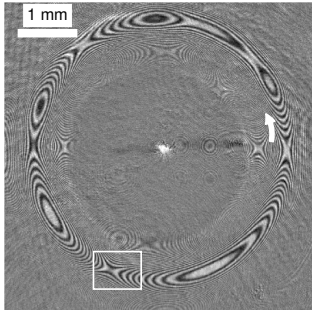
Matplotlib and Scientific Visualization

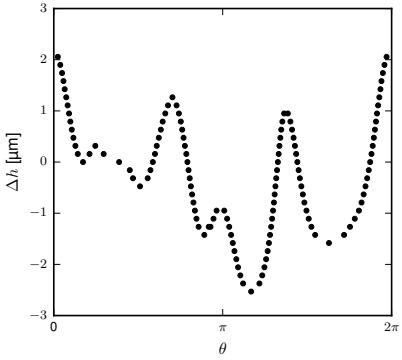
Thomas A Caswell

2021-03-17

Who am I?

- Trained as a physicist
  - Jamming + dynamics of Leidenfrost drops with Nagel and Gardel at UChicago





Who am I?

- Trained as a physicist
  - Jamming + dynamics of Leidenfrost drops with Nagel and Gardel at UChicago
- Currently in Data Science and System Integration program at NSLS-II
- Current Project Lead of Matplotlib

Acknowledgments

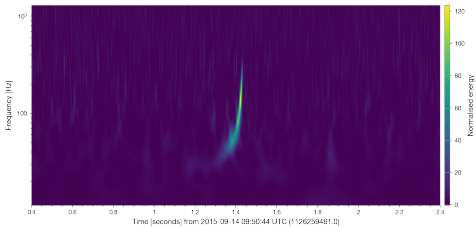
- John Hunter (1968-2012)
- Michael Droettboom
- The whole Matplotlib development team
  - Over 1,250+ have contributed code, many more in bug reports, feature requests, and user support
- Dora Caswell

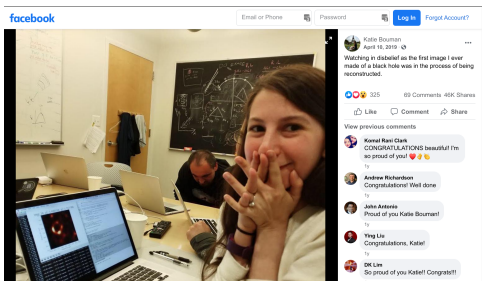
Recent funding from Chan Zuckerberg Initiative (2020-present)

Matplotlib

. . . is a comprehensive library for creating static, animated, and interactive visualizations in Python.

- Widely used through out science
  - LIGO, EHT, LSST, NSLS-II, APS, ALS, SPT, STSci, ATLAS, Mars rovers, . . .
  - Single PI labs in physics, chemistry, oceanography, meteorology, biology, . . .





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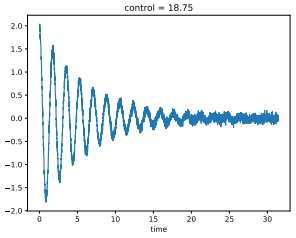
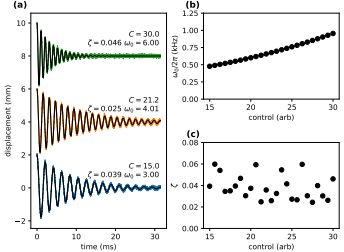
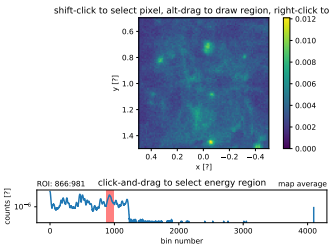
https://mybinder.org/v2/gh/losc-tutorial/quickview/master
https://github.com/losc-tutorial/quickview

What is visualization for?

1. Exploratory data analysis
   - just get the data on the screen in a way *you* can understand as fast as you can
2. Paper figures
   - need to be *just right*
3. Part of a standard (interactive) workflow
   - repeatedly visualize and explore similar data

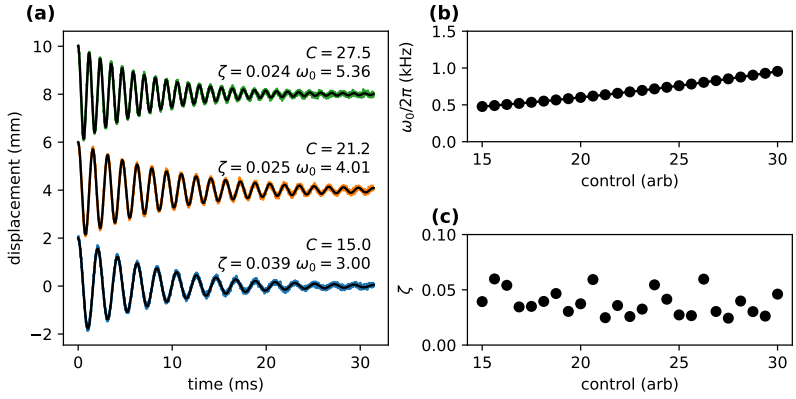






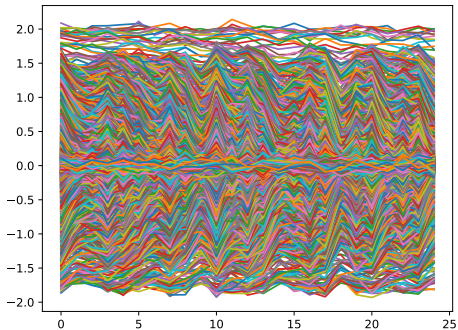
Case Study: Paper Figure

- you have 25 cantilevers, varied something (called 'control') in fabrication
- displace away from equilibrium position and released to watch vibrations ring down
- Goals:
  - go from exploratory visualization to paper ready figures
  - write reusable helper functions



Step 0.0 ("just plot it")

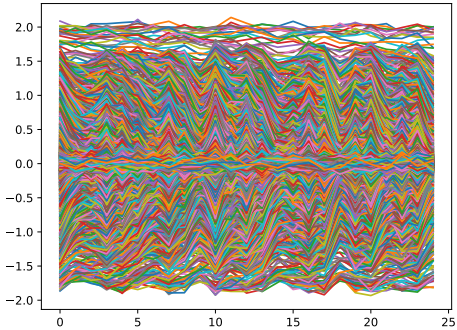
```
1  from gen_data import get_data
2  import matplotlib.pyplot as plt
3
4  d = get_data()
5  plt.plot(d)
```



Step 0.0 ("just plot it")

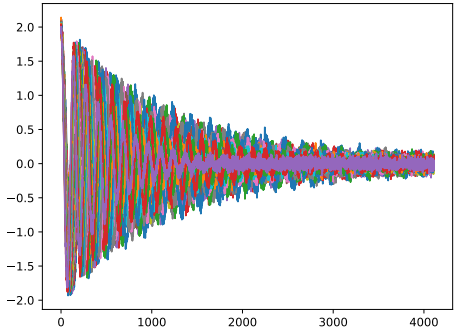
```
1  from gen_data import get_data
2  import matplotlib.pyplot as plt
3
4  d = get_data()
5  plt.plot(d)
```

- #accidentalart



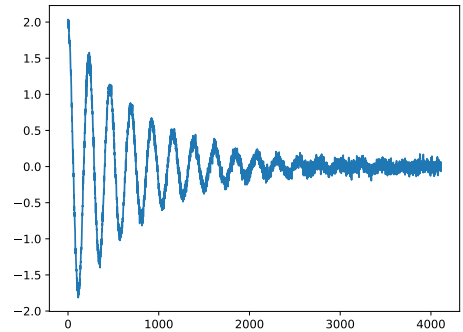
Step 0.1 ("just plot it. . . the right direction")

```
1  from gen_data import get_data
2  import matplotlib.pyplot as plt
3
4  d = get_data()
5  plt.plot(d.T)
```



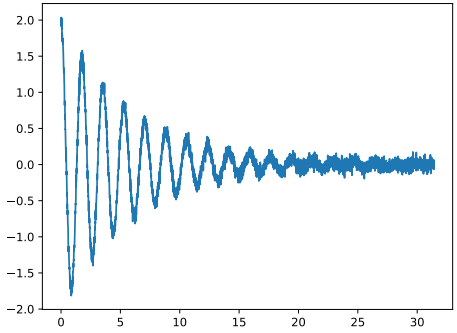
Step 1.0 (plot just one)

```
1  from gen_data import get_data
2  import matplotlib.pyplot as plt
3
4  d = get_data()
5  m = d[6]
6  plt.plot(m)
```



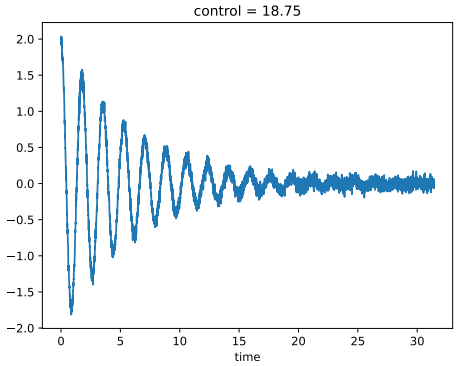
Step 1.1 (use meaningful x-axis)

```
1  from gen_data import get_data
2  import matplotlib.pyplot as plt
3
4  d = get_data()
5  m = d[6]
6
7  fig, ax = plt.subplots()
8  ax.plot(m.time, m)
```



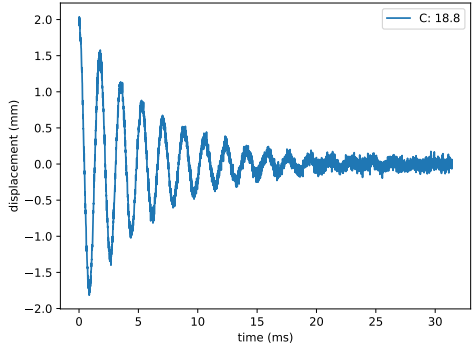
Step 1.1.1 (use xarray's plotting)

```
1  from gen_data import get_data
2  import matplotlib.pyplot as plt
3
4  d = get_data()
5  m = d[6]
6
7  fig, ax = plt.subplots()
8  m.plot(ax=ax)
```



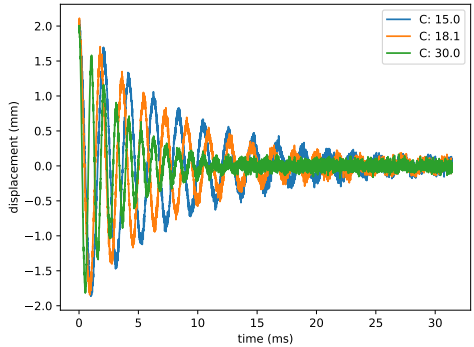
Step 1.2 (add legend and axis labels)

```
1  d = get_data()
2  m = d[6]
3  ctrl = float(m.control)
4  fig, ax = plt.subplots()
5
6  ax.plot(
7      m.time,
8      m,
9      label=f"C: {ctrl:.1f}"
10 )
11
12 ax.legend()
13 ax.set_xlabel("time (ms)")
14 ax.set_ylabel("displacement (mm)")
```



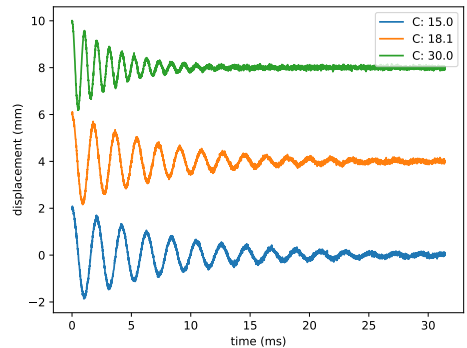
Step 1.3 (make a function)

```
1  def plot_one(ax, m):
2      ...
3      ln, = ax.plot(
4          m.time, m, label=label
5      )
6      ...
7
8  fig, ax = plt.subplots()
9  plot_one(ax, d[0])
10 plot_one(ax, d[5])
11 plot_one(ax, d[-1])
12 ...
```



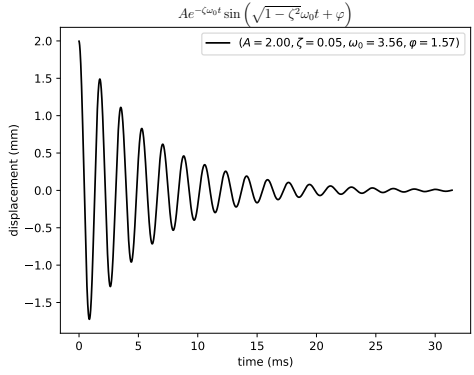
Step 1.4 (add vertical offset)

```
1  def plot_one(ax, m, offset=0):
2      ...
3      ln, = ax.plot(
4          m.time,
5          m + offset,
6          label=label
7      )
8      ...
9  ...
10 plot_one(ax, d[0]. offset=0)
11 plot_one(ax, d[5]. offset=4)
12 plot_one(ax, d[-1]. offset=8)
13 ...
```



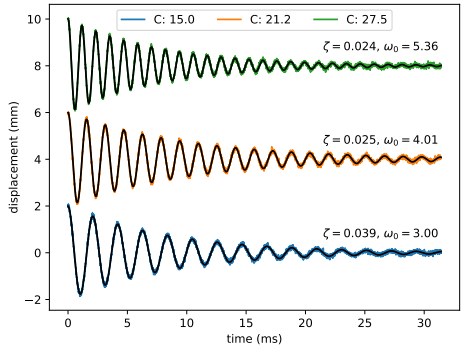
Step 2.0 (fit the data)

```
1  from gen_data import fit
2  ...
3  fit_vals = fit(m)
4  ax.plot(
5      m.time,
6      fit_vals.sample(m.time),
7      label=fit_vals._repr_latex_(),
8      color='k'
9  )
10 plt.gca().set_title(
11     r"$A e^{-\zeta\omega_0t} \sin..."
12     usetex=True
13 )
14 ...
```



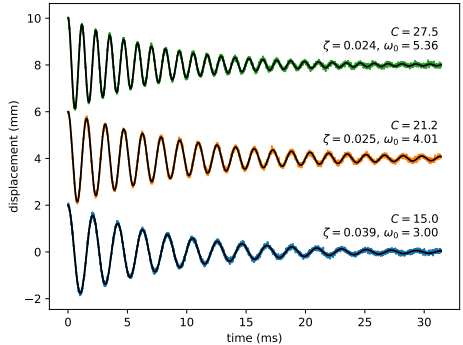
Step 2.1 (plot fit on data)

```
1  def plot_one(ax, m, fv, offset=0):
2      fit, = ax.plot(
3          t, fv.sample(t) + offset
4      )
5      ann = ax.annotate(...)
6      ...
7  ...
8  plot_one(
9      ax, d[10], fit(d[10]), offset=4
10 )
11 ax.legend(
12     ncol=3, loc="upper center"
13 )
14 ...
```



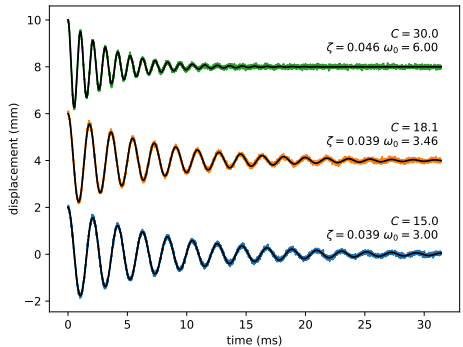
Step 2.2 (move control label to annotation)

```
1  def plot_one(ax, m, fv, offset=0):
2      ...
3      ann = ax.annotate(...)
4      ...
5
6  ...
7  plot_one(
8      ax, d[10], fit(d[10]), offset=4
9  )
10 ...
```



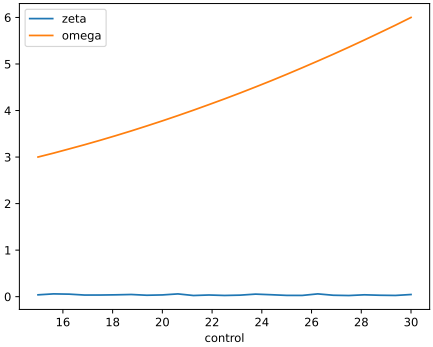
Step 2.3 (write another function)

```
1  def plot_several(ax, d, fits):
2      for j, (m, fv) in enumerate(
3              zip(d, fits)
4      ):
5          plot_one(ax, m, fv, 4*j)
6      ax.set_xlabel("time (ms)")
7      ax.set_ylabel("displacement (mm)")
8
9  fig, ax = plt.subplots()
10 indx = [0, 5, 24]
11 fits = [fit(d[i]) for i in indx]
12 plot_several(ax, d[indx], fits)
```



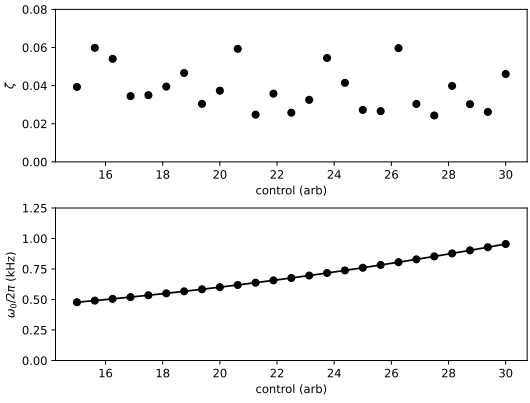
Step 3.0 (look at ω_0 and ζ)

```
1  import pandas as pd
2
3  fits_df = pd.DataFrame(
4      [fit(m) for m in d],
5      index=d.coords["control"]
6  )
7
8  fig, ax = plt.subplots()
9  fits_df.plot(
10     y=["zeta", "omega"], ax=ax
11 )
```



Step 3.1 (helper functions for ω_0 and ζ plots)

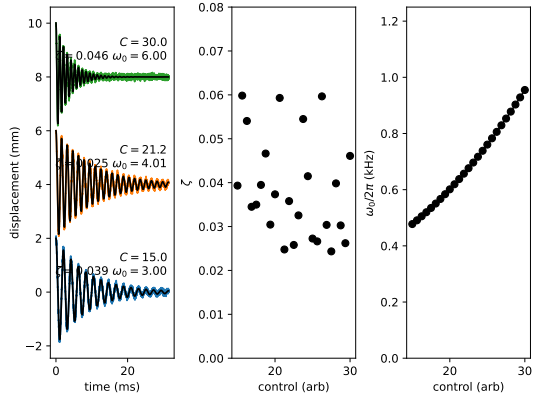
```
1  def plot_zeta(ax, fits_df):
2      ax.set_xlabel(...)
3      ax.set_ylabel(...)
4      return ax.plot(...)
5
6  def plot_omega(ax, fits_df):
7      ax.set_xlabel(...)
8      ax.set_ylabel(...)
9      return ax.plot(...)
10
11 fig, (ax1, ax2) = plt.subplots(2, 1)
12 plot_zeta(ax1, fits_df)
13 plot_omega(ax2, fits_df)
```



Step 4.0 (put it all together)

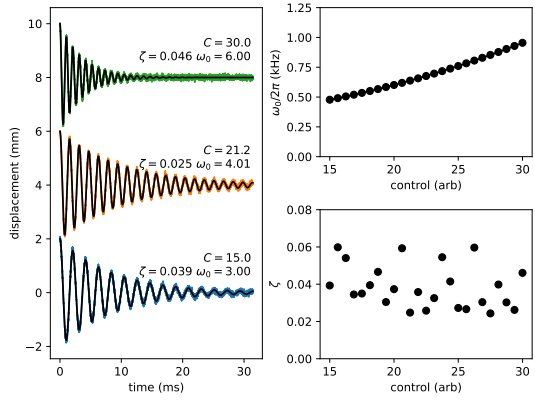
```
indx = [0, 10, 24]

fig, (ax1, ax2, ax3) = plt.subplots(
    1, 3, constrained_layout=True
)
plot_several(
    ax1,
    d[indx],
    [fits[i] for i in indx]
)
plot_zeta(ax2, fits_df)
plot_omega(ax3, fits_df)
```



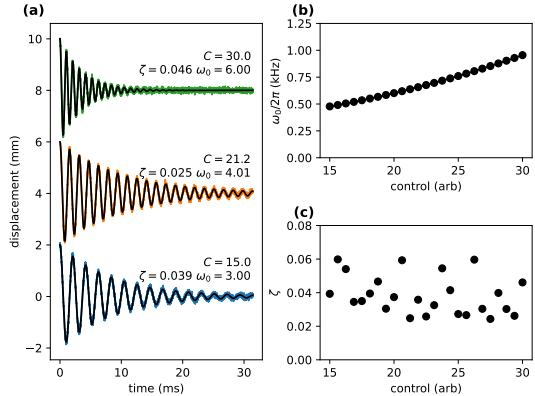
Step 4.1 (improve the layout)

```
1  fig, ad = plt.subplot_mosaic(
2      [["raw", "omega"],
3       ["raw", "zeta" ]],
4      constrained_layout=True
5  )
6  indx = [0, 10, 24]
7  plot_several(
8      ad["raw"],
9      d[indx],
10     [fits[i] for i in indx]
11 )
12 plot_zeta(ad["zeta"], fits_df)
13 plot_omega(ad["omega"], fits_df)
```



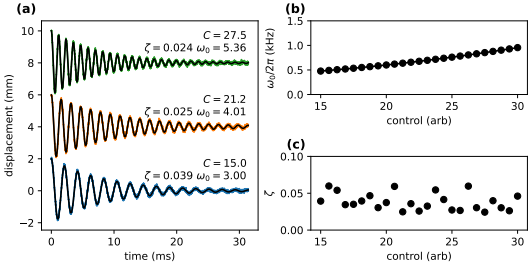
Step 4.2 (label the subplots)

```
1  def subplot_label(ax, text):
2      return ax.annotate(text, ...)
3
4  spm = {
5      "raw": "a",
6      "omega": "b",
7      "zeta": "c"
8  }
9
10 for k, v in spm.items():
11     subplot_label(ad[k], f"({v})")
```



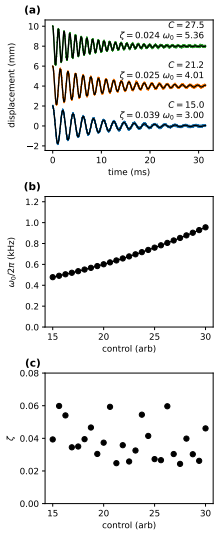
Step 4.3 (set the size to journal specifications)

```
1  def paper_figure_2(
2      fig, layout, d, fits, plot_every
3  ):
4      ...
5
6  dcw = 17.8 / 2.54
7  paper_figure_2(
8      plt.figure(
9          figsize=(dcw, dcw * 0.5)
10     ),
11     [["raw", "omega"], ["raw", "zeta"]],
12     d,
13     fits,
14     plot_every=10,
15 )
```



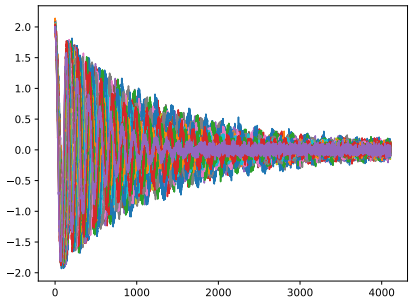
Step 4.4 (try a one column layout)

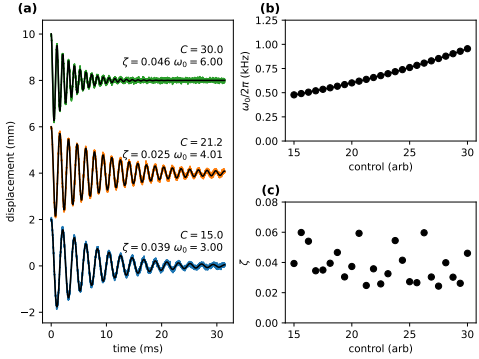
```
1  scw = 8.6 / 2.54
2  paper_figure_2(
3      plt.figure(
4          figsize=(scw, scw * 2.5)
5      ),
6      [["raw"], ["omega"], ["zeta"]],
7      d,
8      fits,
9      plot_every=10,
10 )
```



Case Study Summary

- Went from initial exploratory look at data to a paper-ready figure
- Iterative built a mini-library for this experiment





Interactive Visualizations

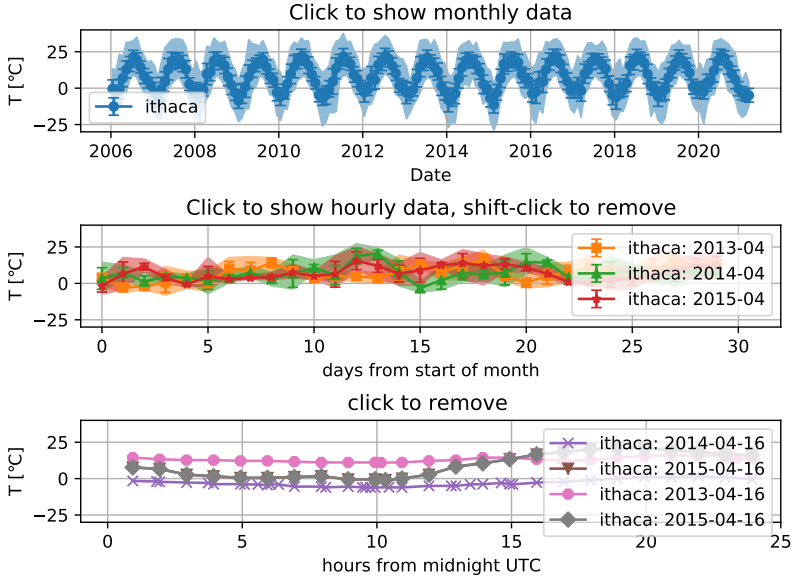
- Matplotlib has framework-agnostic UI tools to get mouse and keyboard events
- several third-party-packages with more complex interactions
  - mplcursors https://mplcursors.readthedocs.io/en/stable/
  - MplDataCursor https://github.com/joferkington/mpldatacursor
  - mpl_interactions https://mpl-interactions.readthedocs.io/en/latest/

LIVE DEMO TIME

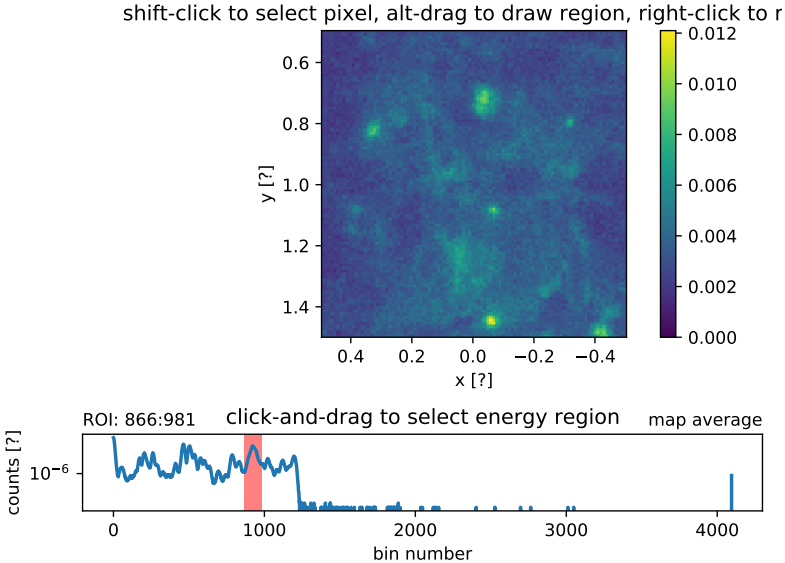
Hello world

- `fig.ginput` in a terminal
- handle mouse click events in a Jupyter notebook

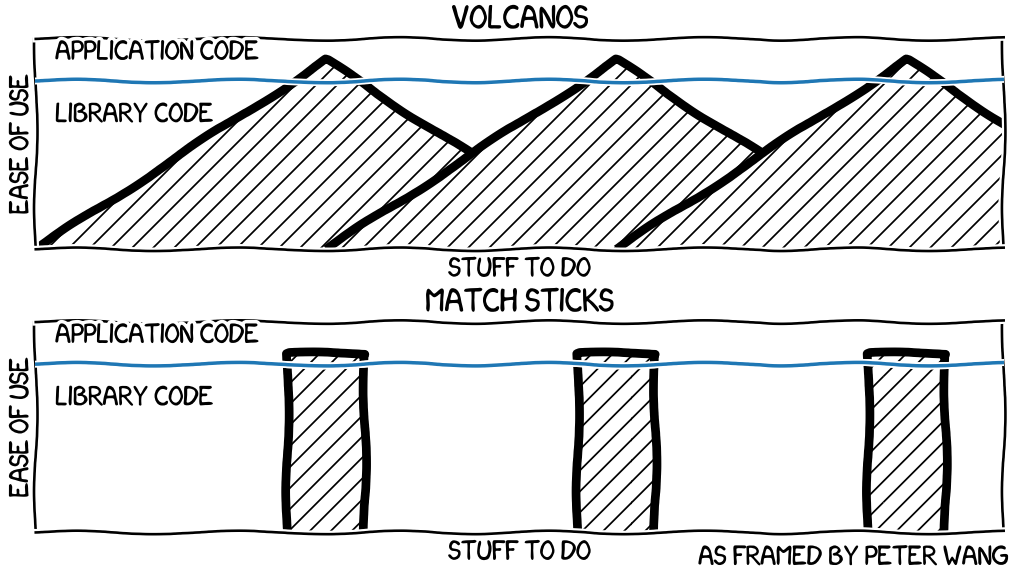
Interactive application (temperature)



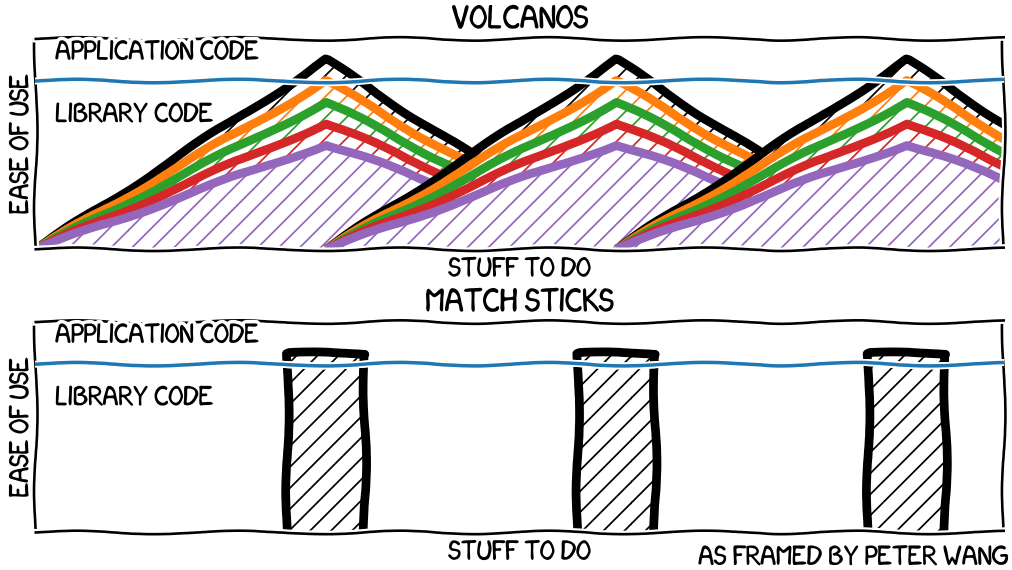
Interactive applications (x-ray fluorescence map)



Iterative software development



Iterative software development



Future Work

- On going incremental improvements, bug fixes, and maintenance
- Improvements to Figure and Axes layout tooling (Jody Klymak)
- Re-designing Matplotlib's internal data model (Hannah Aizenman)

Resources

This material: https://github.com/tacaswell/2021-03_APS

- docs: https://matplotlib.org/stable
- cheatsheets: https://github.com/matplotlib/cheatsheets
- chat: https://gitter.im/matplotlib
- forum: https://discourse.matplotlib.org
- tutorials:
  - https://github.com/matplotlib/interactive_tutorial,
  - https://github.com/matplotlib/AnatomyOfMatplotlib
  - https://github.com/matplotlib/GettingStarted
- Interactive Applications Using Matplotlib, Benjamin V. Root (2015)
- domain-specific libraries
- Building a maintainable plotting library (PyData NYC 2019) https://youtu.be/NV4Y75ZUDJA
- Seperation Of Scales (PyData Gobal 2020) https://youtu.be/P85UIuMovnI