Data and Doughnuts

March, 14th 2025

Agenda - morning 09:00 a.m. - 12:00 a.m.

Scientific Introduction (Harrison)

Data handling and publishing

- Data Handling (Johanna)
- Nice examples from Justin and Jarod
- FAIR data and data publishing (Harrison)
- Dataverse (Johanna)
- Nice example from Jahred

Study design and statistical analysis

Data analysis

- How to work with spreadsheets (Harrison)
- What are jupyter notebooks and hands-on exercises (Johanna)

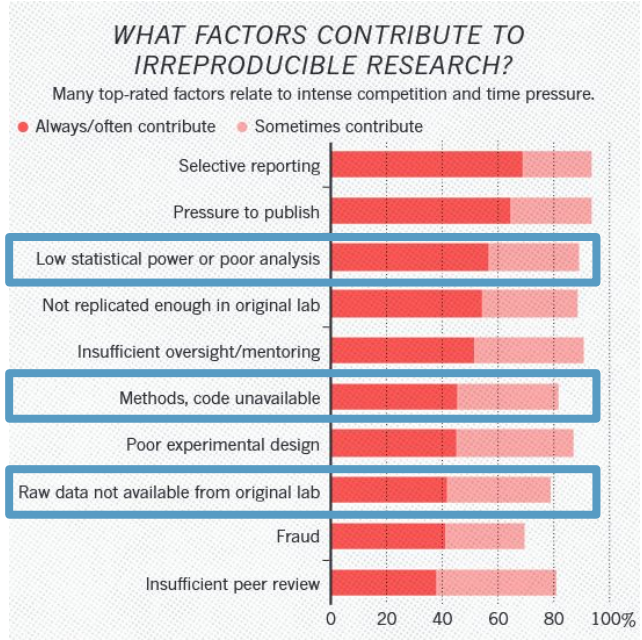
Agenda - afternoon 01:00p.m.-02:30p.m.

Lunch (12:00-01:00 p.m.)

Open session (01:00 p.m. - 02:30 p.m.)

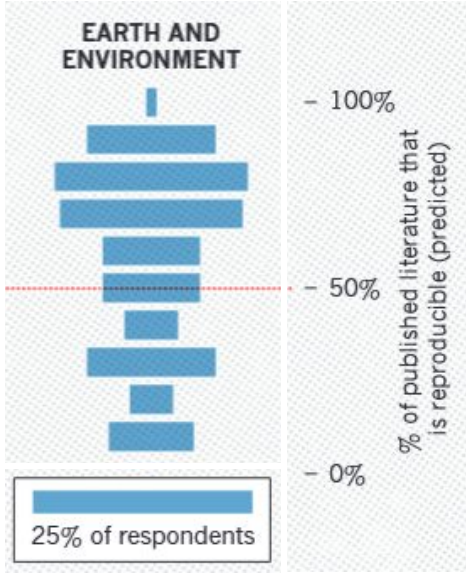
- Open questions
- Hands on exercises

THE UNDERLYING PROBLEM



More than 25 % of 1576 researchers asked in 2016 thought that more than 50% of published science in environmental research was not reproducible.

Baker, M. (2016). 1,500 scientists lift the lid on reproducibility.



BEYOND REPRODUCIBILITY: PROMOTING REUSE

In 2016, the FAIR Guiding Principles for scientific data management and stewardship (Wilkinson et al) were published in *Scientific Data*. The authors intended to provide guidelines to improve the Findability, Accessibility, Interoperability, and Reuse of digital assets. The principles emphasise machine-actionability (i.e., the capacity of computational systems to find, access, interoperate, and reuse data with none or minimal human intervention) because humans increasingly rely on computational support to deal with data as a result of the increase in volume, complexity, and creation speed of data.

Source: https://www.go-fair.org/fair-principles/

Data Handling

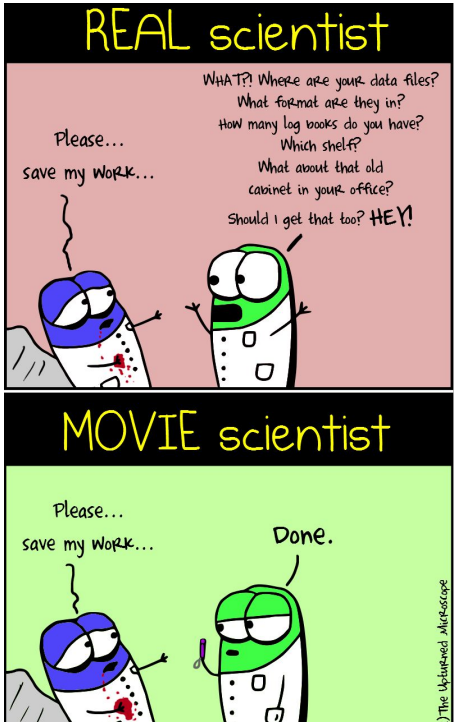
Johanna

Goal: have all necessary data available when writing up your PhD thesis

And how?

- **Delete** ‘useless files’, **archive** relevant data.
- Use meaningful **folder names and structures**
- Use **filenames** that help you navigate your data.
- **Document** your work and data.

“Reproducibility is like brushing your teeth. It is good for you, but it takes time and effort. Once you learn it, it becomes a habit.” - Irakli Loladze, mathematical biologist



https://theupturnedmicroscope.com/comic/real-vs-movie-scientist-2/

Archive relevant data

- Get rid of data and files, not everything is important.
- Archive your important data.
- **Raw experimental data** / simulation inputs are important data!
- Keep track, take notes, and document.
  - **Digitize** and keep your **lab notes**.
- **Backup** your data.

https://www.1800gotjunk.com/us_en/blog/decluttering/organize-your-attic https://www.apge.com/blog/attic-makeover-the-power-of-organized-storage https://chrislovesjulia.com/attic-organization/

Folder names and structures

- What important contextual information can you use to sort data files?:
  - separate data by academic semester?
  - separate data by projects?
  - separate data by measurement or instrument type?
  - ….
- Make a system. Follow the system. Be consistent.
  - **dedicated places for raw data and lab notes**
  - **dedicated places for data analysis/code**
  - …

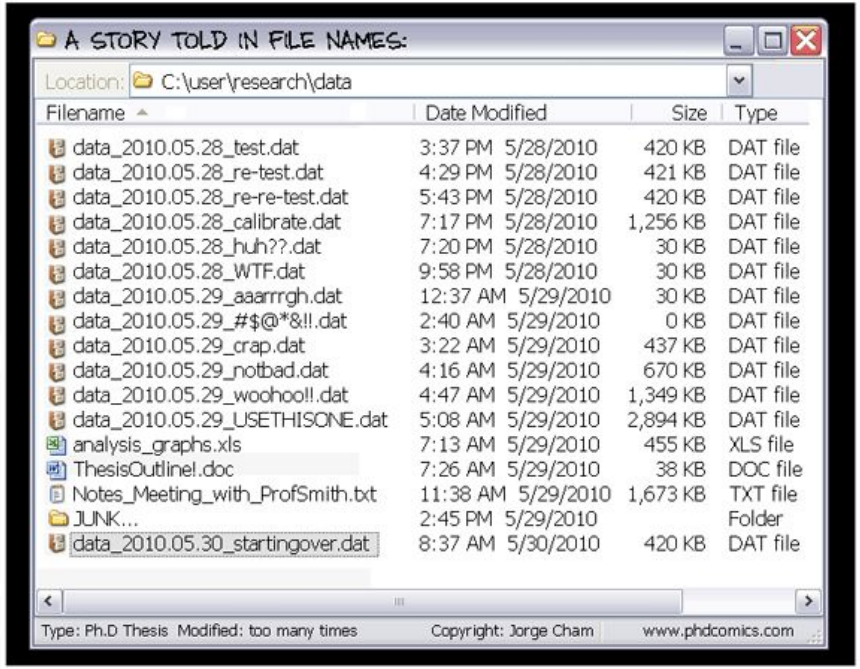
- Where is your data saved? (special care with myDrive and OneDrive)

Filenames

- Avoid white spaces.
- Exclude special characters:

  & ,* % # ;*)(!@$^~' { [?<-.

- Period only before file extension.
- 32 characters or less.
- numeric versioning: _v001, _v002
- ISO 8601 format for dates: 20240101, 2024_01_01



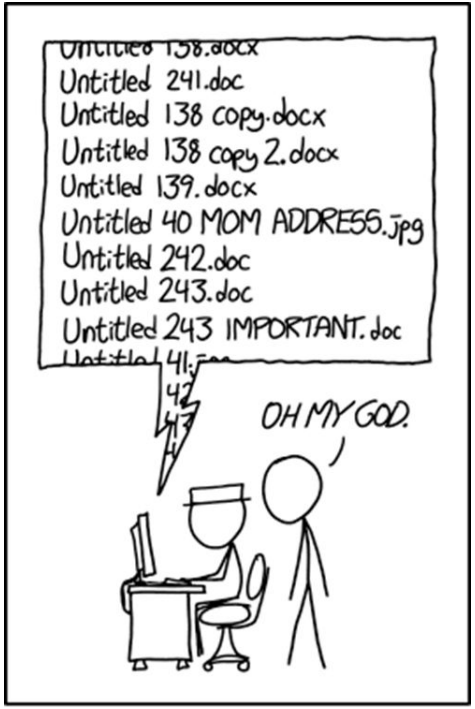
https://phdcomics.com/comics/archive.php?comicid=1323

File naming conventions

- What **information is important** about your files and **makes each file distinct**?
- Choose common naming convention and **stick to it**!

Nice Example			
DOC_WAX_01	SeaW_WAX_01	pH4_WAX_01	pH8_WAX_01_S
DOC_WAX_02	SeaW_WAX_02	pH4_WAX_02	pH8_WAX_02_S
DOC_DEX_01	SeaW_DEX_01	pH4_DEX_01	pH8_DEX_01_S
DOC_DEX_02	SeaW_DEX_02	pH4_DEX_02	pH8_DEX_02_S
DOC_COL_01	SeaW_COL_01	pH4_COL_01	pH8_COL_01_S
DOC_COL_02	SeaW_COL_02	pH4_COL_02	pH8_COL_02_S

Sample Sorbent Number



http://imgs.xkcd.com/comics/documents.png

KEEP YOUR DATA, AND KEEP IT CLEAN!

- **Delete** ‘useless files’, **archive** relevant data.
- Use meaningful **folder names and structures**
- Use meaningful **file names.**
- **Document** your work and data.

https://pub-e93d5c9fdf134c89830082377f6df465.r2.dev/2024/06/Messy-Chaotic-Data.webp

RESSOURCES

- Worksheet: Naming and organizing your files and folders (MIT libraries):
  https://www.dropbox.com/scl/fi/1zd63iszw33rh4hjcu1dl/Worksheet_fileOrg.docx?rlkey=q0t25t1wttp4qx2p1ne39qfhd&dl=0

- File naming conventions worksheet (Caltech Libraries):
  https://authors.library.caltech.edu/records/mmnpf-cez11

- Google Drive for Desktop
  Google Drive for Desktop

- One Drive
  OneDrive

https://pub-e93d5c9fdf134c89830082377f6df465.r2.dev/2024/06/Messy-Chaotic-Data.webp

Data Handling

Justin, Jarod

Data Publishing

Harrison

Five Key Aspects of Data Publishing to Keep in Mind

1. Data Management and Documentation
2. Choosing the Right Repository
3. Licensing and Access Control
4. Citations and Persistent Identifiers
5. Compliance and Ethical Considerations

Understanding these aspects ensures that data publishing adds value to the academic community, boosts research impact, and upholds ethical standards. Let’s explore them a little further.

Data Management and Documentation

Proper data organization, metadata creation, and clear documentation (e.g., methods, formats, and variables) are essential to ensure that others can understand and reuse the dataset. Following standards like the FAIR principles enhances data clarity and usability.

Choosing the Right Repository

Selecting an appropriate repository — whether general-purpose (e.g., Dataverse, Zenodo, Figshare) or discipline-specific (e.g., GenBank for genetic data) — ensures long-term preservation, proper indexing, and greater visibility for the dataset.

Licensing and Access Control

Applying the right license (e.g., Creative Commons) clarifies terms of use and reuse. Researchers should also determine access levels, balancing openness with ethical or legal obligations related to sensitive data.

Citations and Persistent Identifiers

Assigning persistent identifiers like DOIs (Digital Object Identifiers) makes the dataset citable, ensuring proper attribution and enabling other researchers to reference the data in future work.

Compliance and Ethical Considerations

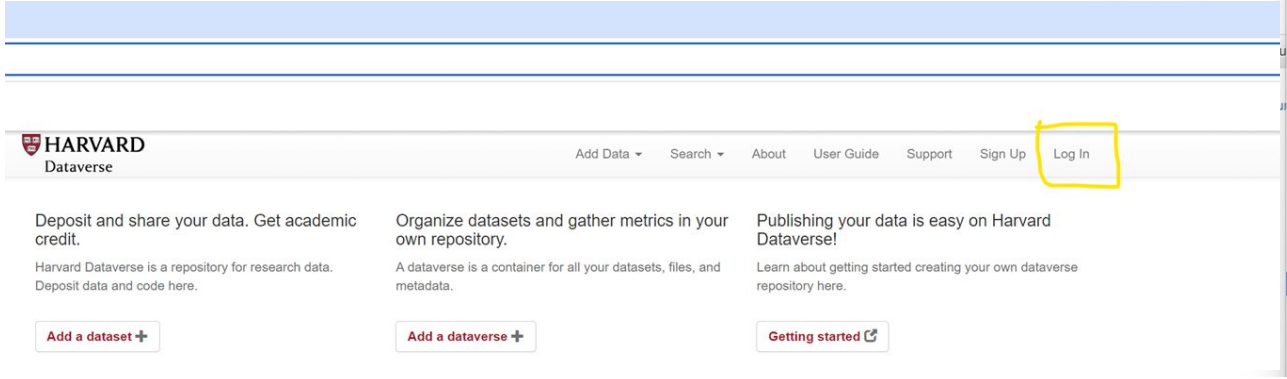
Researchers must comply with institutional, funder, and journal data-sharing policies while addressing ethical concerns, such as obtaining consent for data sharing and protecting sensitive or personal information.

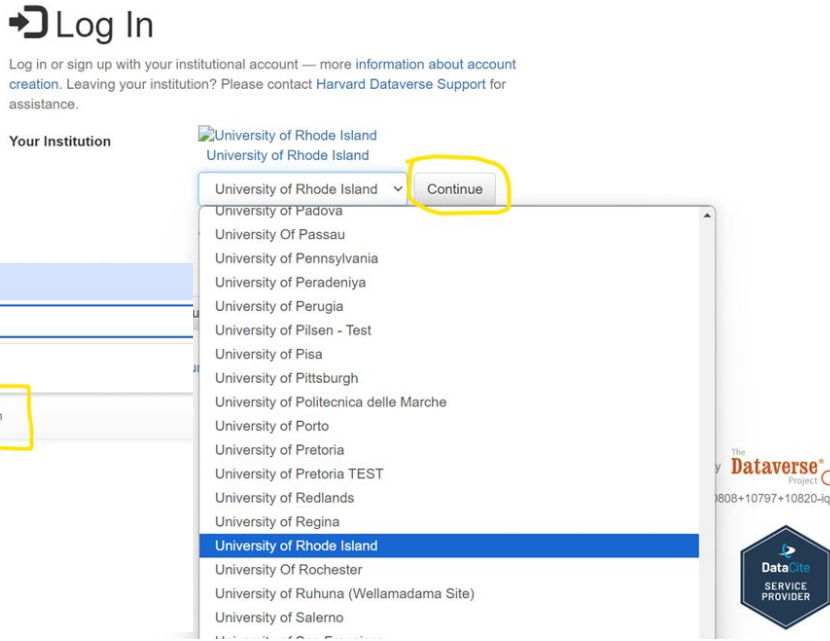
Harvard Dataverse

Johanna

Harvard Dataverse Login

- Go to: https://dataverse.harvard.edu
- Login with your SSO





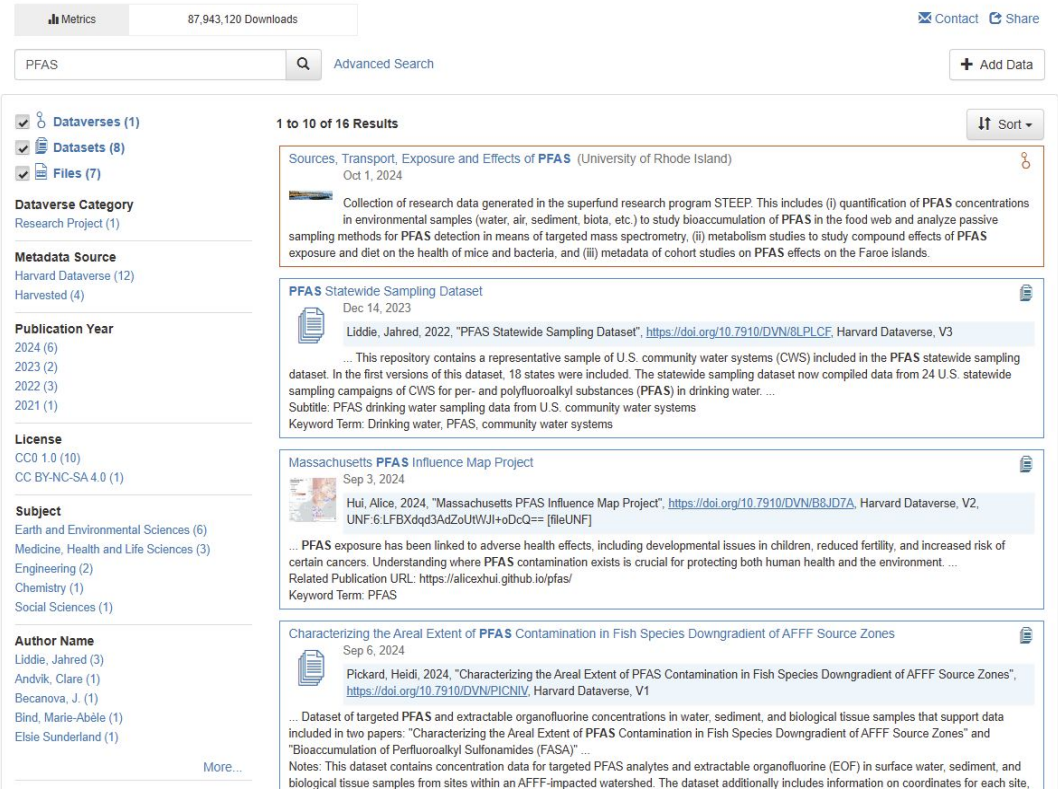
Harvard Dataverse

… is a free repository for research data (and code)

…is commonly used in research (> 75k datasets published)

…'**general repository**' - might not be the best choice for specific data sets (e.g. raw .mzML)

… assigns a DOI to each published data set



Data Publishing in Harvard Dataverse

Jahred Liddie

Best practices with spreadsheets

Harrison

Keeping track of your analyses

When you're working with spreadsheets, during data clean up or analyses, it's very easy to end up with a spreadsheet that looks very different from the one you started with. In order to be able to reproduce your analyses or figure out what you did when Reviewer #3 asks for a different analysis, you should:

- create a new file with your cleaned or analyzed data. Don't modify the original dataset, or you will never know where you started!
- keep track of the steps you took in your clean up or analysis. You should track these steps as you would any step in an experiment. We recommend that you do this in a plain text file stored in the same folder as the data file.

Spreadsheet setup example

survey_data.xlsx

	A	B	C	D	E	F	G	H	I
1	DateCollected	Year	Month	Day	Plot	Species	Sex	Weight	
2	7/16/13	2013	7	16	2	DM	F		
3	7/16/13	2013	7	16	7	DM	M	33g	
4	7/16/13	2013	7	16	3	DM	M		
5	7/16/13	2013	7	16	1	DM	M		
6	7/18/13	2013	7	18	3	DM	M	40g	
7	7/18/13	2013	7	18	7	DM	M	48g	
8	7/18/13	2013	7	18	4	DM	F	29g	
9	7/18/13	2013	7	18	4	DM	F	46g	
10	7/18/13	2013	7	18	7	DM	M	36g	
11	7/18/13	2013	7	18	7	DM	F	35g	

README_surveyData.txt — Carpe...

```
Processing notes on survey_data.xlsx

2014-08-19 work done -------

1. Transferred 2013-raw to 2013-clean,
and 2014-raw to 2014-clean

2. In 2013-clean: created a 'Species'
column and moved information from header
to that column

3. In 2013-clean, put all the different
tables together into one table with
columns: date collected, plot, species,
sex, weight

4. In 2013-clean, separated
month/day/year column into three columns
```

Structuring data in spreadsheets

The cardinal rule of using spreadsheet programs for data is to keep it “tidy”:

1. Put all your variables in columns - the thing you’re measuring, like ‘weight’ or ‘temperature’.
2. Put each observation in its own row.
3. Don’t combine multiple pieces of information in one cell. Sometimes it just seems like one thing, but think if that’s the only way you’ll want to be able to use or sort that data.
4. Leave the raw data raw - don’t change it!
5. Export the cleaned data to a text-based format like CSV (comma-separated values) format. This ensures that anyone can use the data, and is required by most data repositories.

Exercise - Data Cleaning

1. Download the data by clicking here to get it from FigShare.
2. Open up the data in a spreadsheet program (e.g. Excel or Google Sheets).
3. You can see that there are two tabs. Two field assistants conducted the surveys, one in 2013 and one in 2014, and they both kept track of the data in their own way in tabs `2013` and `2014` of the dataset, respectively. Now you're the person in charge of this project and you want to be able to start analyzing the data.
4. With the person next to you, identify what is wrong with this spreadsheet. Also discuss the steps you would need to take to clean up the `2013` and `2014` tabs, and to put them all together in one spreadsheet.

Important: Do not forget our first piece of advice: to create a new file (or tab) for the cleaned data, never modify your original (raw) data.

Introduction to jupyter notebooks

Johanna

Introduction to jupyter notebooks

- **interactive computing environment:**
  - Load and cleanup data
  - Execute data analysis
  - Visualize data
  - **Document all steps**

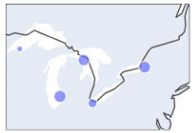
- **Why jupyter notebook?**
  - reproducible
  - automated workflow
  - helpful packages and features

Show off example

Mapping in jupyter notebook is easy. In the code block below you find three code lines used to show PFAS interactive map. You might have to zoom in.

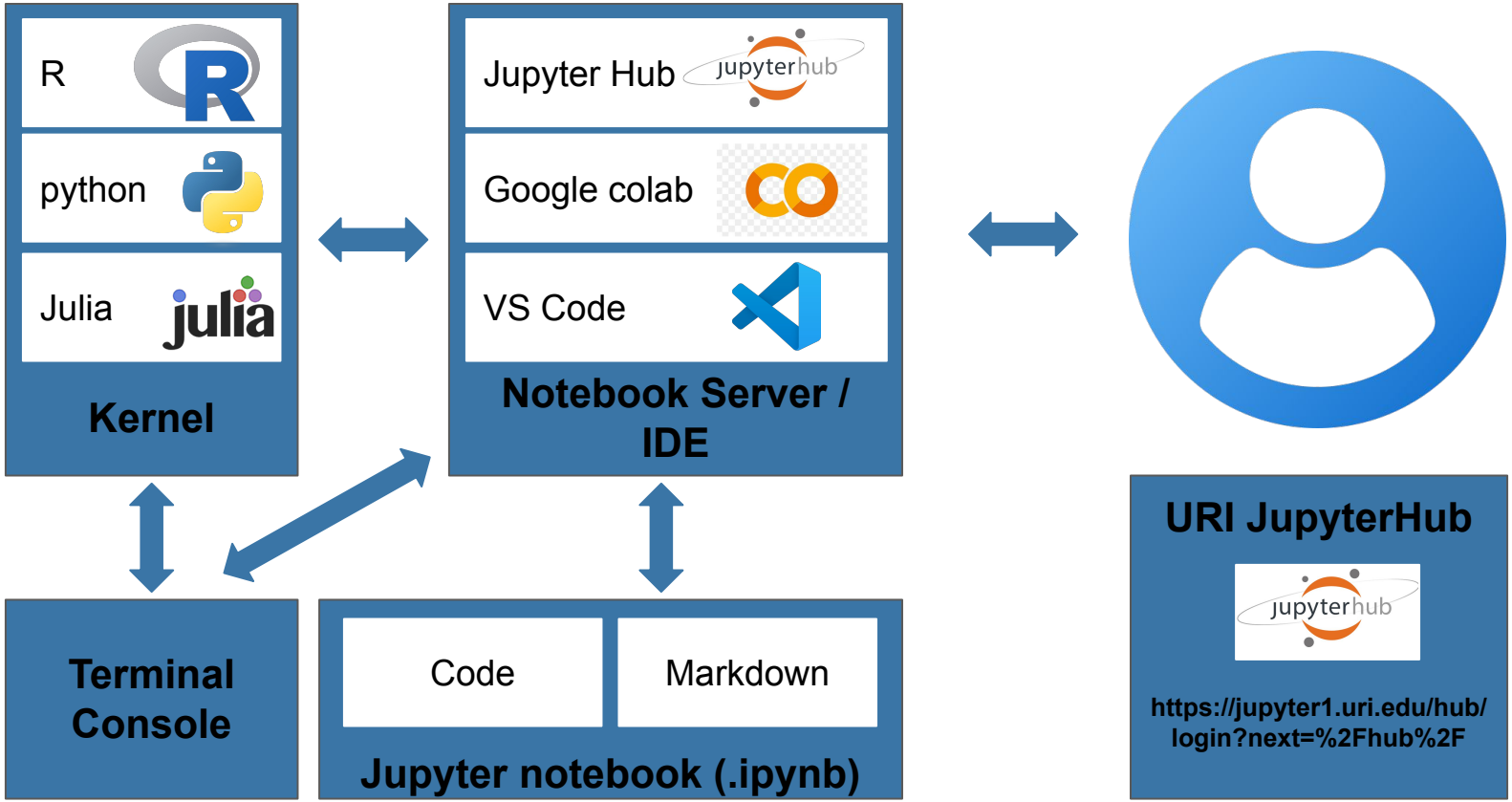
[70]:
```
import plotly.express as px

fig = px.scatter_geo(fish_data_pfos_mean, lat='Latitude', lon='Longitude',
                     hover_name="Lake", size=selected_compound,
                     animation_frame="Year",
                     scope='north america',
                     title="Great Lakes")
fig.show()
```

Great Lakes



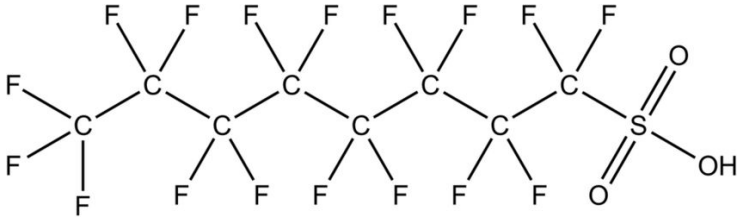
Year=2022

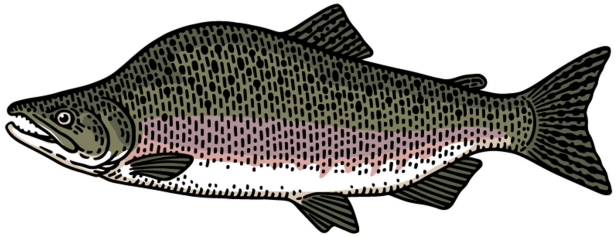
Jupyterhub - relevant terms



Example of today

- Great Lakes Environmental Database
- PFAS concentrations of fish caught at 10 stations at the great lakes from 2011 - 2022.
- Goal: Read in data, filter data, average data, plot data,...
- **Notebook and example data provided in your jupyterhub account**





Further ressources

(1) basic introduction: https://www.dataquest.io/blog/jupyter-notebook-tutorial/
(2) pandas: https://pandas.pydata.org/docs/getting_started/intro_tutorials/index.html
(3) matplotlib: https://www.w3schools.com/python/matplotlib_plotting.asp
(4) General data science: https://github.com/engineersCode/EngComp1_offtheground

and many more...

Your account for URI's jupyter lab will be open **until the end of summer semester**. Download all relevant work beforehand and contact johanna.ganglbauer@uri.edu, if you want to use it in the long term.