

A PhD in oceanography and open source software

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Atmospheric Sciences







Before open source

After open source

Contents

- Example of poor data/code sharing (content warning: excel)
- An attempt at doing better
- Why you should care & what you can do

My first data set

- 1000s of files scattered across directories
- No canonical version of processed files
- Processing in excel spreadsheets

•	No	READM	
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This is not a database

	Α	В	C	D	E	F	G	H	L	J	K	L
1	0 1								1.00158934			
2									-3.01383708			
2	*				.mrk file		02	Winkler	residual			CTD 9.11
4		Niskin	Botella	Presion	Temperatura	Salinidad	21/09 A	O2 µmol/Kg	(-1111)			Tmp CTD
5	21/09/2010	11	6A	5	16.88	35.63	254.9	252.64	4.86			16.8878
6	1	8	5A	12.5	16.05	35.67	238.3			234.80	6.19	16.2192
7		7	4A	20	14.3	35.84	205.7	208.79	-0.42			14.2785
8		5	ЗА	50	13.33	35.85	197.8	200.94	-0.40			13.3336
8		3	2A	80	13.08	35.83	188.2	194.21	-3.35			13.0304
10	8	1	1A	127	12.98	35.82	170.5	174.11	-0.92			12.9874
11							21/09 B					
12	21/09/2010	11	6B	5	16.9	35.62	254.7	257.37	-0.02			16.9368
13	1	9	5B	12.5	16.45	35.64	249.5					16.0897
14		7	4B	20	14.68	35.82	212.6	212.01	3.24			14.5952
15		5	3B	50	13.31	35.84	199.3	202.00	-0.01			13.2942
16	9	4	2B	80	13.06	35.83	188.7	190.09	1.35			13.0512
17		1	1B	124	13.03	35.83	178.2	183.01	-2.13			13.0263
18												
19	8			estadillo								
19		Latitu	Longitu	Z (real)	Temperatura	Salinidad	15/09 loo	O2 µmol/Kg				Tmp CTD
21	15/09/2010	42.23	-8.788	5	17.0025	35.5145	253.0474	200		243.55	12.12	
22	9			10	15.6445	35.6085	190.5372			176.40	16.87	15.5691

My first data set

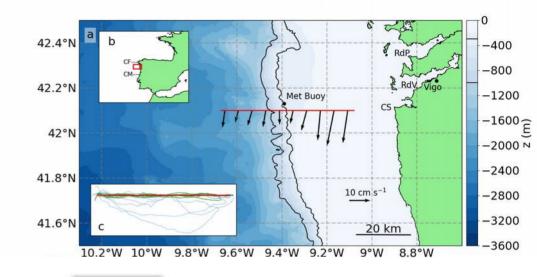
End result >> Reprocess from scratch

This took two years

Substantial duplication of effort

My first data set

A happy ending at least



JGR Oceans

Research Article 👶 Open Access 📵 🕦

Glider Observations of the Northwestern Iberian Margin During an Exceptional Summer Upwelling Season

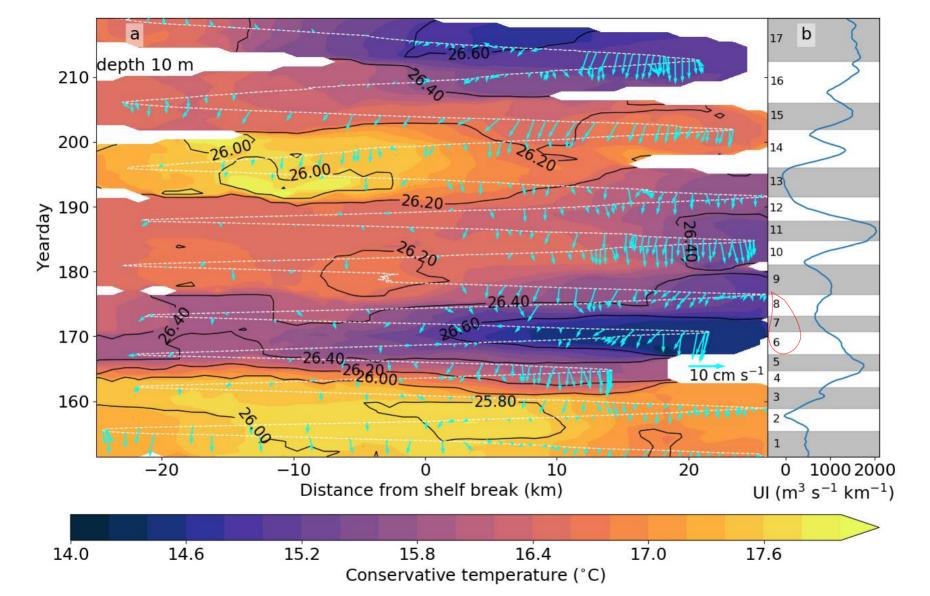
Callum Rollo M, Karen J. Heywood, Rob A. Hall, Eric Desmond Barton, Jan Kaiser

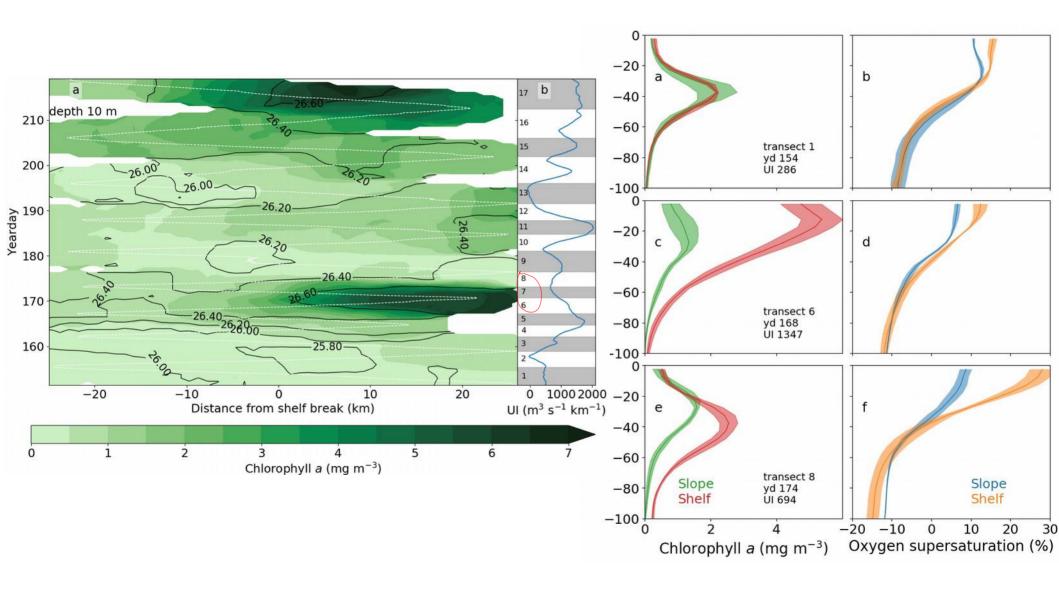
Figures References Related Information

Volume 125, Issue 8

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Oceans





Why is this an problem?

- Effort to collect data >> effort to preserve/share data
- Undocumented datasets easily lost
- Duplication of effort
- "Bus factor"
- Shared code often poorly documented/unusable
- The replication crisis
- When a global pandemic stops field/lab work, how much work can you do?

Principle Issues

Poor data organisation

Multiple conflicting data files

No data archival

No processing notes

Use of proprietary/closed formats

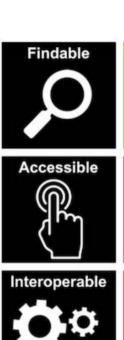
Combined storage and processing

No environment information

Principle Issues

Poor data organisation Multiple conflicting data files No data archival No processing notes Use of proprietary/closed formats Combined storage and processing No environment information

>> Data and scripts are not FAIR





















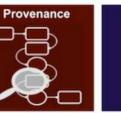














Principle Issues

Solutions I use

Poor data organisation

Multiple conflicting data files

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Combined storage and processing

No environment information

Add a README and structure data logically

One canonical dataset, no duplication

Archive at BODC or zenodo

Work in Jupyter Notebooks

Data in csv or NetCDF

Absolute border between data and scripts

Anaconda environment stored with scripts

A better way, "me and my glider"

SG637 *Omura* (rare species of fin whale)

- Custom sensor integration
- No documentation
- No development notes
- No processing code
- No tests

So, let's make them!



How is it organised?

- All tracked with git
- Includes READMEs
- Manual written in plain text
- Converted to pdf, html etc. automatically with makefile
- Hosted on Github, updates pushed live
- Code to generate plots included
- Timestamped copies archived on zenodo
- Open source FOSS license (GPL3)

What does it look like?

adcp-glider-manual

- manual
 - images
 - sensor-diagram.png
 - signal-test.png

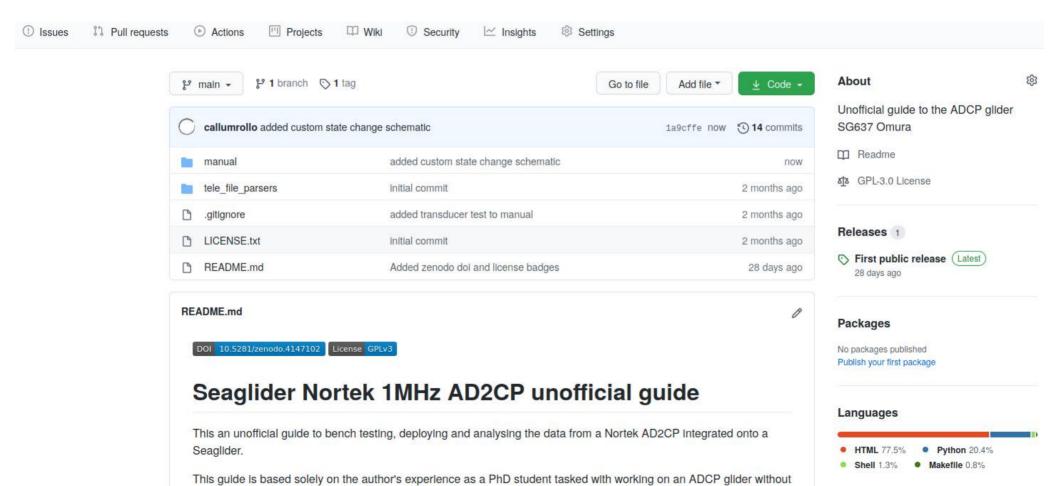
. . .

- adcp-manual.md
- adcp-manual.pdf
- adcp-manual.html
- Makefile

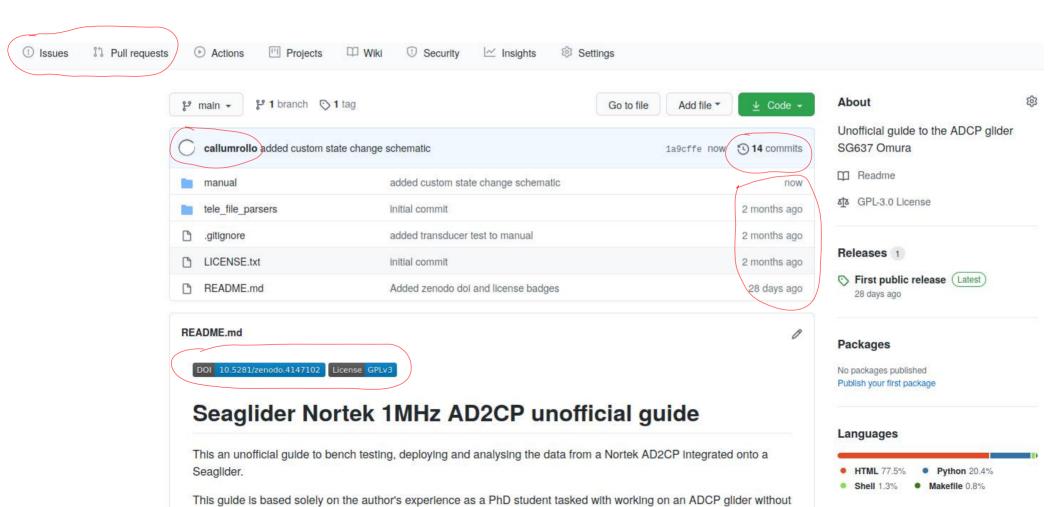
- scripts

- README.txt
- script.py
- helper-script.sh
- README.md
- LICENSE.txt
- .git

What does it look like?



What does it look like?

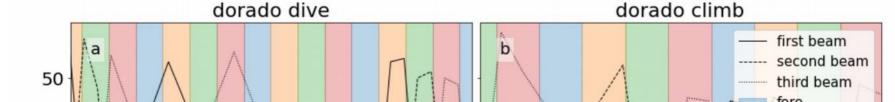


Beam bench test

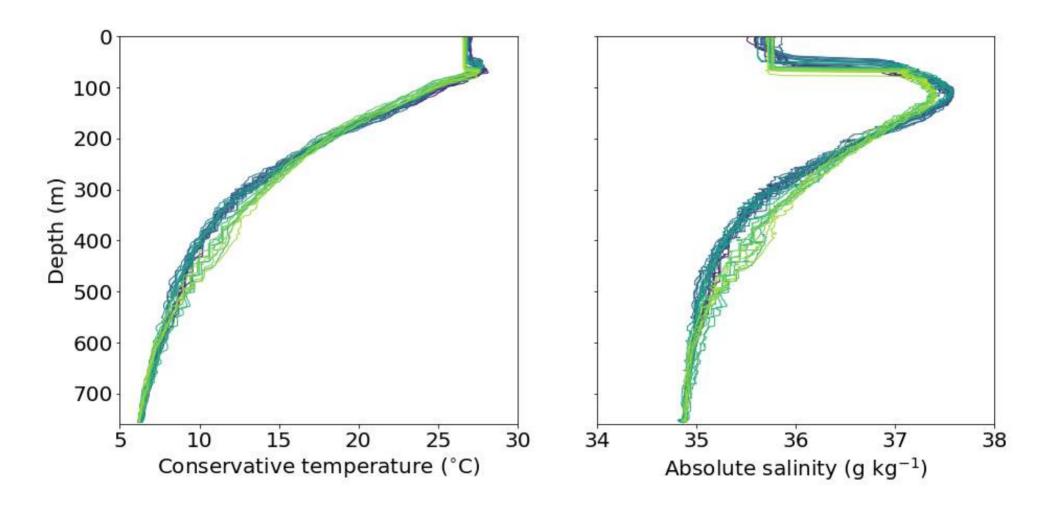
Following bench test instructions in the ADCP glider manual transducers can be tested for firing order.

The following plot shows the results when operating under the DORADO and EAGLERAY firmware versions

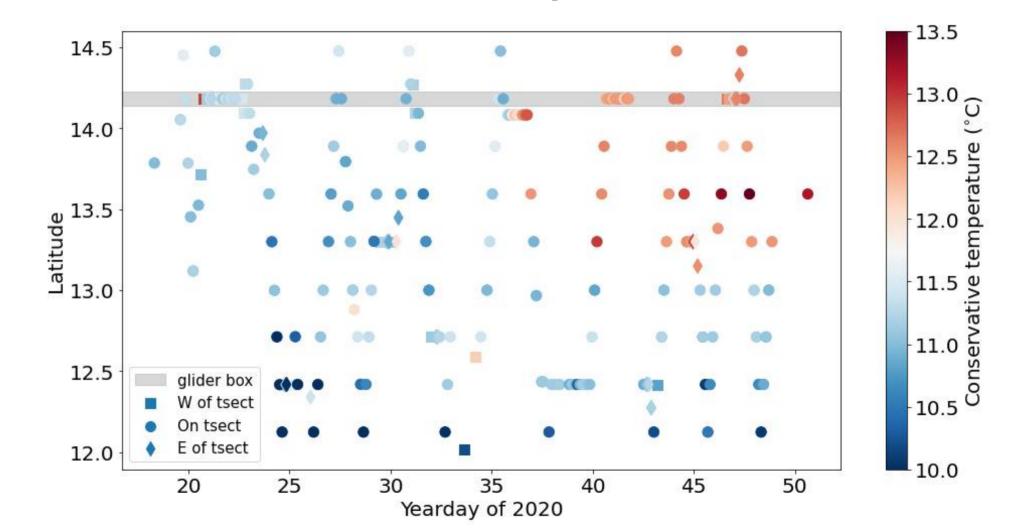
```
fig, ax = plt.subplots(2,2,figsize=(16,10), sharey='row', sharex=False)
fig.subplots adjust(hspace=0.1, wspace=0.02)
ax = ax.ravel()
datasets = [dorado dive, dorado climb, eagle dive, eagle climb]
ds names = ["dorado dive", "dorado climb", "eagle dive", "eagle climb"]
for ax no, dataset in enumerate(datasets):
    ax[ax no].plot(dataset.time, dataset.amp beam[:,1,0], color='k', linestyle='-', label="f
    ax[ax no].plot(dataset.time, dataset.amp beam[:,1,1], color='k', linestyle='--', label="
    ax[ax no].plot(dataset.time, dataset.amp beam[:,1,2], color='k', linestyle='dotted', labe
    ax[ax no].set(xlim=[dataset.time[0], dataset.time[15]], xticks=[],title=ds names[ax no])
    beam shade(ax[ax no])
    fig.autofmt xdate()
ax[2].set(xlabel='Time',ylabel='Return amp (dB)')
ax[1].legend(loc=1);
letterboxes(ax)
fig.savefig('../reports/bench test figures/transducer tests.png')
```



Awkward sidestep into science



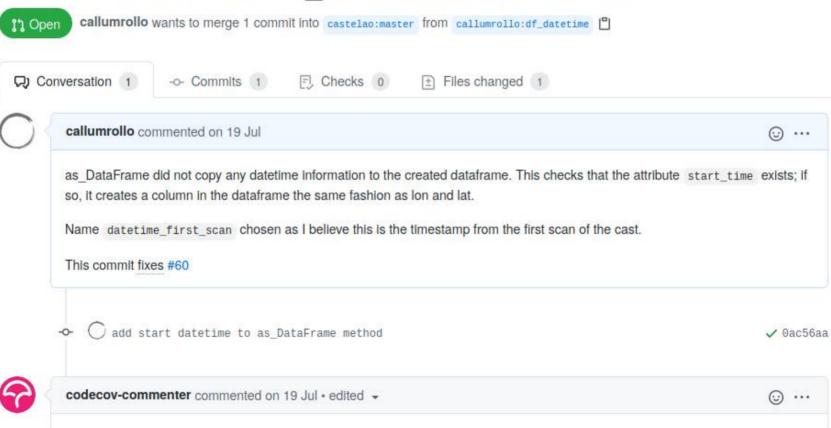
Awkward sidestep into science



What's this got to do with open source?

- Open source library to read CTD data
- Library lacked a feature I needed
- I implemented it
- Pushed to Github
- This would be impossible with proprietary software

add start datetime to as_DataFrame method #61



Open source is good (and fun). You should use it



It doesn't have to be perfect

- Every step is worthwhile. Start with a README
- Easy if you do it from the beginning of a project
- There are courses to help e.g. git, Python
- Start with a small/personal project
- This presentation has been shared, typos and all

It doesn't have to be perfect

We all write horrible messy code. It's ok

The CRAPL

"Academics rarely release code, but I hope a license can encourage them."

"An open source license for academics... should absolve authors of shame, embarrassment and ridicule for ugly code."

- Matt Might

Sounds like effort, why should I do this?

- Will remind you in 6 months what your code means
- Reduce duplication of effort
- Lead by example/golden rule
- Encourage collaboration
- Recognition outside of academia
- The wind blows toward open science
- Increasingly a requirement of publication/funding



OK I'm sold, what now?

An hour

- Comment your code and add a README
- Note the environment you ran it in
- Archive to zenodo

A day

- · Learn to use git
- Refactor code for readability
- Upload to github*

A new project

- Use open source languages and formats
- Structure your project e.g. cookiecutter
- Make your code into a reusable module and share it



Better coding == Better practices science

How did you get into this?

- Leading the UEA Python group
- Running a server
- Syncing data during glider deployments
- Automating boring stuff
- Shell scripting
- Making a personal website
- Breaking things and fixing them
- Attending Ocean Hack Week (blog post)
- Contributing to projects on GitHub
- Using Linux





Training you can take

- Jennifer Graham and Tiago Silva run an excellent introductory git training course for ENV and Cefas researchers https://github.com/CefasRepRes/Git_Training_2020/wiki
- Join the UEA Scientific Python group (contact Callum). We teach half day courses in Python and hold occasional seminars and drop in sessions
- Self teach from the 3 day intro to Python we run with Cefas
- Take a PPD course in R, particularly good for statistical analysis
- Attend Ocean Hack Week

Links and resources

- Good enough practices for scientific computing basically this talk but good
- Getting started with GitHub
- Top quality data science courses from software carpentries
- ANDS' FAIR data webinars
- JPO letter from editors on supporting FAIR principles November 2020
- Zenodo data archival policies (any project up to 50 GB, indefinite storage and free DOI)
- Pangeo project for open source atmospheric science and oceanography
- Software sustainability institute, Southampton
- The journal of open source software (JOSS)
- Cookiecuttter template for data science
- Matt Might's CRAPL academic licence
- Great minimalist example of open source from geosciences. Commented code, readme and licence Try it out on Binder here
 (launches interactive notebook in your browser).
- Ten Years Reproducibility Challenge
- Stackoverflow all of your programming questions answered

```
The wall of logos on slide 22 are:
git github zenodo
Python netCDF R
Linux Project Jupyter British Oceanographic Data Centre
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Footnotes

This talk was presented as a seminar at the Centre for Atmospheric and Ocean Sciences, University of East Anglia 2020-11-27

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- FAIR graphic on slide 11 from ANDS
- -Image of Bartelbey the Scrivener on slide 25 from Broken Brilliant