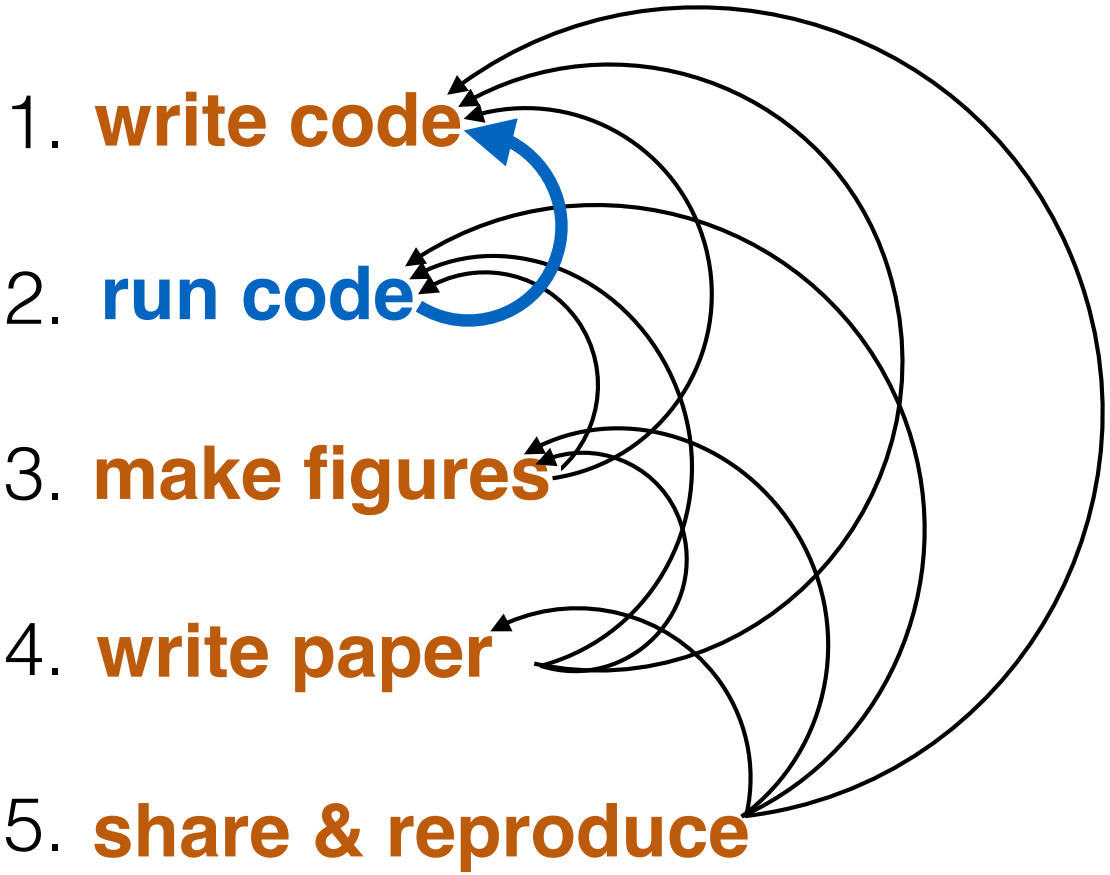
IPython
Interactive Python

helps run code

- tab completion
- introspection
- %magics



What about Jupyter?

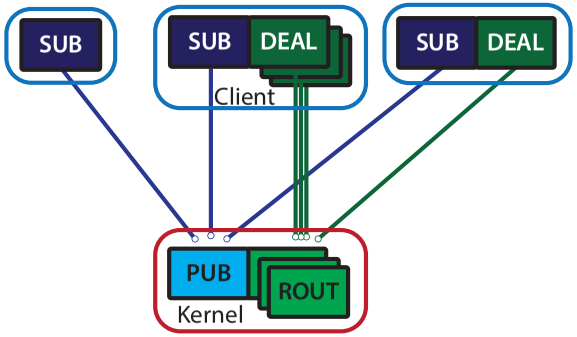


IPython

jupyter

What is Jupyter?

Network Protocol



ØMQ + JSON

Document Format

We have already computed $P(X|A)$ above. On the other hand, $P(X|\sim A)$ 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 $P(X|\sim A) = 0.5$. Then

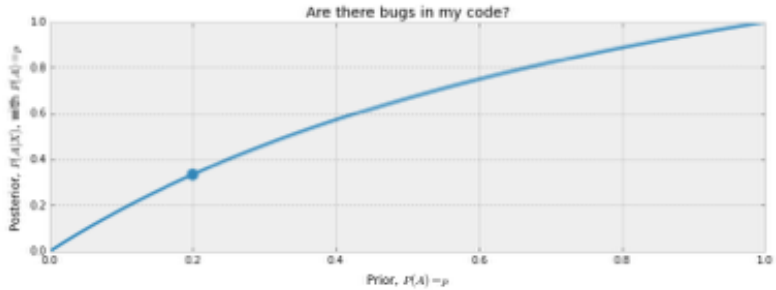
$$P(A|X) = \frac{1 \cdot p}{1 \cdot p + 0.5(1-p)}$$

$$= \frac{2p}{1+p}$$

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="#348ABD", lw=3)
# plt.fill_between(p, 2*p/(1+p), alpha=.5, facecolor=["#A60628"])
plt.scatter(0.2, 2 * (0.2) / 1.2, s=140, c="#348ABD")
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>
```



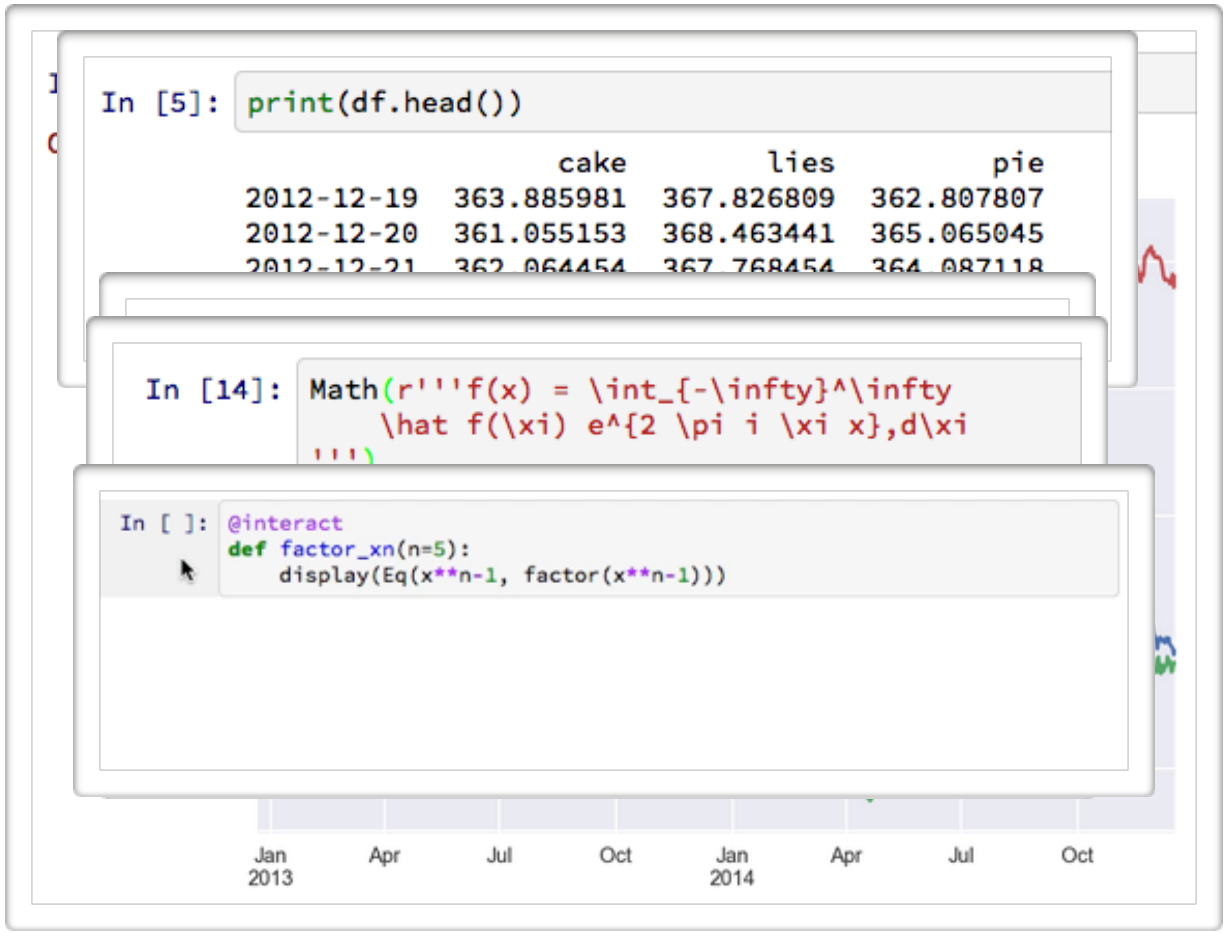
https://github.com/CamDavidsonPilon/Probabilistic-Programming-and-Bayesian-Methods-for-Hackers

Jupyter Protocol

supercharge the P in REP*L

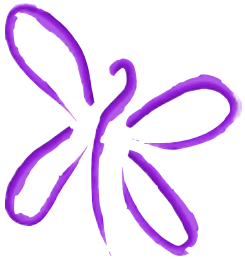
any mime-type output

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



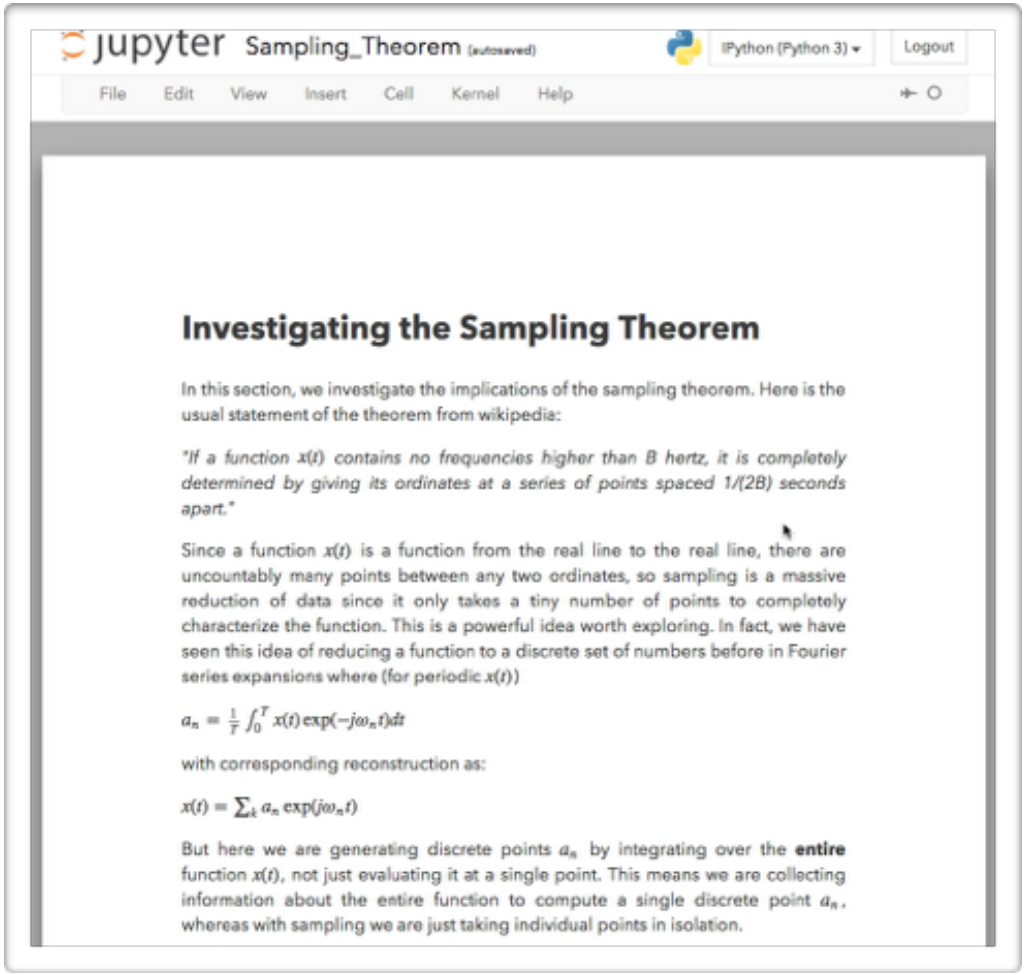
Jupyter Protocol

is language agnostic



Jupyter Notebooks

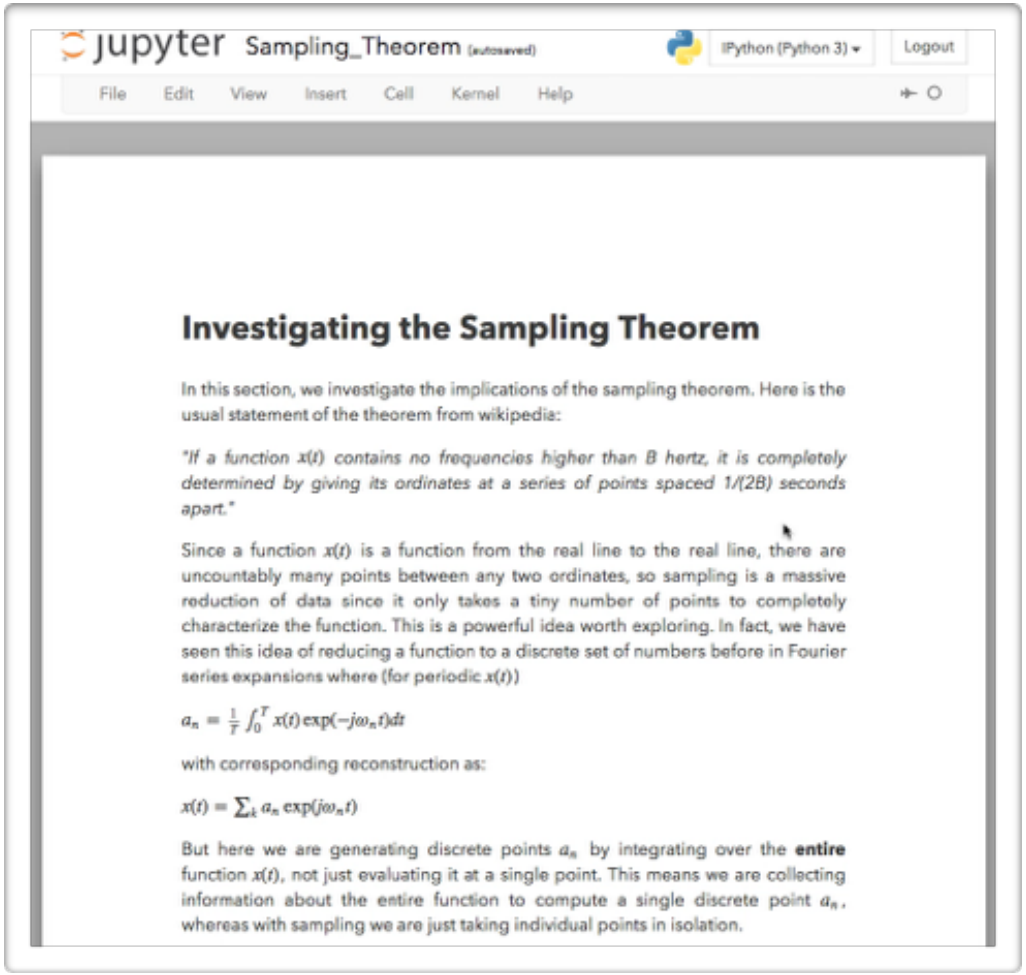
- notebook = sequence of cells
- text cell = markdown + latex)
- code cell = REP (input + output)
- metadata everywhere



https://github.com/unpingco/Python-for-Signal-Processing

Jupyter Notebooks

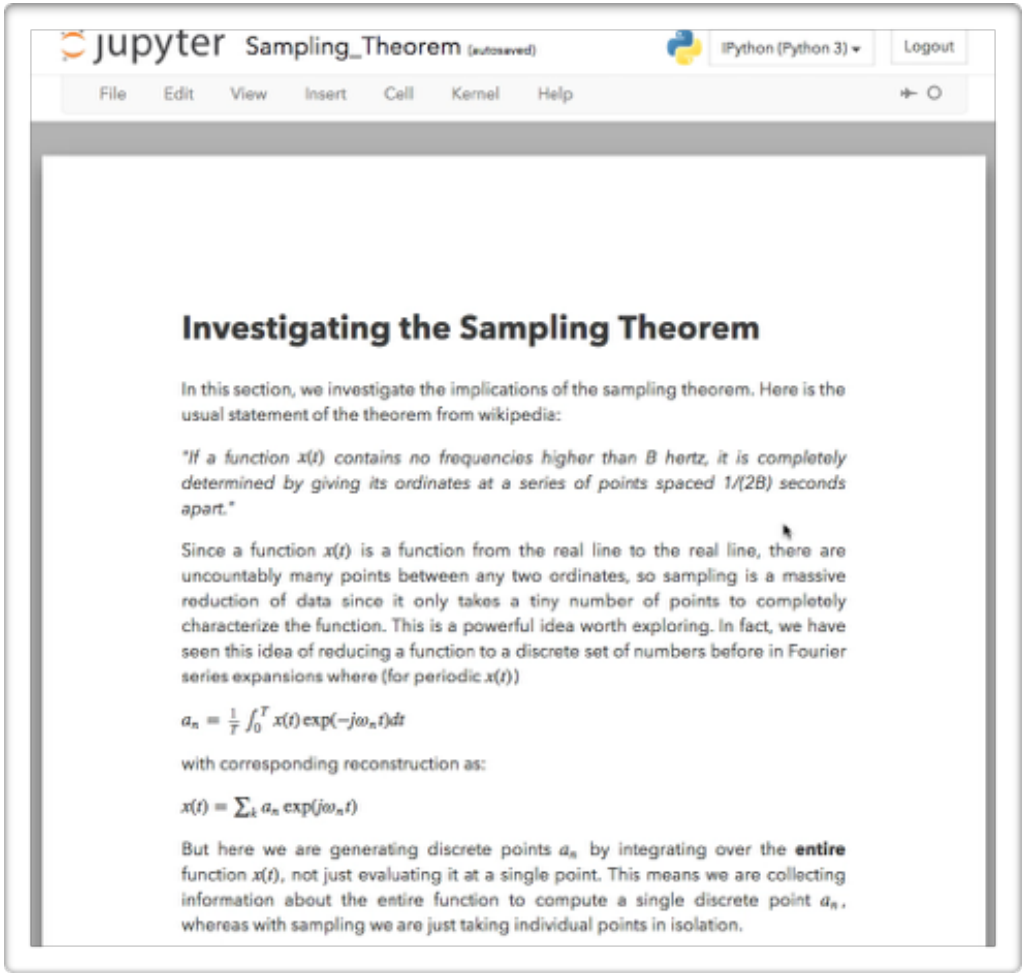
- Plain Text (JSON)
- Publicly documented schema
- Machine readable, easy to understand
- Transformable (nbconvert)



https://github.com/unpingco/Python-for-Signal-Processing

Jupyter Notebooks

- interactive environment
- input format
- output format



https://github.com/unpingco/Python-for-Signal-Processing

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

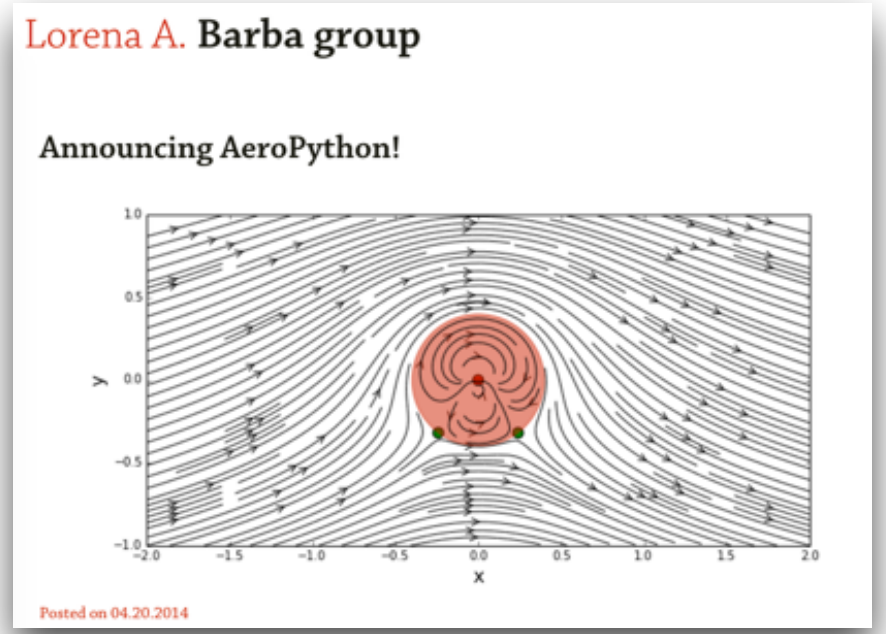
Applications of Jupyter Notebooks

- **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

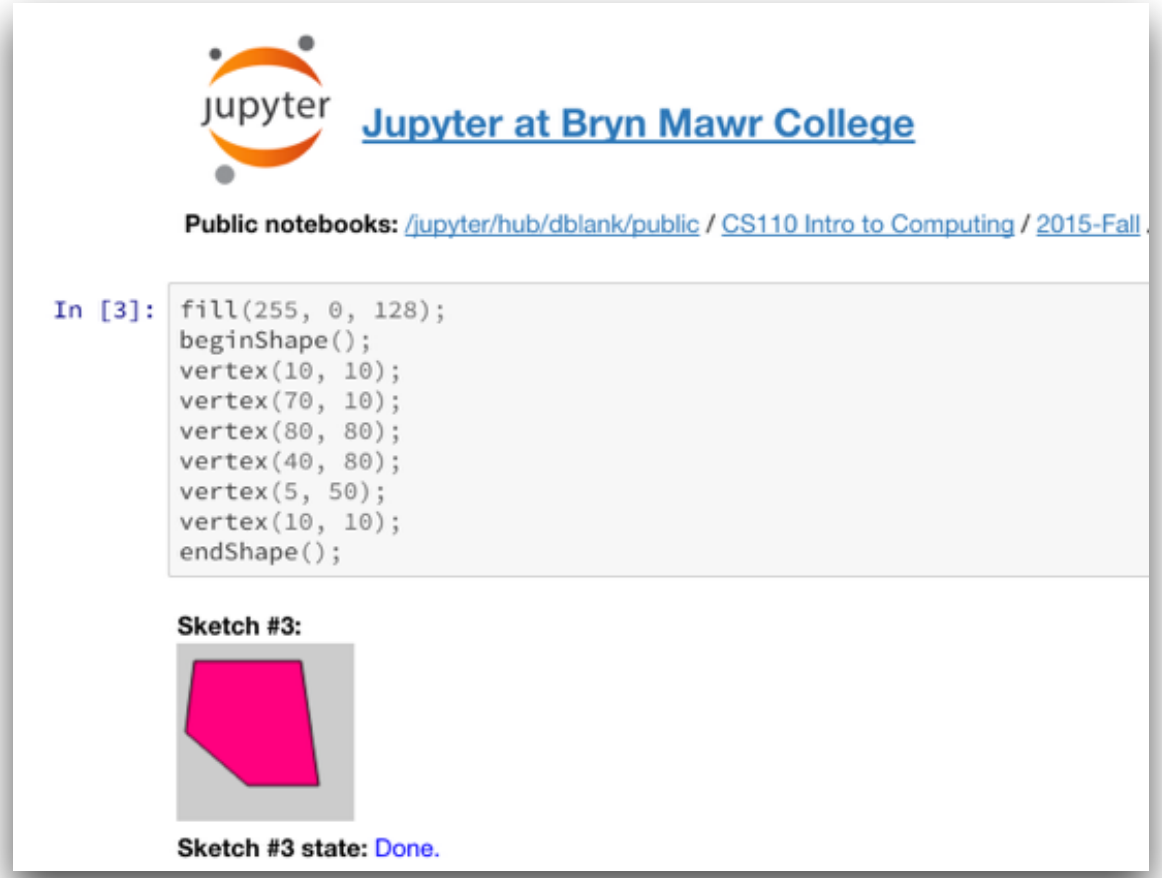
Jupyter in the Classroom

Lorena Barba
AeroPython
Aerodynamics, George Washington U
Flipped Classroom



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

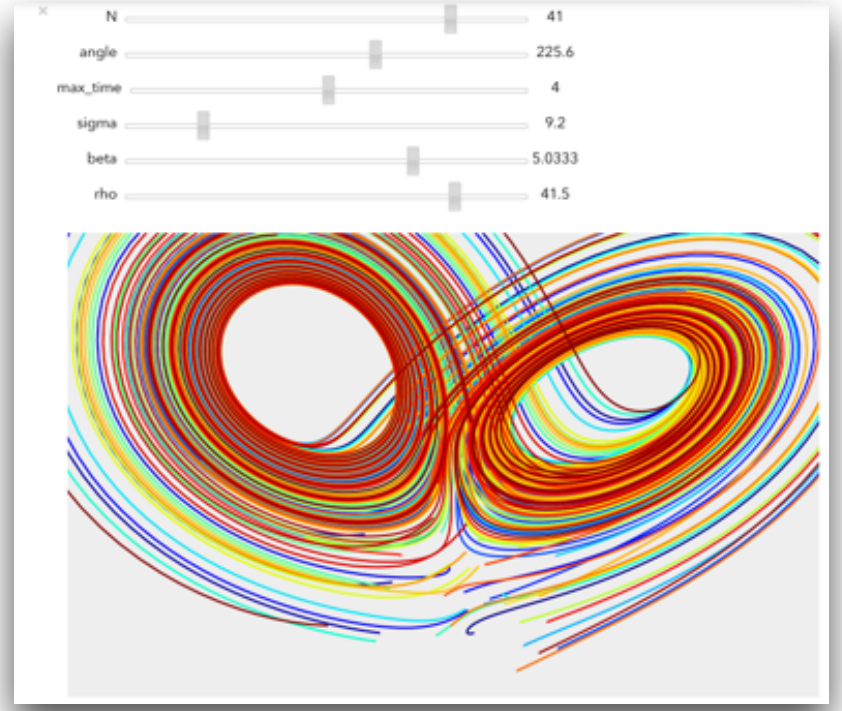
Jupyter in the Classroom



Doug Blank
CS, Brynmawr
Calysto (Multiple languages, not Python)
JupyterHub

Jupyter in the Classroom

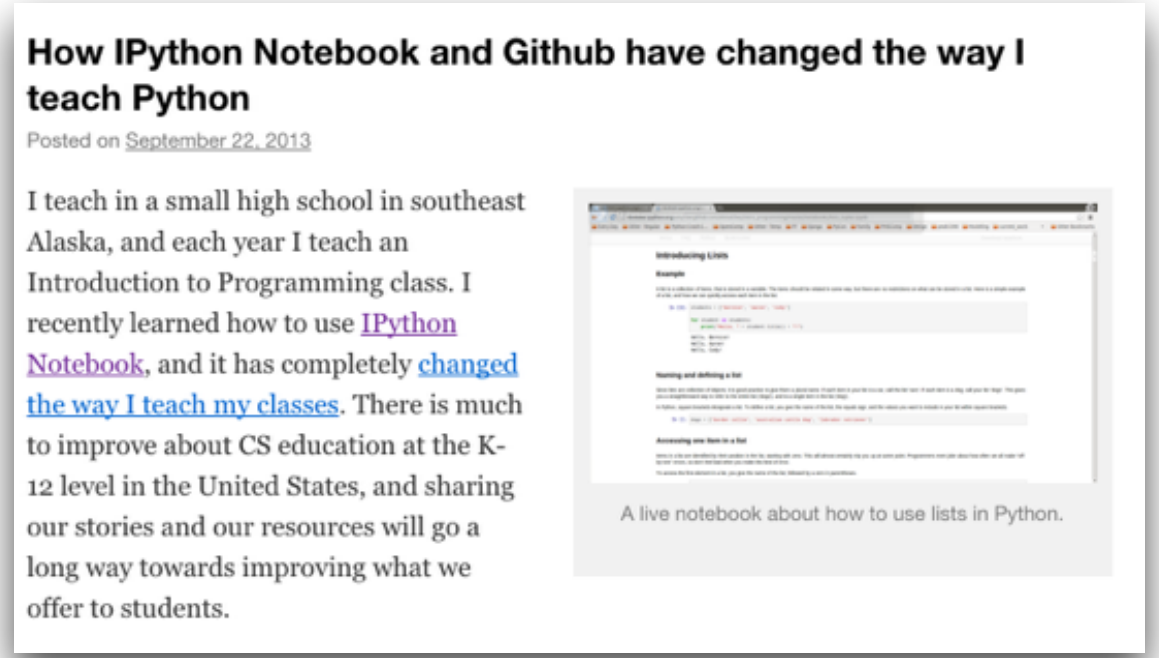
Brian Granger
Computational Physics, Cal Poly
JupyterHub



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

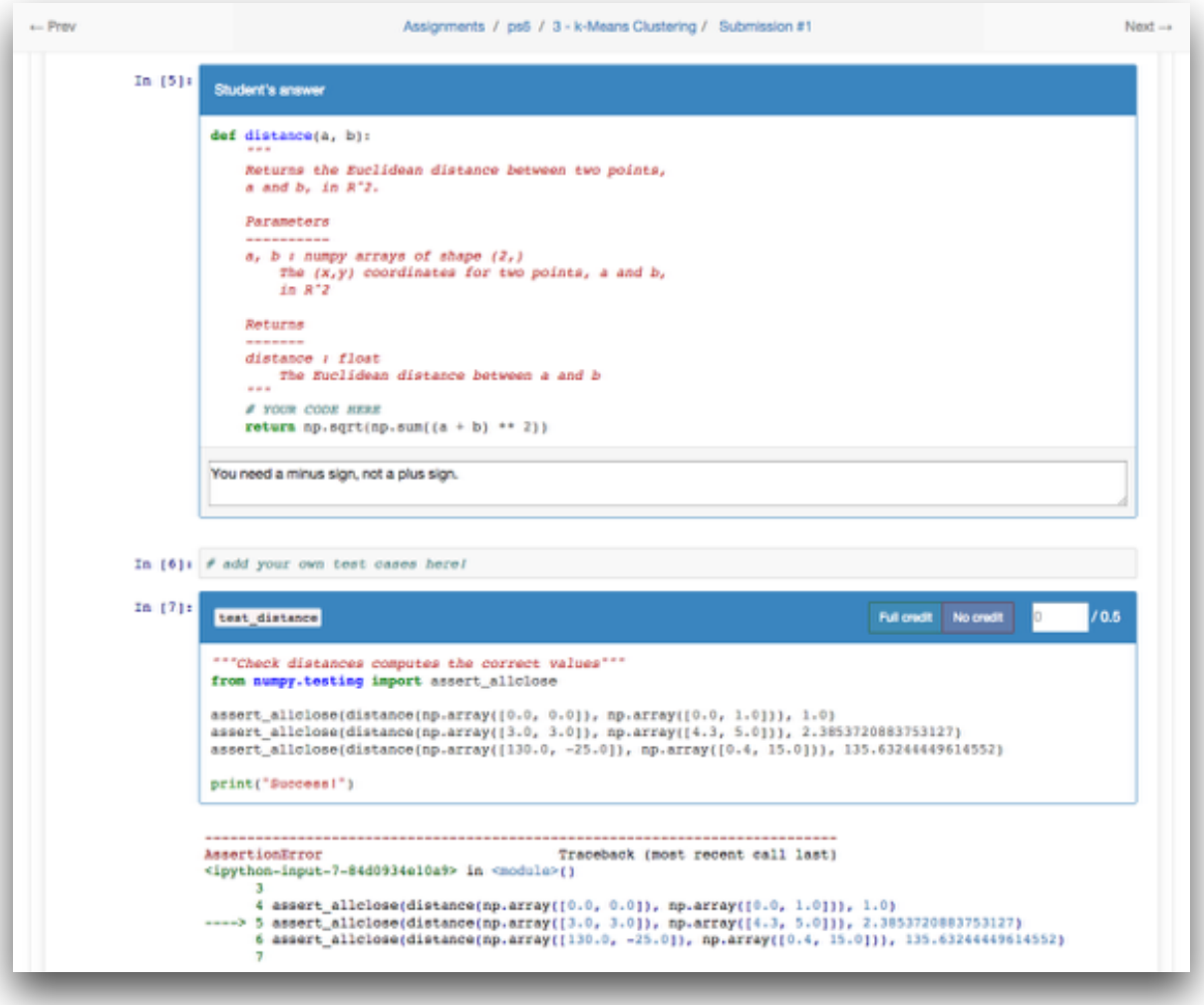
I teach in a small high school in southeast Alaska, and each year I teach an Introduction to Programming class. I recently learned how to use IPython Notebook, and it has completely changed the way I teach my classes. There is much to improve about CS education at the K-12 level in the United States,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

A live notebook about how to use lists in Python.

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



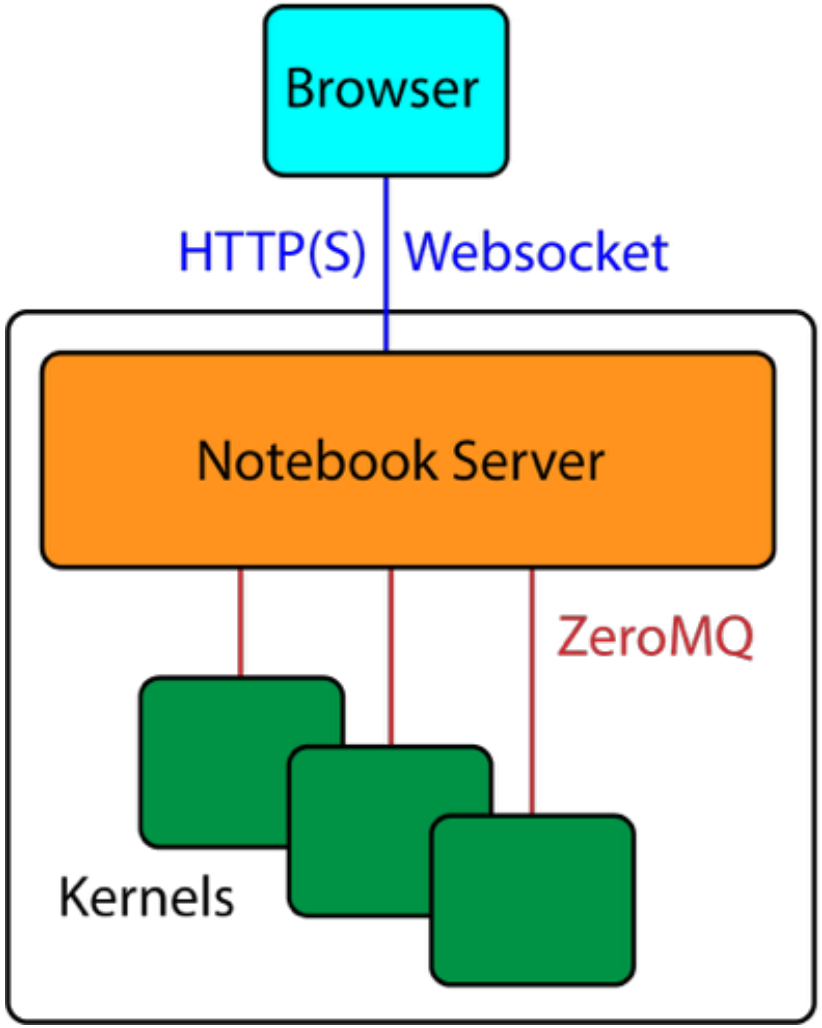
NBGrader

Notebooks as assignments

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

jupyterhub

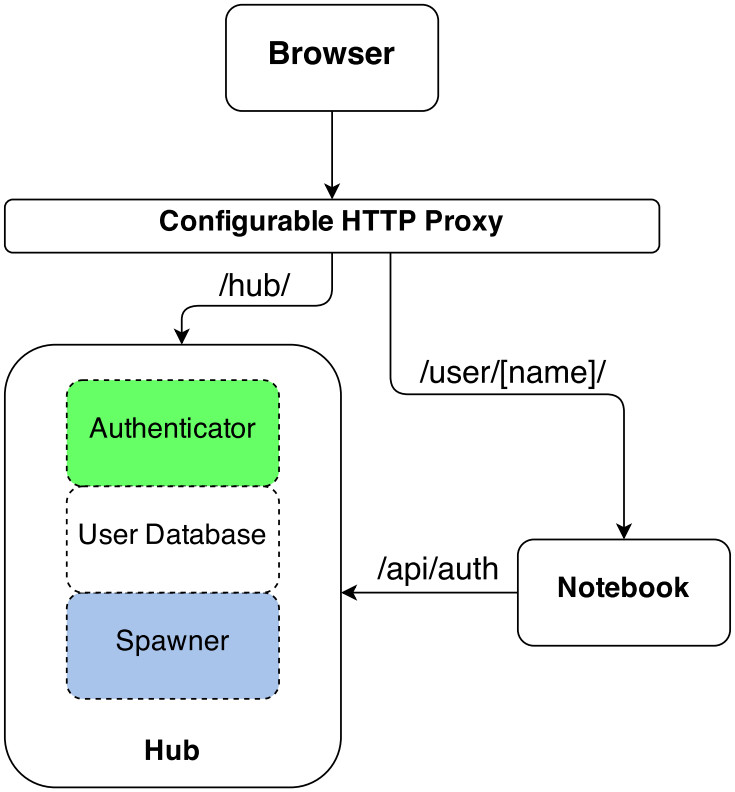
multi-user notebook server



Notebook Application

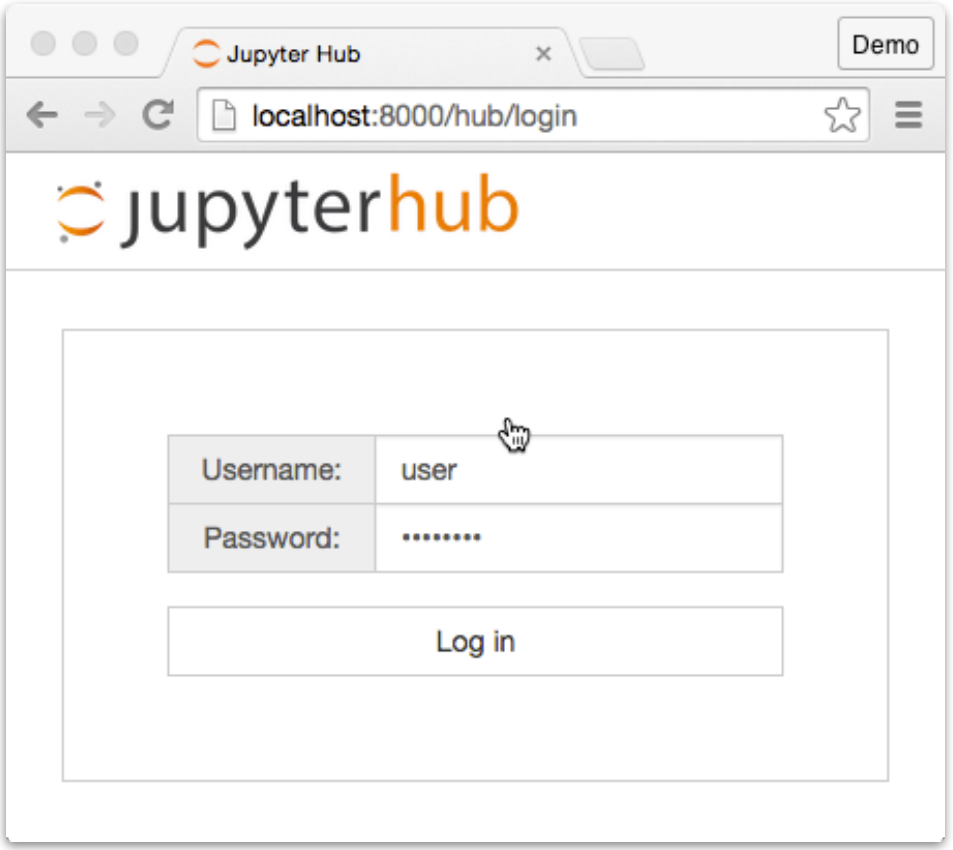
jupyterhub

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



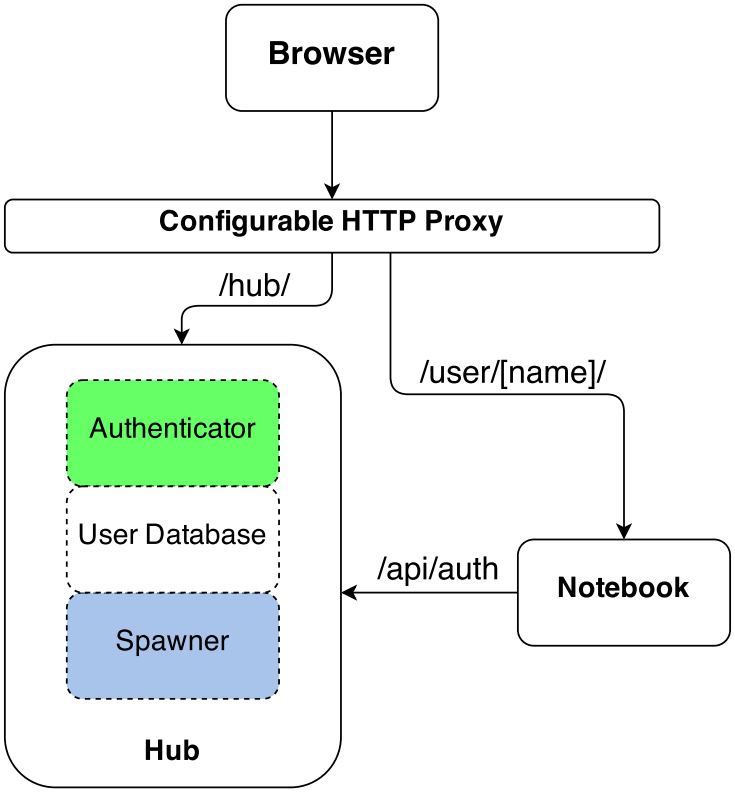
jupyterhub

- 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



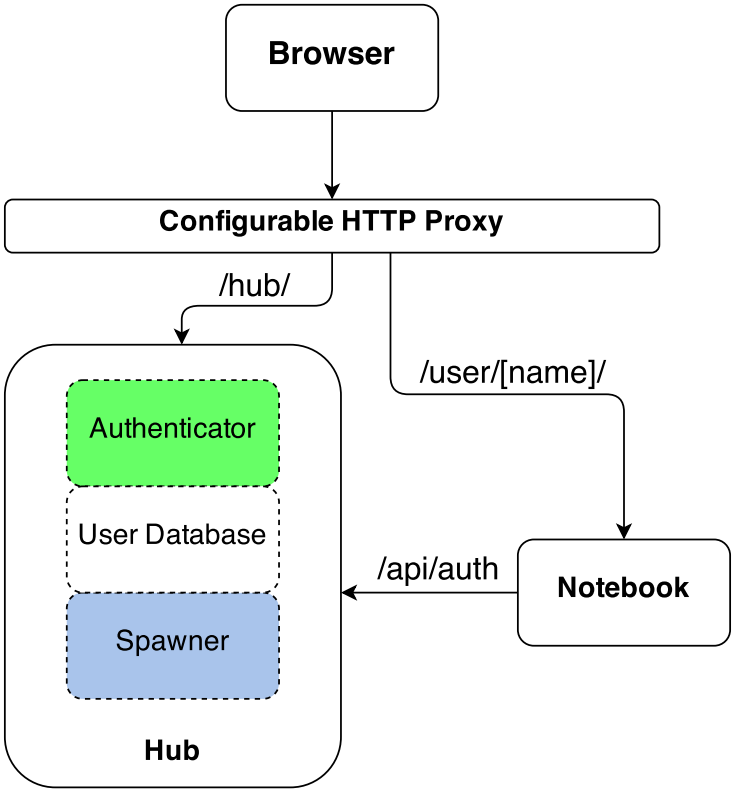
jupyterhub

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



jupyterhub

- 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

jupyter