

How I work

and



Contents

- cool stuff
- nbflow
- jupyter lab
- spyder 3.0
- bokeh
 - holoviews
 - datashader
- parallel python

cool stuff

> conda environment

```
> conda create env -n name_of_env python=3.5 matplotlib  
> source activate name_of_env  
> conda env list
```

> python IDE

```
> wingIDE (https://wingware.com/)  
> pyCharm (https://www.jetbrains.com/pycharm/)  
> eclipse  
> spyder  
> jupyter lab (soon)
```

wingIDE

The screenshot displays the wingIDE Integrated Development Environment (IDE) interface. The main window features two code editors side-by-side, both showing the same file: `main.py`. The code is a Python script for a graphical application, likely a reflectometer, involving QWidgets and QML. The right editor has several lines of code highlighted in yellow, indicating they are selected or being edited.

Below the code editors is a status bar with tabs for "Search", "Stack Data", "Exceptions", "Breakpoints", and "Testing".

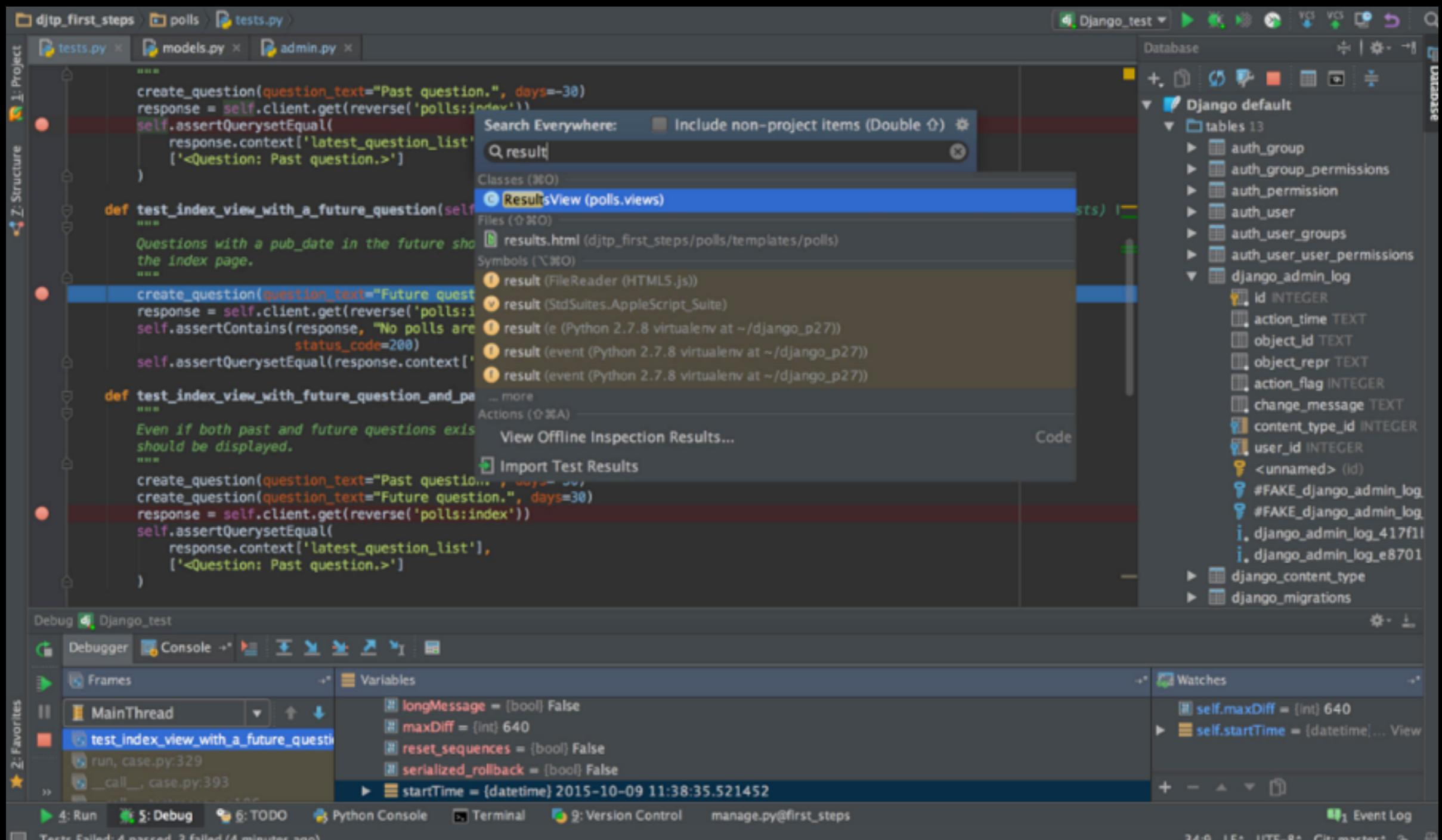
To the left of the main window is a vertical "Project Files" sidebar showing a tree view of the project structure, including files like `MANIFEST.in`, `setup.cfg`, and `setup.py`.

On the right side of the main window, there are several floating panes:

- A "Project" pane listing all files in the project, such as `main.py`, `main.qml`, `main.cpp`, etc.
- An "Editor" pane showing the source code of the currently selected file.
- A "Source Browser" pane listing symbols from the current file, with `splash.showMessage` currently selected.
- A "Call Stack" pane showing the call stack for the selected symbol.
- A "Symbol" pane displaying detailed information about the selected symbol, including its type (callable method), signature, and documentation.
- A "Documentation" pane providing links to external documentation for the selected symbol.
- A "Help" pane at the bottom right containing general help text and links.

The top of the screen has a standard Mac-style menu bar with options like "File", "Edit", "Search", "Project", "Python Environment", "Project Properties", "Break", "Debug", "Step Into", and "Debug To Cursor".

pyCharm



unit testing using travis

The image shows two side-by-side screenshots illustrating the integration of GitHub and Travis CI for continuous integration.

GitHub Repository Page:

- Repository:** ornlneutronimaging / BraggEdge
- Code:** 179 commits, 1 issue, 0 pull requests, 2 branches, 5 releases
- Branch:** master
- Commits:** A list of recent commits by JeanBilheux, including: Improved code, Improved code, Added docs and rREADME.rst, Added docs and rREADME.rst, Improved code, Improved code, Trying to fix the unit test coverage on travis, Adding versioneer, Move list of structure to top config file. Updated test and added som..., still trying to understand why _versioneer can not be found on Travis, Added non python files to build, Update README.md, Improved demo.py, Improved coverage of experiment by, Update setup.cfg, Improved code, and README.md.
- Status:** version 1.0.1, build passing, codecov 98%, gitter, join chat
- Page Title:** Work concerning the Bragg Edge LDRD — Edit

Travis CI Build Status Page:

- Repository:** ornlneutronimaging / BraggEdge
- Build Status:** build passing
- Build Details:** master · Improved code · Commit fad4ef · Compare bocl108..fad4ef · JeanBilheux authored and committed
- Build Jobs:** 162.1 (Python 2.7), 162.2 (Python 3.4)
- Build Metrics:** Elapsed time 8 min 21 sec, Total time 14 min 50 sec, 3 months ago

documentation using sphinx



orlneutronimaging.github.io/BraggEdge/index.html

Apps Google Maps Gmail Google Contacts Google Calendar Adobe Aviation Python Temporary Programme soiree TweetDeck SciPy2016

braggedge 1.0.0 documentation

WELCOME TO BRAGGEDGE'S DOCUMENTATION!

Contents :: How to use This library »

Welcome to braggedge's documentation!

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 - [Lambda Calculation](#)
 - [Distance source-Detector Calculation](#)
 - [Detector Offset Calculation](#)
 - [Lattice Calculator](#)
- [The API Reference](#)
- [The Material Handler Reference](#)
- [The BraggEdges Handler Reference](#)
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Indices and tables

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documentation using sphinx

The image shows two side-by-side code editors. Both editors have tabs at the top labeled "braggiedge.py_demo.rst". The left editor displays a Python script with code examples and explanatory text. The right editor displays the generated reStructuredText (rst) file, which is used by Sphinx to generate documentation.

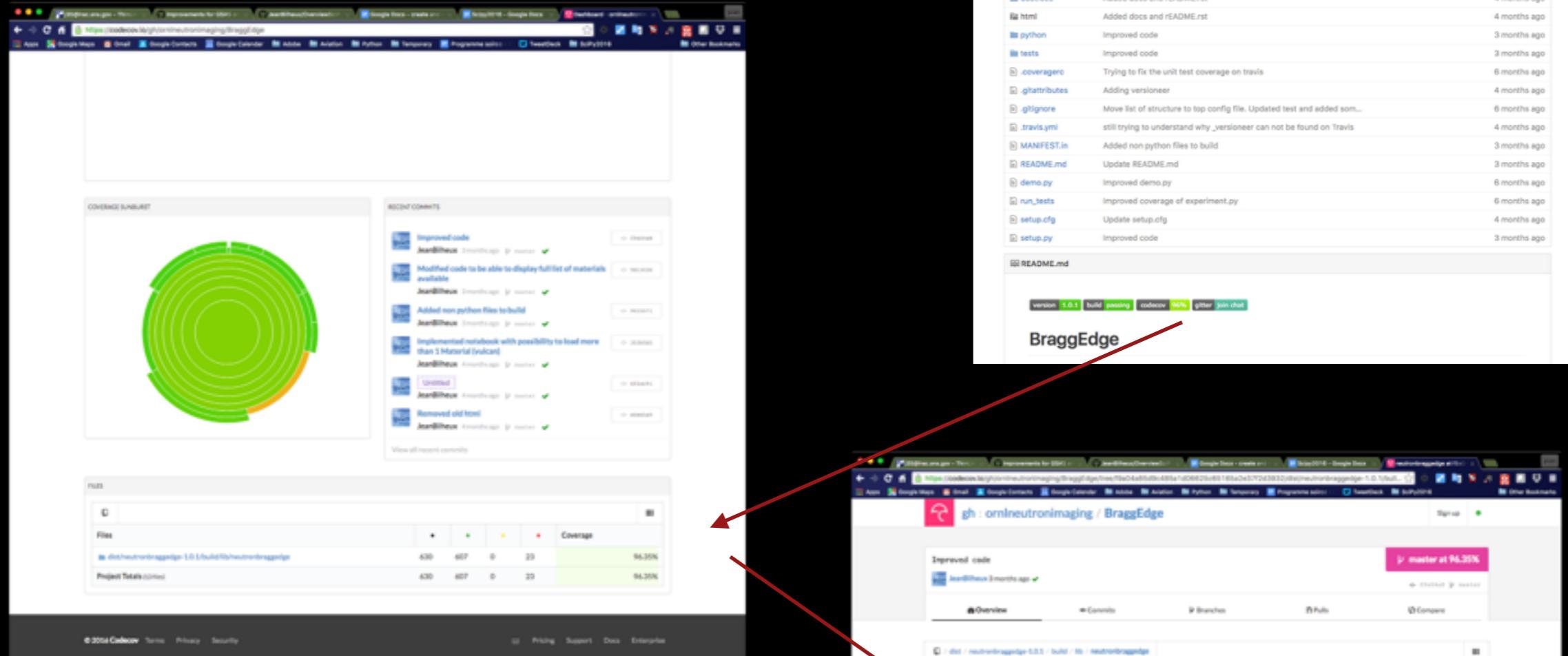
Left Editor (Python Script):

```
1 How to use This library
2 -----
3
4 >>> import neutronbraggiedge
5
6 From **python***, first you need to import the package
7
8 >>> from neutronbraggiedge.braggedge import BraggEdge
9
10 Metadata of Elements
11 -----
12
13 For a particular element, or a list of elements, you can retrieve:
14   - lattice parameter
15   - h, k and l values
16   - Crystal structure
17   - bragg edges values
18
19 For this example, we are retrieving the data for *Fe* and we are only
20 interested by the first *** crystal orientation.
21
22 >>> _handler = BraggEdge(material = 'Fe', number_of_bragg_edges = 4)
23 >>> print("Crystal Structure is: %s" %_handler.metadata['crystal_structure'])
24 'BCC'
25 >>> print("Lattice is %.2f" %_handler.metadata['lattice'])
26 2.87
27 >>> print("hkl are: ", _handler.hkl)
28 hkl are: [(1,1,0),(2,0,0),(2,1,1),(2,2,0)]
29 >>> print("bragg edges are: ", _handler.bragg_edges)
30 bragg edges are: [2.0268, 1.4332, 1.1782, 1.0134]
31
32 It is also possible to display all metadata at once
33
34 >>> print(_handler)
35 -----
36 Material: Fe
37 Lattice: 2.8664A
38 Crystal Structure: BCC
39 Using local metadata Table: True
40
41 h | k | l | d(A) | BraggEdge
42
43 1 | 1 | 0 | 2.8269 | 4.0537
44 2 | 0 | 0 | 1.4332 | 2.8664
45 2 | 1 | 1 | 1.1782 | 2.3484
46 2 | 2 | 0 | 1.0134 | 2.0269
47
48
49
50
51 In this example, we are retrieving the data for *Fe* and *Al*
52
53 >>> _handler = BraggEdge(material=['Al', 'Fe'], number_of_bragg_edges = 4)
54 >>> print("Crystal Structure of Al is: %s" %_handler.metadata['crystal_structure']['Al'])
55 'FCC'
56 >>> print("Lattice of Al is: %.2f" %_handler.metadata['lattice']['Al'])
57 4.45
58
59 Here, we display the metadata for a list of material
60
61 >>> print(_handler)
62 -----
63 Material: Al
64 Lattice : 4.0466A
65 Crystal Structure: FCC
66 Using local metadata Table: True
```

Right Editor (reStructuredText File):

```
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```

test coverage



<https://codecov.io/>



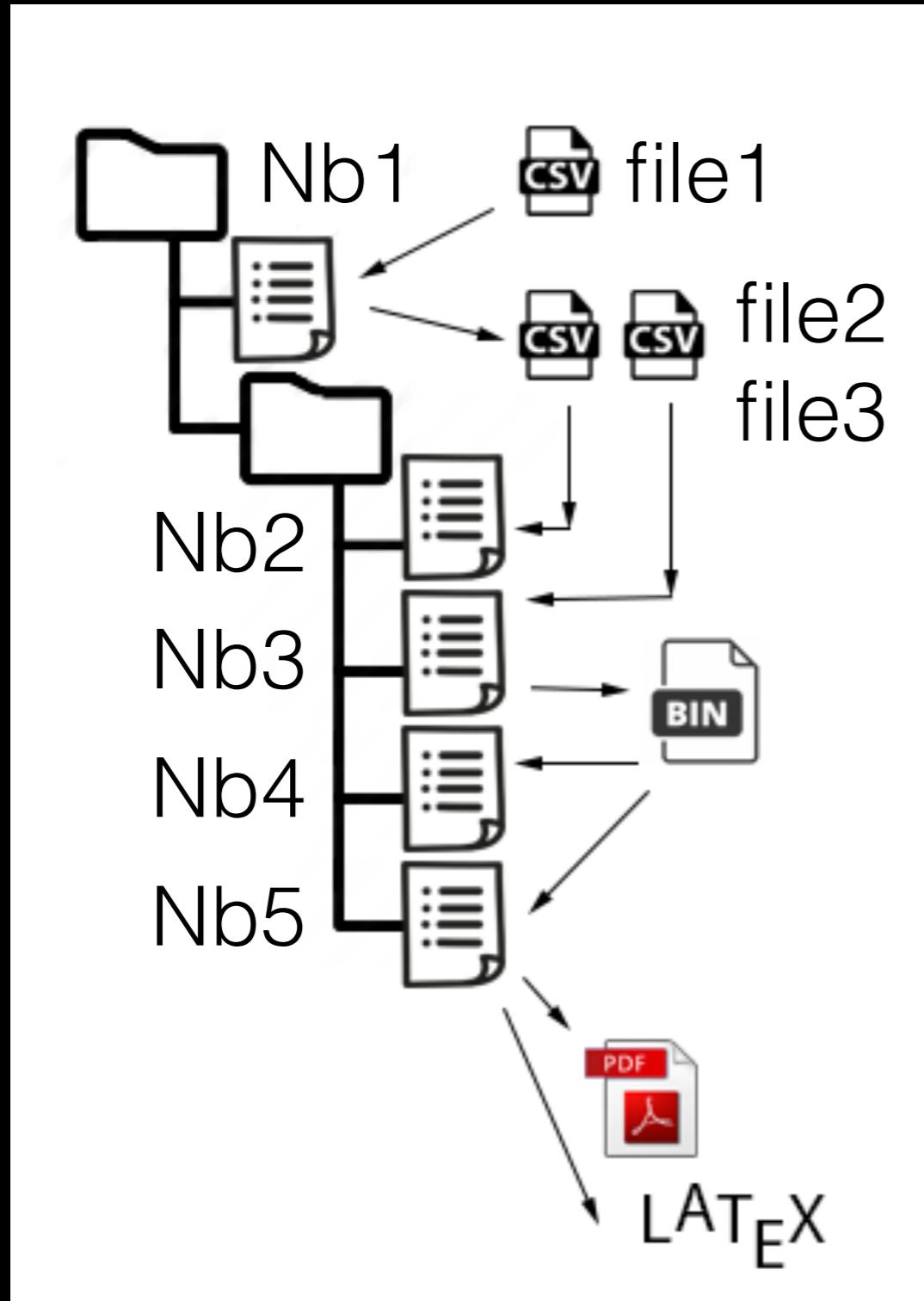
SciPy2016

Contents

- nbflow
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nbflow

Problem



If I modify Nb3, which other notebooks do I need to run ?

Solution

Define in each notebook its dependencies

nbflow

Define the dependencies at the top of the notebook

```
__depends__ = ["..../results/data.json"]
__dest__ = "..../results/stats.json"
```

A screenshot of a Jupyter Notebook cell. The cell contains the following Python code:

```
92 lines (91 sloc) | 1.73 KB
Raw Blame History ⚡ 🖊 🗑
```

```
In [ ]: __depends__ = ["..../data/human_raw.json"]
        __dest__ = "..../results/human.csv"

In [ ]: import pandas as pd
        import json
        import datetime

In [ ]: # Load the JSON formatted data
        with open(__depends__[0], "r") as fh:
            data = json.load(fh)
        data[0]

In [ ]: # Convert it to a pandas DataFrame
        df = pd.DataFrame(data).set_index(["participant", "stimulus"]).sortlevel()
        df['timestamp'] = df['timestamp'].apply(datetime.datetime.fromtimestamp)
        df.head()

In [ ]: # Save it to CSV
        df.to_csv(__dest__)
```

nbflow

To run the magic library

install nbflow

> pip2 install git+git://github.com/jhamrick/nbflow.git

Move to top folder and edit SConstruct file

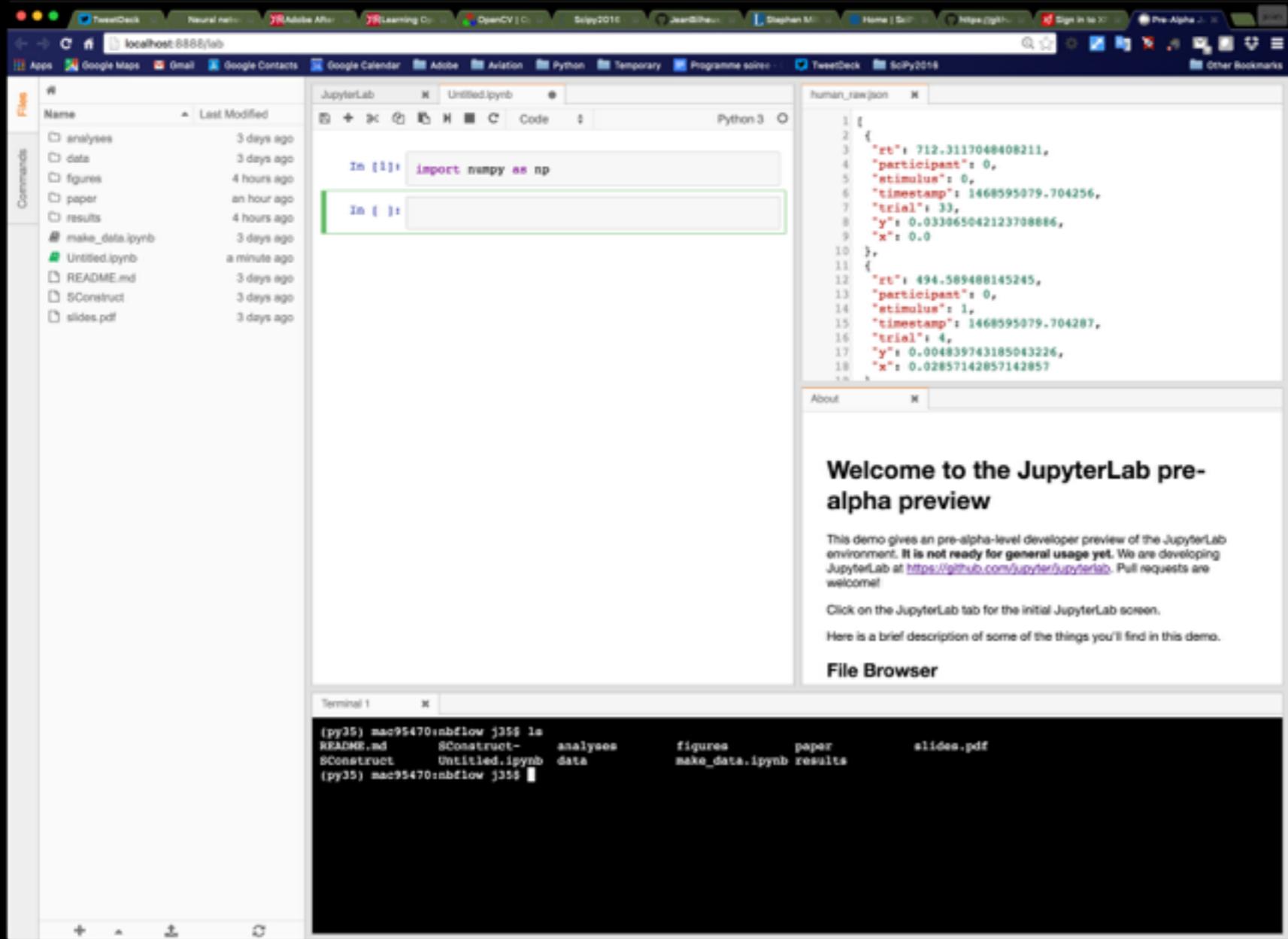
```
12 lines (9 sloc) | 300 Bytes

1 import os
2 import glob
3 from nbflow.scons import setup
4
5 env = Environment(ENV=os.environ)
6 setup(env, ["analyses"])
7
8 results = sorted(glob.glob("results/*.tex"))
9 figures = sorted(glob.glob("figures/*.pdf"))
10 env.PDF("paper/paper.pdf", "paper/paper.tex")
11 env.Depends("paper/paper.pdf", results + figures)
```

Then run library

> scons

jupyter lab



Current version should not be used for development!

<https://github.com/jupyter/jupyterlab>

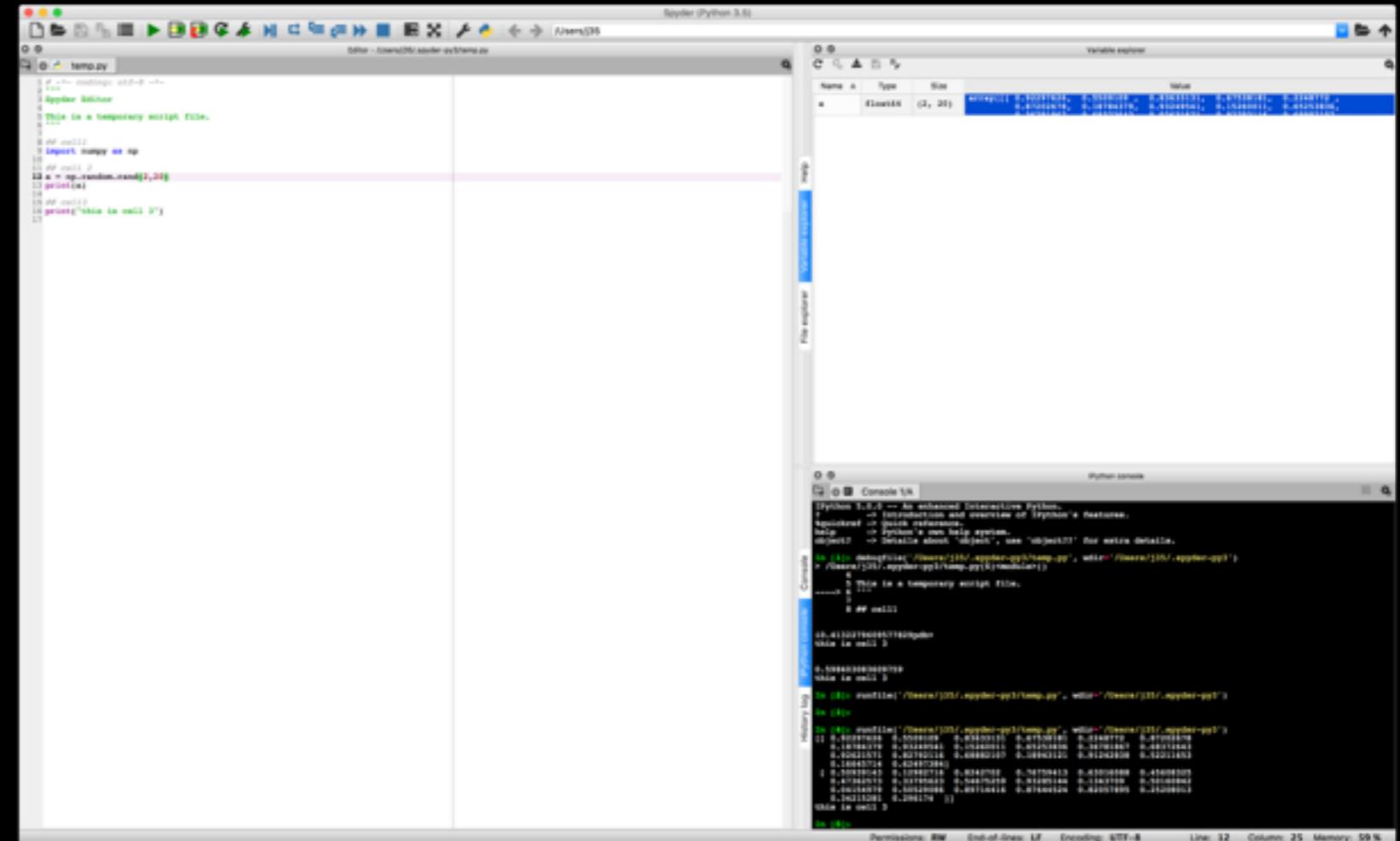
File browser,
notebooks,
terminal, file
editor, all in one
window, inside
the browser.

beta version
and
aiming for a
1.0 release
before next
SciPy

spyder 3.0

What's new

- work with projects
- plugins
 - ex: new buttons
- conda graphical installer
- line profiler

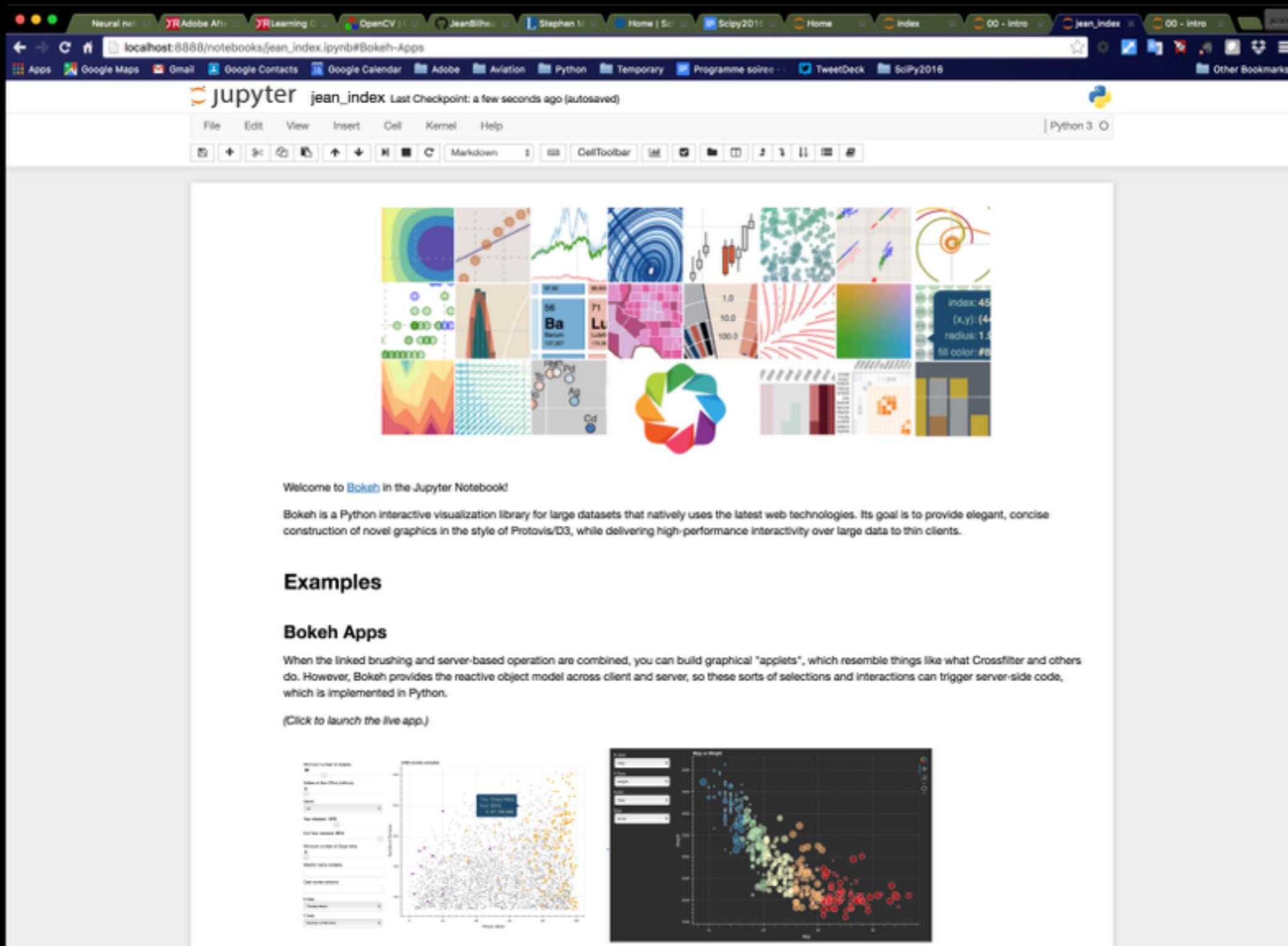


Tool to make python looks like matlab IDE

My opinion

- concurrent of jupyter lab
- will be a great tool for playing with data
- still has some GUI issues

bokeh (0.12.0)



demo -> OverviewSciPy2016/bokeh/jean_index.ipynb

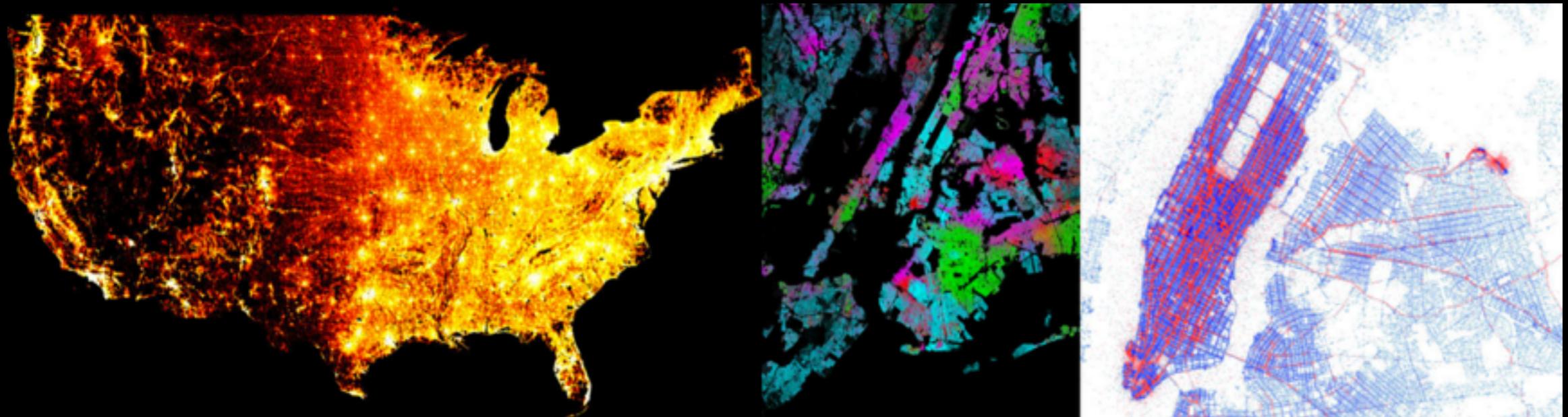
holoviews

Stop plotting your data -
annotate your data and let it
visualize itself

```
> conda install bokeh pandas ipython-notebook ipywidgets
```

demo -> Overview/SciPy2016/holoviews/index.ipynb

datashader: visualizing big data sets



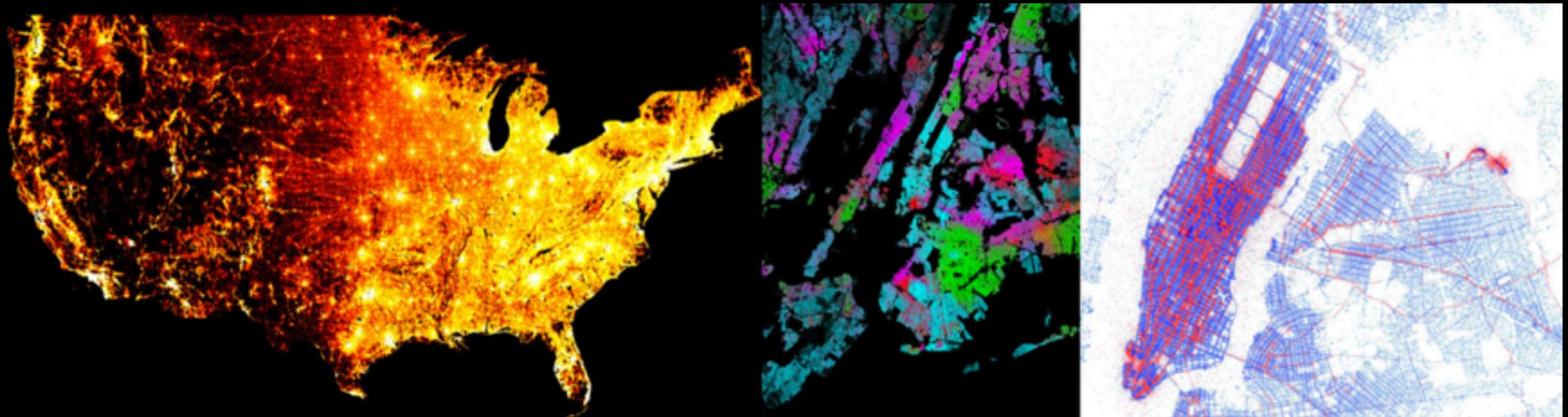
When not to use data shader

- Plotting less than 1e5 or 1e6 data points
- When every datapoint matters; standard Bokeh will render all of them
- For full interactivity (hover tools) with every datapoint

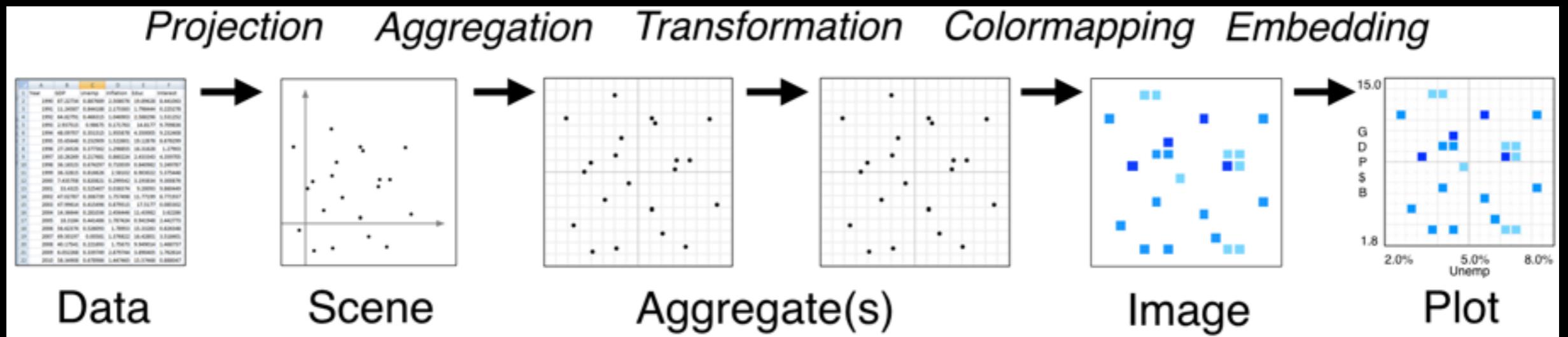
When to use data shader

- Actual big data; when Bokeh/Matplotlib have trouble
- When the distribution matters more than individual points
- When you find yourself sampling or binning to better understand the distribution

datashader: visualizing big data sets

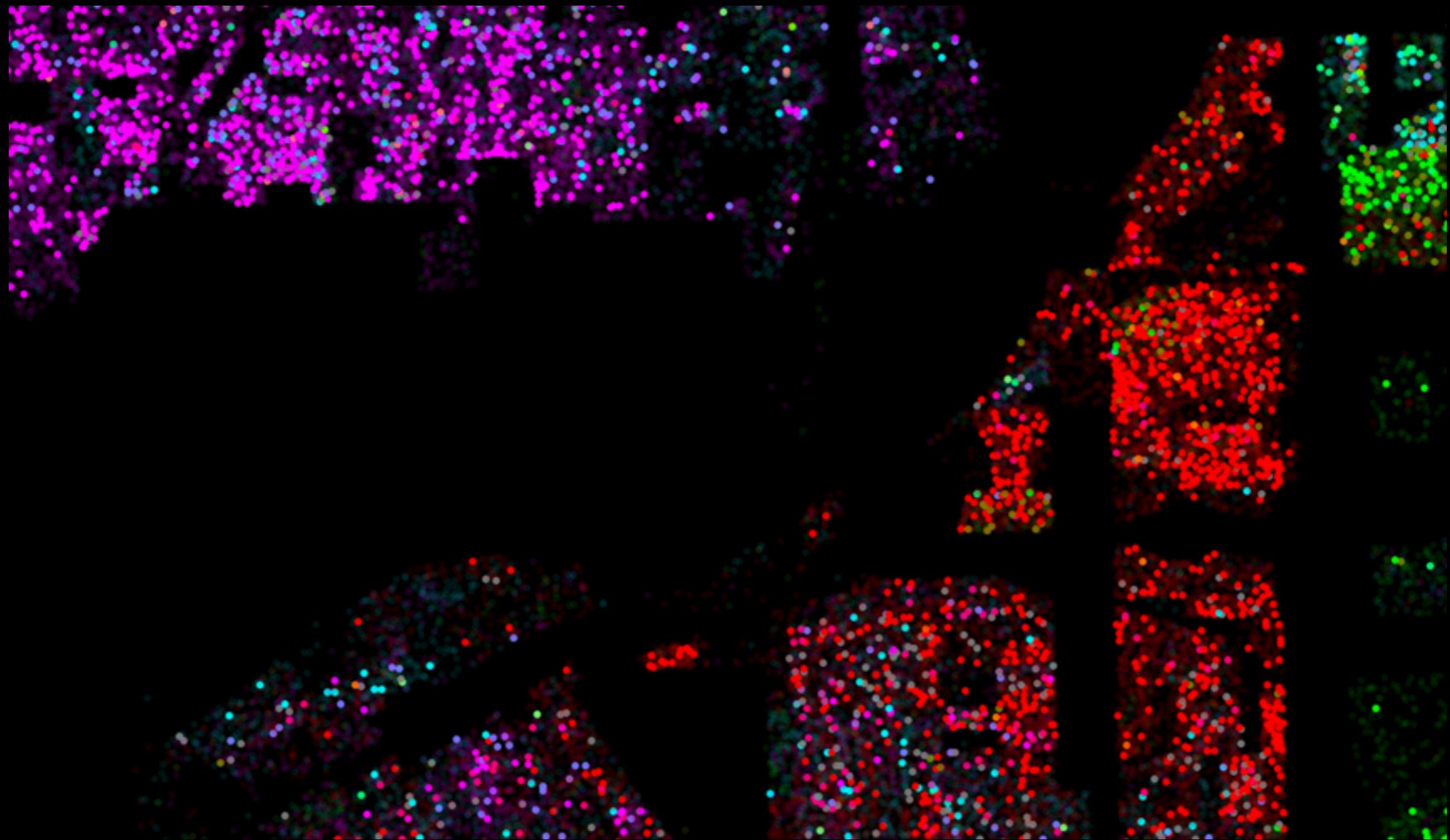


How does it work



demo -> OverviewSciPy2016/datashader/index.ipynb

datashader: visualizing big data sets



parallel python

- mpi4py
(https://github.com/JeanBilheux/python_tutorial/tree/master/python/parallelization)
- map
- Submit

<http://matthewrocklin.com/scipy-2016-parallel/algorithms.html#/0/1>

demo -> Overview/SciPy2016/parallel/



Thank you

github.com/JeanBilheux/OverviewSciPy2016