From Science to Open Source and Back Again

Thomas A Caswell

2022-11

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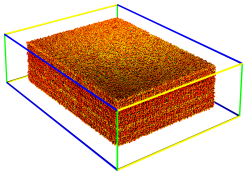

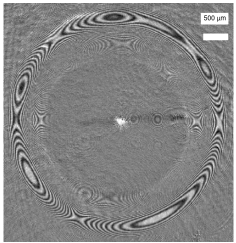

Who is this guy talking to you?

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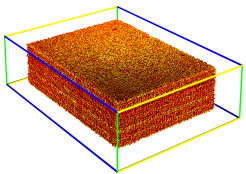
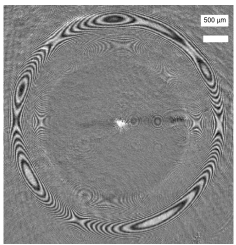
  - studied jammed amorphous systems + dynamics of Leidenfrost drops
- Currently developing data acquisition at NSLS-II
- Current Project Lead of Matplotlib
- PSF Fellow (Q2 2022)





matplotlib

bluesky

Acknowledgments

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- Dora Caswell

Software is core to the future of science

- Software is critical to (almost) all modern experimental science [1].

[1] https://doi.org/10.5281/zenodo.7295423

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- ... lets you ask different questions.
- ... encapsulates techniques in a re-usable and transferable way.

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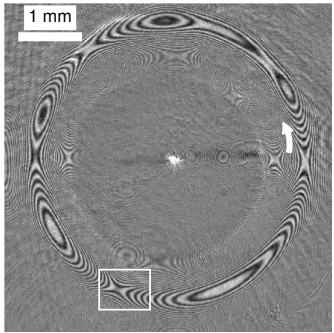
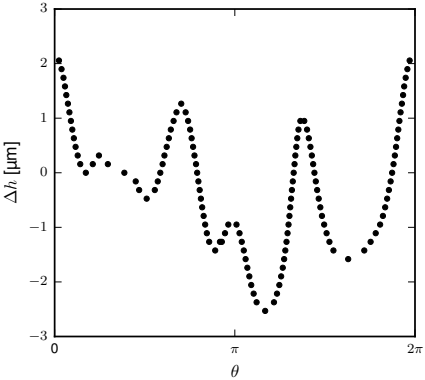
  - 20,000 particles per frame over thousands of frames
  - could only (practically) be done with software

tracking fringes

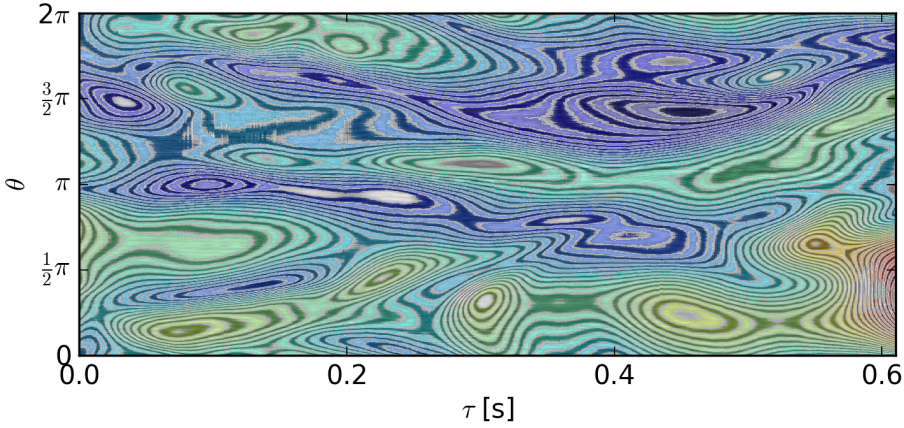




- Justin Burton manually counted fringes, got science out!
- "I bet you can automate that and get a time series of the profile" - Me

- 2011-11 got prototype working
- 2012-06 pulled `trackpy` out
- 2013-12 defended PhD & paper

tracking fringes



- 1TB of high-speed video to extract dynamics of the rim
- Could not have done this "by hand"

Software is a team sport

Oct 11, 2012, 7:55 PM
Subject: tracking.py

Hi Thomas,

I'm a physics grad at JHU working for Bob Leheny, who is himself a former student of Sidney Nagel. I came across your website a few years ago by way of Eric Weeks' page. Today I checked in on your site and found your pure Python implementation of track.pro.

Over the last few months I implemented the Crocker/Weeks particle location algorithm in pure Python (with a little C). I know you have done the same in C++. Currently, I'm still calling IDL to do the trajectory-linking step, but I am about to try switching to your tracking.py. I'm letting you know that I'm using it, as you request on your web page. Also, maybe we should consider contributing to each other's repositories.

Here's mine: https://github.com/danielballan/mr

Cheers, Dan

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- This led to merging our code bases
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  - About 30 people have now contributed to `trackpy`
- Dan joined me at BNL and is my closest collaborator

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- Myth of "lone genius" is harmful in both science and software

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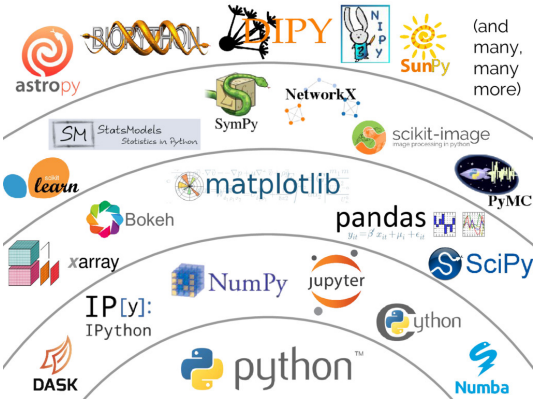
- Useful software is bigger than one person can physically write
  - particularly if you include the whole stack!
- Every piece of software I've written together is better than any I wrote alone

"If I have seen further it is by standing on the shoulders of Giants" -Newton

All of this was made possible by the Scientific Python ecosystem



Credit: Jake VanderPlas's SciPy 2015 Keynote

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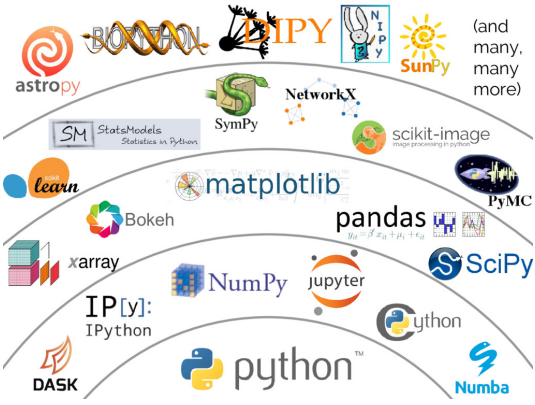

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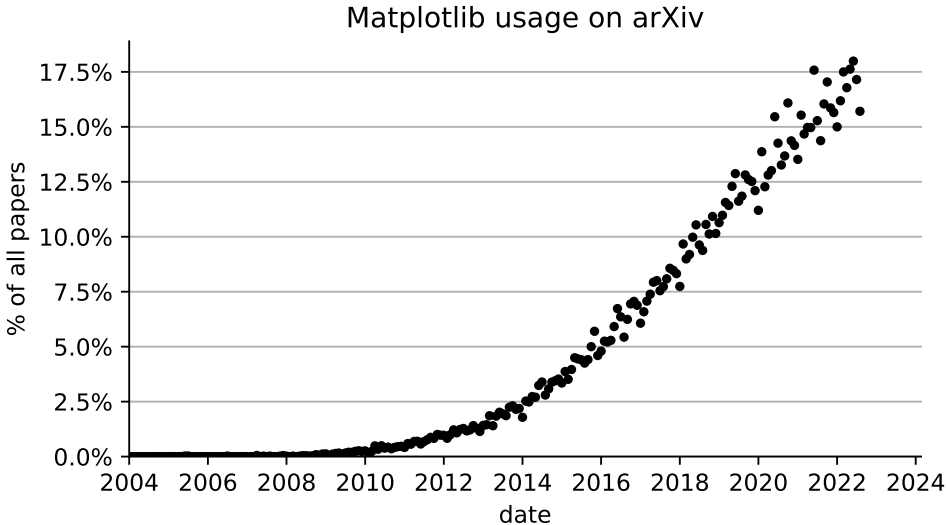
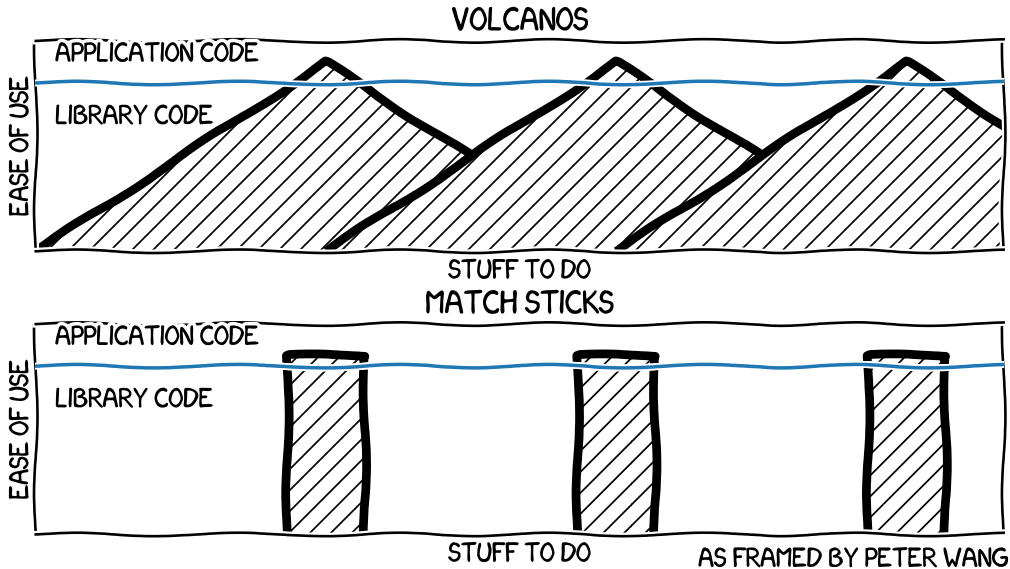
- trackpy has been cited 296 times
- Leidenfrost paper cited 40 times (Physical Review E 90 (1), 013014)

Matplotlib's impact



https://www.coiled.io/blog/how-popular-is-matplotlib

Build volcanos not match sticks



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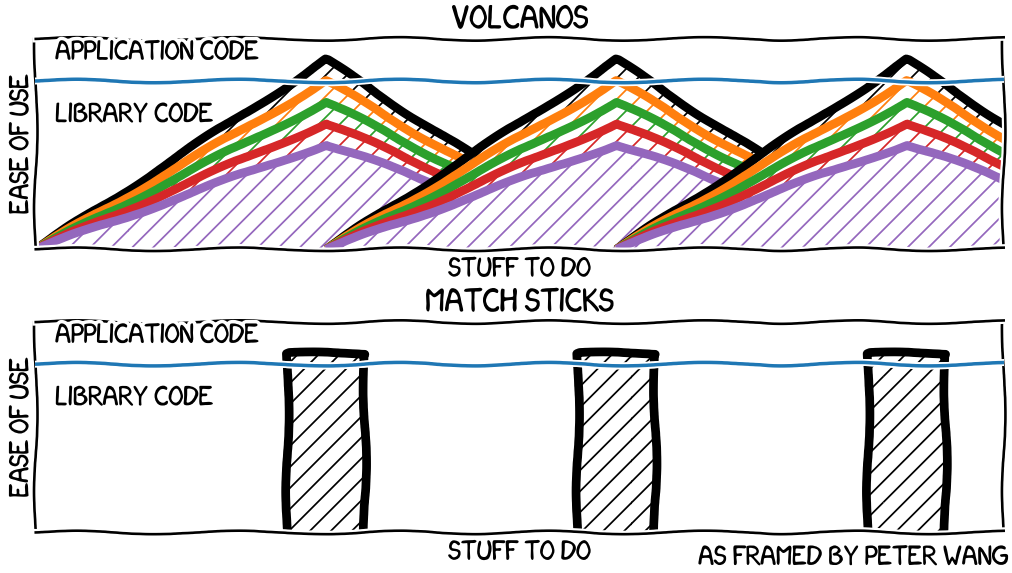

Application vs Library

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- never fail

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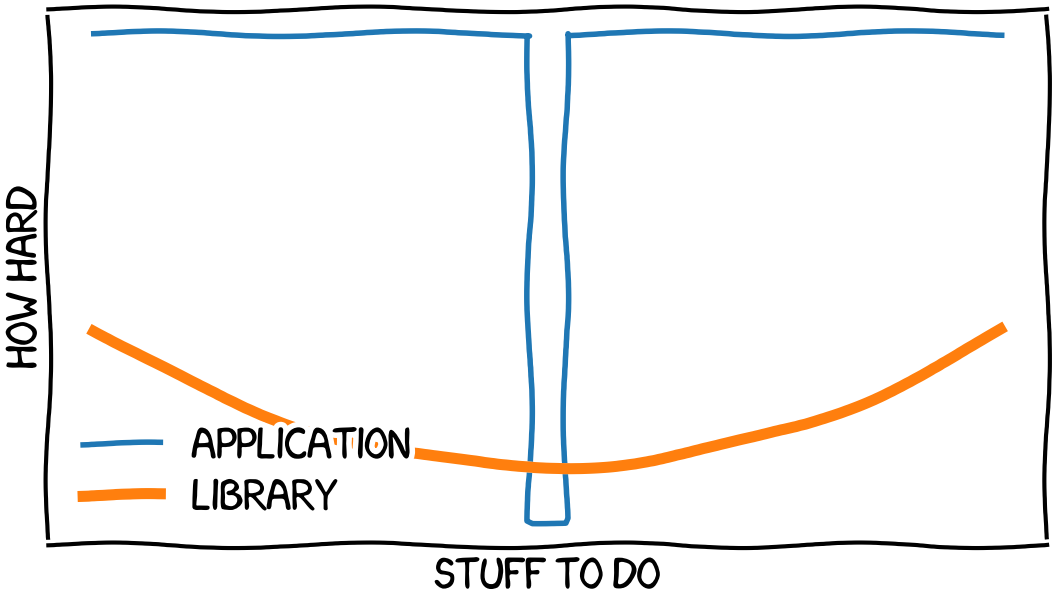
- agnostic (as possible) to I/O
- fail hard and fast

Application vs Library



Case Study

Directory of images named like `./{sample_name}/x_y_{T}C_z.tiff`

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g = Path(".").glob("**/*.tiff")
out = {}
for f in g:
    data = tifffile.imread(f)
    sample = f.parents.parts[-1]
    fn = f.name
    T = int(fn.split("_")[2][:-1])
    out[sample] = data.sum() / T
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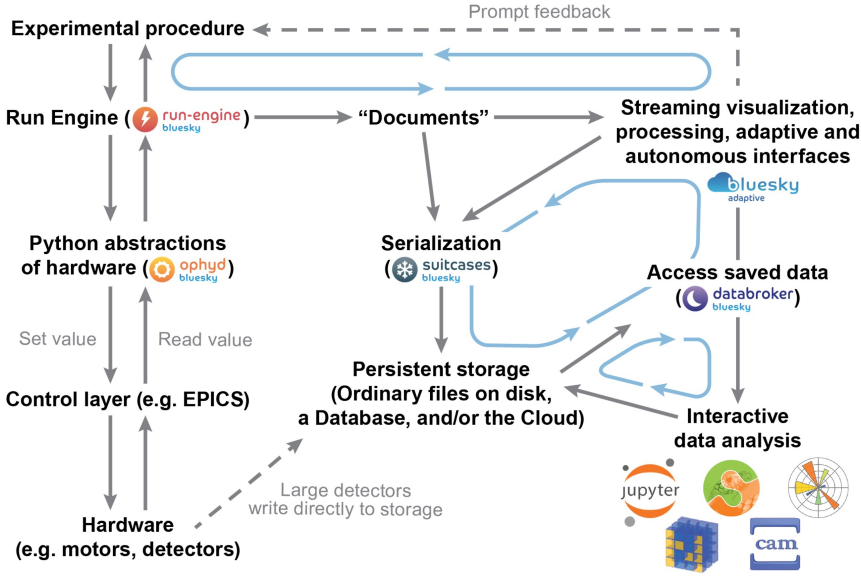
- If I make this change who do I break?

Dawn of Bluesky



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Impact and adoption

- Running NSLS-II user operations
  - (1.3k+ researchers|550+ papers)/yr

If you have experimental apparatus you want to automate talk to me!

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Why did this work?

- co-designed but independent libraries
- Developed in the open from the start
  - anyone can see the code
  - anyone can see and join discussions
  - anyone can influence the code
- invite users to become collaborators

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- Technical skills
  - "the easy part"

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Enter the Research Software Engineer (RSE)

"We like an inclusive definition of Research Software Engineers to encompass those who regularly use expertise in programming to advance research. This includes researchers who spend a significant amount of time programming, full-time software engineers writing code to solve research problems, and those somewhere in-between"

https://us-rse.org/about/what-is-an-rse/

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What a RSE role is not?

- Computer Science research

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  - where are the likely extension points?
  - What are the right trade offs?
- Partnership and Collaboration
  - RSE conversant in domain
  - Domain scientist conversant in SW

https://us-rse.org | https://us-rse.org/jobs/

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- Make friends! Build collaborations! Have fun!

Links

- US-RSE home page: https://us-rse.org
- CSCCE home page: https://www.cscce.org
- Bluesky project homepage: https://blueskyproject.io
- My blog: https://tacaswell.github.io
- Use VC: https://tacaswell.github.io/how-i-learned-to-love-vcs.html
- mpl on arXiv source: https://github.com/mrocklin/arxiv-matplotlib
- Daniel Katz talk: https://doi.org/10.5281/zenodo.7295423
- These slides: https://github.com/tacaswell/talk_2022-11_pydataNYC

tcaswell@gmail.com | tcaswell@bnl.gov | @tacaswell@fosstodon.org

backup buffer

How did I start to work on Matplotlib?

- opened a PR to solve a problem I had (10yrs ago in August)
  - https://github.com/matplotlib/matplotlib/pull/1062
- started answering questions on StackOverflow about Matplotlib while procrastinating my research (sorry Sid)
- eventually started reporting & fixing bugs upstream
- was offered commit rights and asked to start reviewing other PRs
- was offered co-lead in 2014
- was offered lead in 2016