

# Software for research(ers)

\*Plus bonus cat photos

Andy Boughton / [Center for Statistical Genetics](#)

July 2017







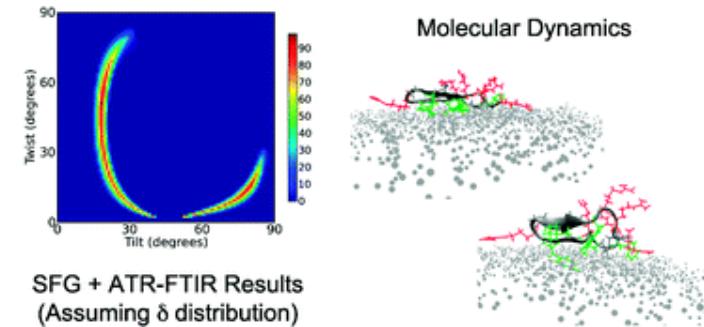
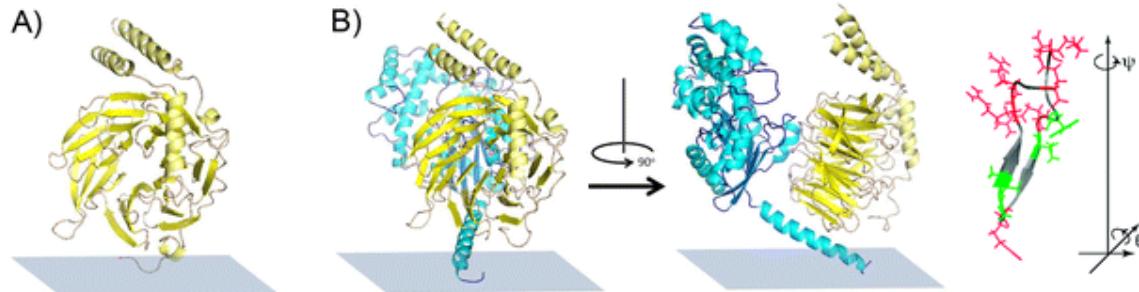
# What I do here

- Applications Programmer/Analyst (I write code)
  - Python (various)
  - JavaScript/ full stack web development
  - Solve problems and languages will follow
- Topics I can drone on about
  - Usability / Accessibility
  - Front-end security considerations
  - Open science/ open data



# Act I: Chemistry (PhD, 2011)

- Studied the behavior of proteins at interfaces
  - Molecular Dynamics Simulations
  - Sum Frequency Generation Vibrational Spectroscopy





# Act II: Life among the engineers

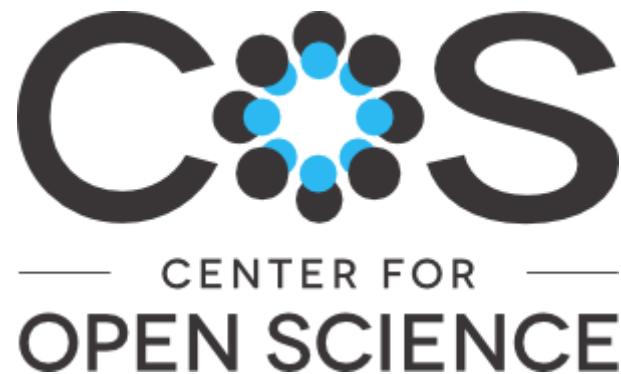
- DARPA AVM project: crowdsourced vehicle designs
- Built tools to collaboratively capture component designs
- Wrote code to predict vehicle properties based on geometry models





# Act III: Thinking about collaboration

- Nonprofit technology startup (Charlottesville, VA)
- Web applications to help researchers share data
- Emphasis on reusable libraries and APIs
- Preprint service, participant recruiting, many other projects





# How it all ties together

Modern instruments are slowly turning data collection  
from an artisanal good to a commodity

New opportunities if you can make sense of the data

The really good discoveries require combining  
approaches

...and incentives to make it happen



# Software... for researchers

- Evolve requirements but preserve communities
- "What can we get away with breaking?"
- Central servers are fragile- be agnostic about entry points
- Tools are fragile- ambiguous code will break
- Tools may outlast students, eventually documentation is wrong

\* Opinions my own, if even that



*In thinking about why the technique has been so widely used, I've come to the following conclusions. First, it solves a common problem... Second, the method was spelled out in detail... including... a sample computer subroutine.*

Abraham Savitzky, commentary on journal's 5th most cited paper 1945-1999:  
[Analytical Chemistry, 1989, 61 \(15\), pp 921A-923A](#)



# Thanks!









