Reproducible Science

August 30, 2019

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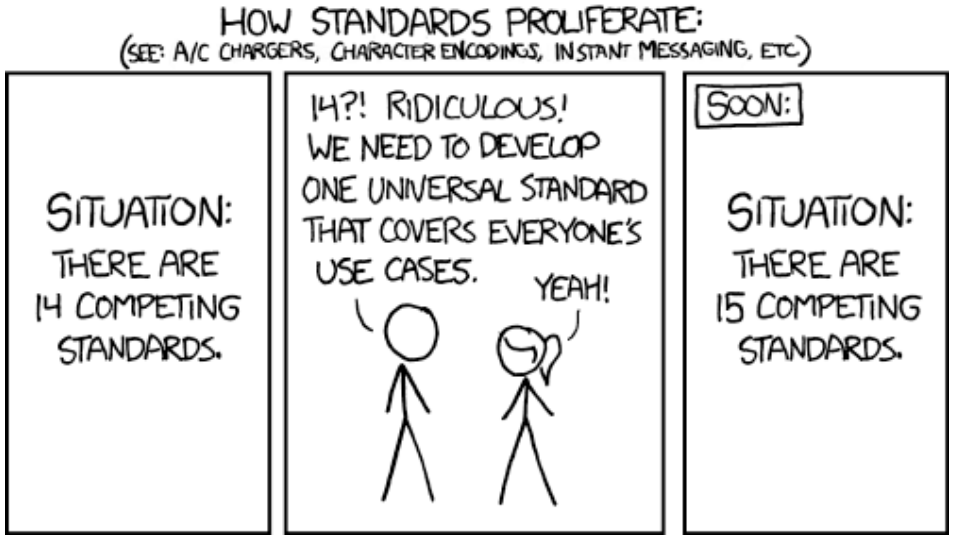
Quiz time!

- What is a repository?
  - Differences between code and data repositories?
- Who do you turn in your data/results to?
- Name a version control software (VCS)
- What is a branch in git?
- What is a package in Python?



- Have you had trouble running code from others, or sharing your code?
- Is interoperability important to you?
  - Do you feel there are too many standards to understand?

(Oceanography) Data Stewards Salad

- ESIP
- RDA
- EarthCube
- FAIR
- Ocean Best Practices
- DataONE
- IEDA
- Force11
- And so on…

An Opinion of Two Cities: Science and Software

- Science focused:
  - Repeatability, Replicability, Reproducibility
  - FAIR principles
  - Data centers/repositories
  - Methods repository - Ocean Best Practices
- Software focused:
  - Community decisions in oceanography
  - Working environment: package managers, virtualization
  - Online interactive notebooks: Binder
  - Version control: git, Github
  - Code readability: formatters
  - Code readability part 2: docstrings/comments, autodocs
  - Variable names and standard vocabularies
  - Advanced software engineering
  - Licensing code and data
  - DOIs for code and data

Repeatability, Replicability, Reproducibility

- **Repeatability**: Same team, same experimental setup
- **Replicability:** Different team, same experimental setup
- **Reproducibility:** Different team, different experimental setup

- **Methods reproducibility**: provide sufficient detail about procedures and data so that the same procedures could be exactly repeated.
- **Results reproducibility**: obtain the same results from an independent study with procedures as closely matched to the original study as possible.
- **Inferential reproducibility**: draw the same conclusions from either an independent replication of a study or a reanalysis of the original study.

Plesser HE (2018) Reproducibility vs. Replicability: A Brief History of a Confused Terminology. *Front. Neuroinform*. 11:76. doi: 10.3389/fninf.2017.00076

FAIR Principles

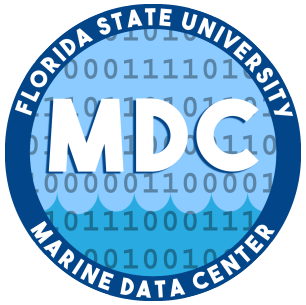
- Make data easier to use: “guidelines to improve the findability, accessibility, interoperability, and reuse of digital assets”
- **What does FAIR mean?**
  - **Findable**
  - **Accessible**
  - **Interoperable**
  - **Reusable**

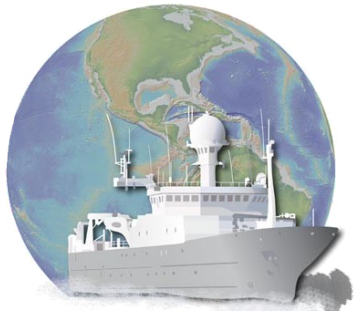
- “Is your data FAIR?” vs “Does your data follow FAIR virtues?”
  - Absolutes versus relatives – start with the relatives

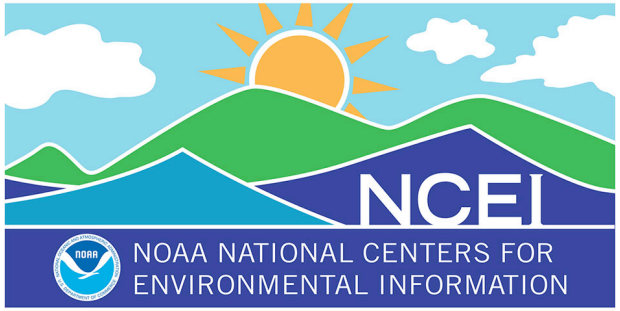
https://www.go-fair.org/fair-principles/

Data Centers/Repositories

- Data centers are paid to make your data available – talk to us!
  - (It's also a requirement of your grant to submit your data)
- Use our libraries to read our data holdings, or ask us to make them
  - Feel free to contribute too!







Repository of Methods – Ocean Best Practices

- DOIs for manuals and handbooks
  - How to do fieldwork, make models, etc.
- UNESCO/IOC project
- Internationally agreed upon methods…
  - …and publically submitted methods

United Nations Educational, Scientific and Cultural Organization
Intergovernmental Oceanographic Commission
Ocean best practices

https://www.oceanbestpractices.org/

Reproducible Software: Opinionated Practices

Why spend effort for reproducibility?

- Faster deployment of code
- Faster understanding of code
- Easier extension of code
- It’s good for you and the community!

What is reproducibility?

- Read more than write – can you read it one month, year from now?
- New installs over current- can you install it one month, year from now?
- Code brittleness – can you extend it one month, year from now?

Lets see what some people have said about software, data before:

The ~dangers~ of big data

- Data may be hosted in several different places, which is a waste of resources
- Reproducibility of published analyses:
  - If code isn't readable it is difficult to check
  - Code is often written in proprietary languages
- Data may be used without understanding it or updating it (QC status)
- Where should this data be hosted? Who should maintain it?

PODS-DISCO 2018, Hawaii

How should we organize and share our datasets?

Access and reproducibility are key!
Projects like BCO-DMO and Earthcube are creating standards and improving access

Coding standards are important for sharing and reproducibility (IPython/Jupyter notebook/Github)

How can we discover the relationships in large multi-instrument data streams? How can we relate data collected from new technology to old data?

How to encourage scientists to participate?
Requirements by journals and funding bodies
Building community and tools to keep data sustainable
Are there non-science funding resources to facilitate this? Creating positions such as "Information Officer"

PODS-DISCO 2018, Hawaii

How do we standardize our coding practices?

- “Opinionated” guidelines – PEP-20, ”This is the way we are doing things”
- More people following the same opinionated practices – easier to share code!
- Software tools to help write opinionated Python
  - Conda/Conda-forge
  - Black
  - isort (non-notebooks, production code)
- Software tools to help facilitate opinionated Python
  - Git/Github
  - Binder
  - Sphinx (numpy docstrings)
- Science decisions made by communities
  - netCDF-CF
  - Pangeo

Community Decisions - Oceanography

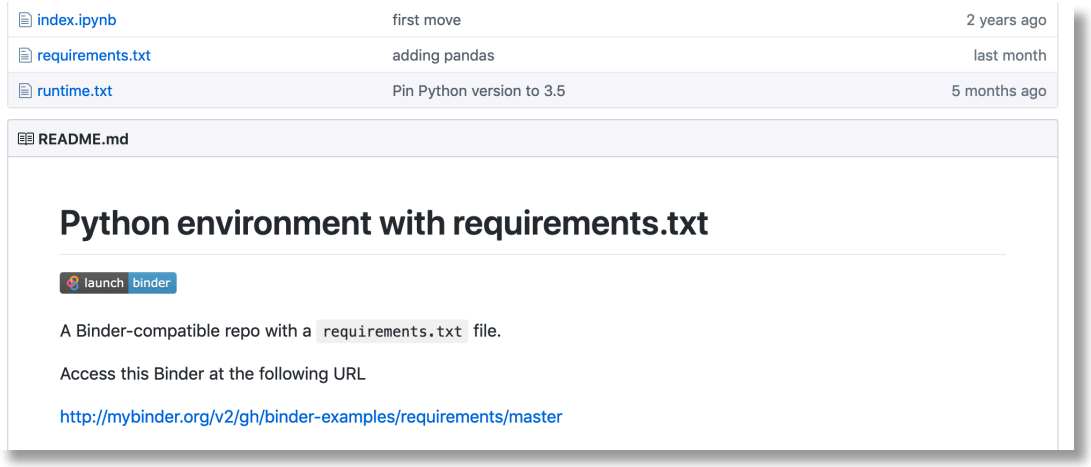
- Formats: NetCDF (as opposed to CDF)
  - Backends: HDF5, NetCDF3, zarr (cloud native, coming soon™!)
- Formats: ASCII/CSV (old)
  - Easier for initial view, quickly lacking flexibility and metadata
- Standard Vocabularies
  - Regulated vocabularies with strict definitions
  - Propose new names, pass committee approval
  - CF – Physical parameters
  - BODC lists – Biogeochemical parameters
- Cloud: Pangeo
  - Standardizing environments to make it easier to run code

Working environments

- Simplify installing and setting up an environment to run code
- Compartmentalization makes it easier to prevent unforseen mixing that leads to problems
- Package manager:
  - Conda + conda-forge: easier installation of dependencies, environments
  - Pip: standard Python tool; if all of your packages are in there, fine! (probably not)
- Virtualization:
  - Conda provides virtual environments like virtualenv
  - Docker, other tools are good for deployment

Binder

- A platform for making notebooks runnable online
  - Plug-in to Github
  - Google has a similar platform called Colab
- Allow others to experiment with your code before downloading
- Make DOI notebooks runnable

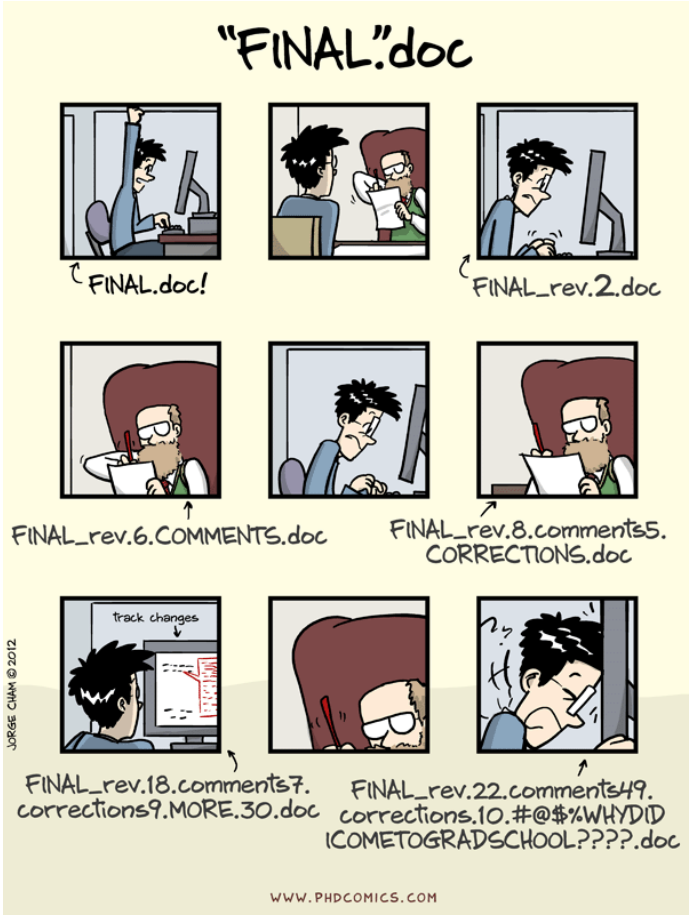


Version Control: git, Github

- Easier to keep track of yours/others changes
- Remote copies as failsafes in case of computer failure – but not a replacement for backups

- Commits should be “atomic”
  - Commits are fully formed, not half-done
  - Related edits are grouped into a single commit
  - Commits are small (one change) and often
- Use branches to try new ideas without polluting the master
- Want more git tutorials?

- Github – one of many places hosting code repos



Code Formatting

- Black: “The Uncompromising Code Formatter”
- isort: Sort and trim imports; for production code, not notebooks

```
# in:

def very_important_function(template: str, *variables, file: os.PathLike, engine: str, header: bool = True
    """Applies `variables` to the `template` and writes to `file`."""
    with open(file, 'w') as f:
        ...

# out:

def very_important_function(
    template: str,
    *variables,
    file: os.PathLike,
    engine: str,
    header: bool = True,
    debug: bool = False,
):
    """Applies `variables` to the `template` and writes to `file`."""
    with open(file, "w") as f:
        ...
```

Code Readability part 2: comments and autodocs

- Docstrings: format for writing documentation in Python
- Flavors: Numpy, Google
  - Use **numpy** for your projects!
- Document/Autodocs: Sphinx
  - Automatically generate code documentation
  - Make html, latex, pdf, plain text, etc.
  - Use with Read the Docs for free hosting

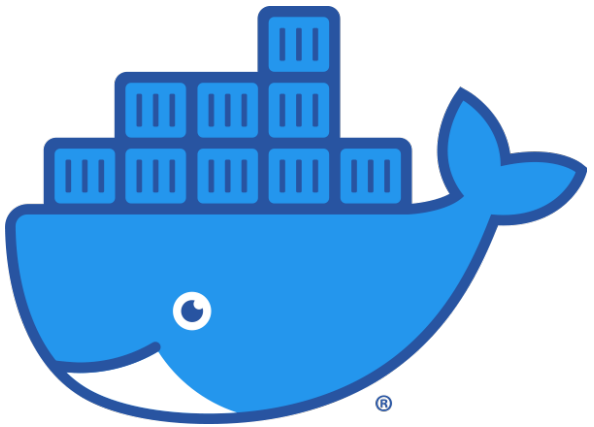

```
class Photo(ndarray):
    """
    Array with associated photographic information.

    ...

    Attributes
    ----------
    exposure : float
        Exposure in seconds.

    Methods
    -------
    colorspace(c='rgb')
        Represent the photo in the given colorspace.
    gamma(n=1.0)
        Change the photo's gamma exposure.

    """
```

Code readability – variable names

- Context is important
  - Internal functions vs public API vs data products?
  - Equations implemented in code can make sense to use shorter names
- Variable names
  - Temperature: temperature, temp, tmp, T, sea_water_temperature, sea_surface_skin_temperature, TEMPP681, TMESOT01
- Those names in blue are from standard vocabularies
  - Controlled, publically available, names added after proposal process
  - Group Examples: CF, SeaVox, BODC
- Someone should write a tool that checks files and converts to standard vocabulary names?

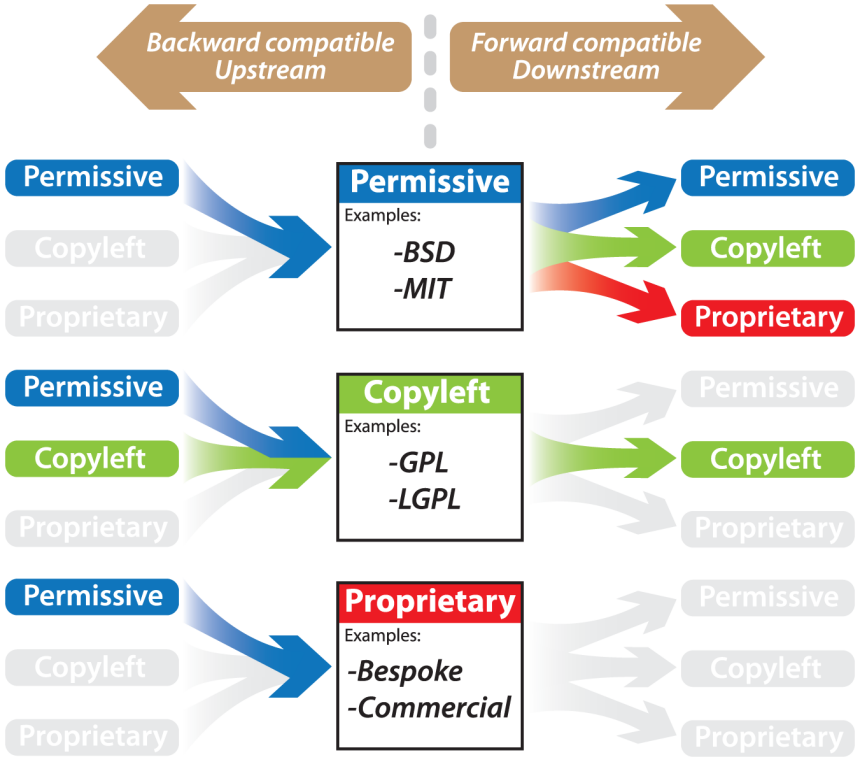
Advanced Software Engineering

- Python language power features:
  - Factories, list comprehensions, etc.
- APIs
  - Data: JSON, YAML, XML, REST, SOAP, etc.
- Packaging
  - Version schemes
- Continuous Integration (CI)
  - Special mention: Pre-commit
- Tests
  - Unit, system/holistic
- Images/Containers
- “Better is the enemy of good”



Licensing Code and Datasets

- Tool to help you choose: https://choosealicense.com/
  - Software: MIT, BSD
  - Data: CC
- USA government data licenses: ODC, CC, GNU
- Publically funded data must be open access, and will be assumed to be open access if none is stated (to date?)



doi: https://doi.org/10.1371/journal.pcbi.1002598.g002

DOIs for Fun and Profit: Pt. 1

- DOI – Digital Object Identifier, can be made by many organizations
  - Your institution may do so, but you don't need to use them
  - We'll work with Zenodo, an EU group
- Making DOIs for code
  - https://guides.github.com/activities/citable-code/
- Making DOIs for data
  - https://www.zenodo.org/
  - Your institution may be able to make DOIs

DataCite
FIND, ACCESS, AND REUSE DATA

DOIs for Fun and Profit: Pt. 2

- Citing DOIs:
  - Zenodo: lets look at **10.5281/zenodo.1256998**
    - Choose citation style
  - Online tool: https://citation.crosscite.org/
    - 10.7942/C2008W, “american-geophysical-union”, “en-US”
- These tools depend on the DOI fields being filled out properly, so you don’t have to manually form them
  - Otherwise, follow recommended style

Thank you for attending OceanHackWeek 2019!