Simple and Effective Methods for Managing and Sharing Scientific Data

The CZ Hub Team November 10, 2021



Critical Zone Network

Data are first-class products of research

Data and Models as Research Products

Some principles from the FORCE11 Data Citation Synthesis Group:

- 1. Data should be considered legitimate, citable, products of research
- 2. Data citations should facilitate giving scholarly credit and normative and legal attribution to all contributors to the data
- 3. In scholarly literature, whenever and wherever a claim relies upon data, the corresponding data should be cited



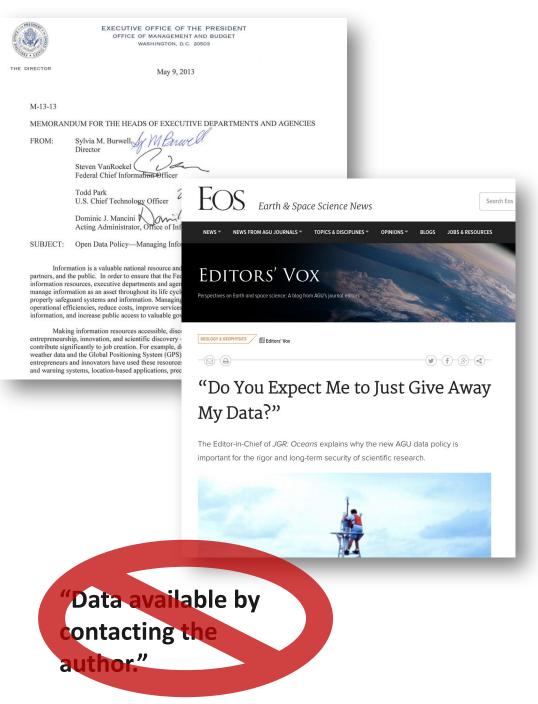
4. .

Data Citation Synthesis Group: Joint Declaration of Data Citation Principles. Martone M. (ed.) San Diego CA: FORCE11; 2014 <u>https://doi.org/10.25490/a97f-egyk</u>

Data Sharing: Requirements

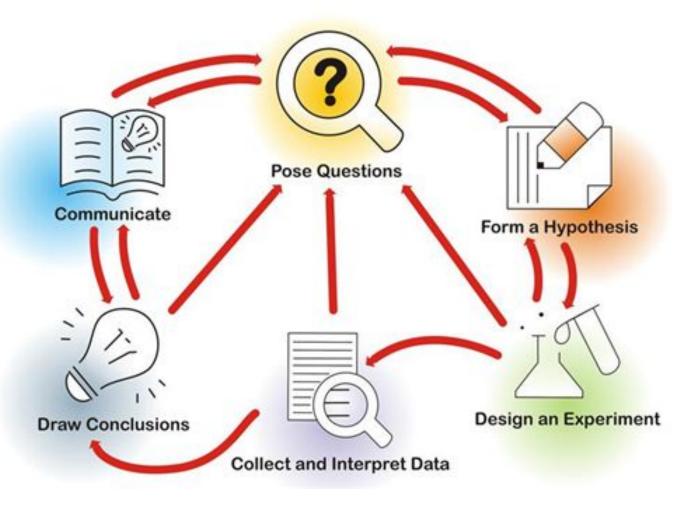
- Federal grants require data sharing and availability (data management plans)
- Many scholarly journals (all AGU journals)
- Data is defined broadly (per AGU policy):
 - Data used to generate, or be displayed in, figures, graphs, plots, videos, animations, or tables in a paper.
 New protocols or methods used to generate the data in a paper.
 - •New code/computer software used to generate results or analyses reported in the paper.
 - •Derived data products reported or described in a paper.

"When you publish a research paper, you are also simultaneously publishing the data that supports your work. The readers of your article have equal rights to see both the words and the numbers – they are inseparable."



Data Sharing: Reproducibility

- Communicating and sharing data is an essential compone of the scientific process
- If our science is not reproducible, we haven't completed the loop
- The value of data sharing ha not yet been fully realized



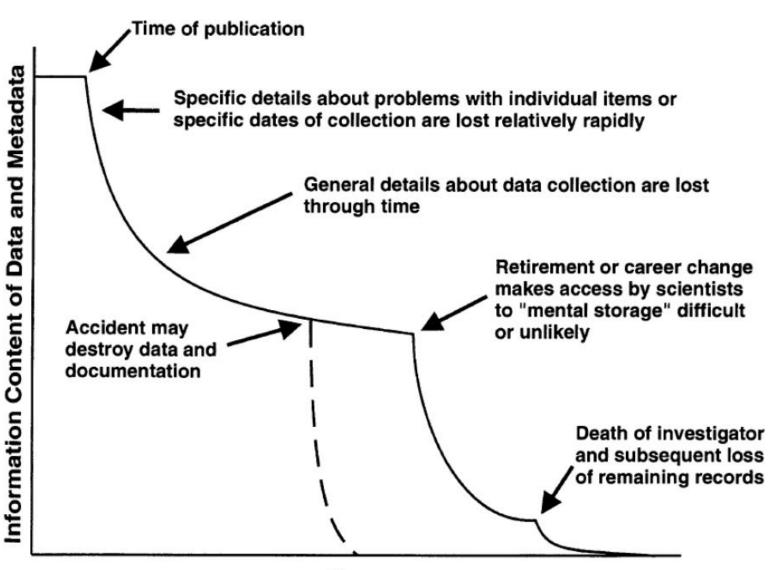
Availability and reproducibility of 360 papers in 2017 (Stagge et al., 2019 in Nature-*Scientific Data*)

Q5. How accessible Q6. Where Q7. What is Q11. Do outputs verify results? to users? available? present? Fully replicable Directions, code [4] & data [20] Some Some Some replicable availability online [175] All 2 of 3 primary [2] [253] papers artifacts [24] [360] Not replicable Contact 1 of 3 primary [4] first author [68] artifacts [80] Availability failure [10] Not specified No primary where [73] Contact artifacts [51] third party [10] Dataless or review [34]

Environmental Modeling & Software	Water Resources Research	J. American Water Resources Association
Hydrology and Earth System	Journal of Hydrology	J. Water Resources Planning &
Sciences	Journal of Hydrology	Management

Stagge, J.H., Rosenberg, D. E., Abdallah, A.M., Akbar, H., Attallah, N.A., James, R. (2019). Assessing data availability and research reproducibility in hydrology and water resources, Scientific Data, 6, 190030, https://doi.org/10.1038/sdata.2019.30

Information Entropy



Example of the degradation of information content associated with data and metadata over time

Michener, W.K. (2006) Meta-information concepts for ecological data management, Ecological Informatics, 1(1):3-7. https://doi.org/10.1016/j.ecoinf.2005.08.004

Information Entropy

"Do not underestimate your ability to forget details about a study!"

Borer, E.T., Seabloom, E.W., Jones, M.B., Schildhauer, M. (2009). Some simple guidelines for effective data management. Bulletin of the Ecological Society of America 90:205-214. <u>https://doi.org/10.1890/0012-9623-90.2.205</u>

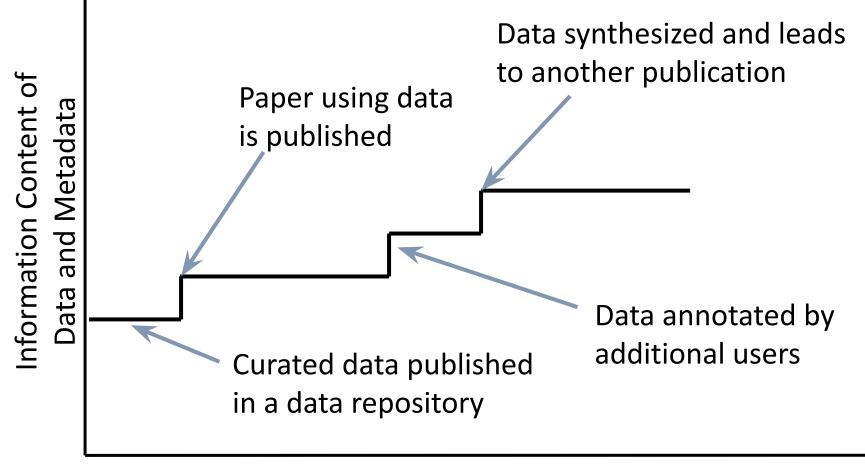
"If the information on an observation is lost, it is lost forever because it is almost impossible to measure the observation again in the original context."

Specht, A., Guru, S., Houghton, L., Keniger, L., Driver, P., Ritchie, E.G., Lai, K., Treloar, A. (2015). Data management challenges in analysis and synthesis in the ecosystem sciences. Science of the Total Environment. <u>https://doi.org/10.1016/j.scitotenv.2015.03.092</u>

"If the rewards of the data deluge are to be reaped, then researchers who produce those data must share them, and do so in such a way that the data are interpretable and reusable by others."

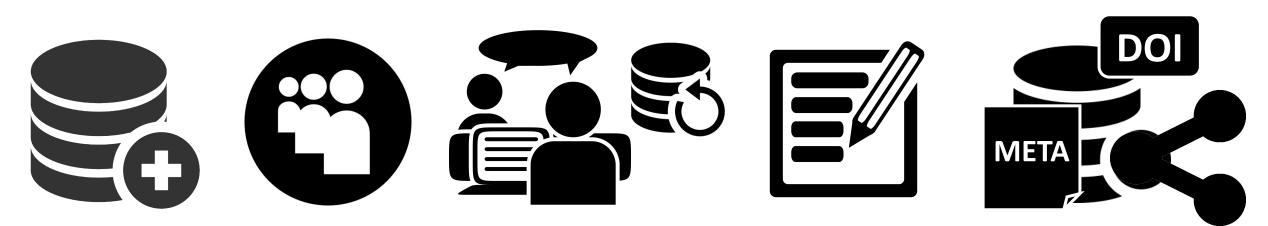
Borgman, C.L. (2012). The conundrum of sharing research data. Journal of the American Society for Information Science and Technology 63(6): 1059-1078. https://doi.org/10.1002/asi.22634

Information Entropy: What if instead?



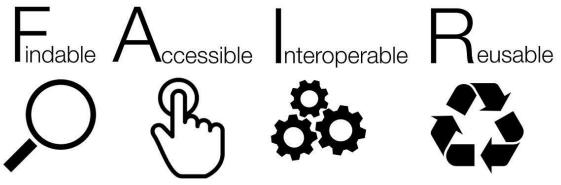
Investigator Data Workflow

- Easily create a digital instance of a dataset or model
- Quickly share it with colleagues (perhaps privately at first)
- Add value through collaboration, annotation, and iteration
- Describe with metadata
- Eventually...share publicly or formally <u>P</u>ublish



How do you go about doing this?

What does it mean for data to be FAIR?



A set of 14 guiding principles to make data:

- <u>Findable</u>: Data have sufficient metadata and a unique, persistent identifier making data discoverable on the Web
- <u>Accessible</u>: Metadata and data are understandable to humans and machines and are available via a trusted repository
- Interoperable: Metadata use formal community standards
- <u>Reusable</u>: Data have clear metadata, usage license, and information about provenance

The extent to which data are FAIR affects their value and extent of reuse.

Wilkinson, M. D. et al. (2016). The FAIR Guiding Principles for scientific data management and stewardship. Scientific Data, 3:160018, <u>https://doi.org/10.1038/sdata.2016.18</u>.

Some Data Management Resources

• Guidelines for Structuring and Formatting Data

- Borer, E.T., Seabloom, E.W., Jones, M.B., Schildhauer, M. (2009). Some simple guidelines for effective data management, Bulletin Ecological Society of America, 90(2), 205-214, <u>https://doi.org/10.1890/0012-9623-90.2.205</u>
- Broman, K. W., & Woo, K. H. (2018). Data Organization in Spreadsheets. The American Statistician, 72(1), 2–10. <u>https://doi.org/10.1080/00031305.2017.1375989</u>
- Goodman, A., Pepe, A., Blocker, A. W., Borgman, C. L., Cranmer, K., Crosas, M., Di Stefano, R., Gil, Y., Groth, P., Hedstrom, M., Hogg, D. W., Kashyap, V., Mahabal, A., Siemiginowska, A., & Slavkovic, A. (2014). Ten Simple Rules for the Care and Feeding of Scientific Data. PLoS Computational Biology, 10(4), e1003542. <u>https://doi.org/10.1371/journal.pcbi.1003542</u>
- Hart, E. M., Barmby, P., LeBauer, D., Michonneau, F., Mount, S., Mulrooney, P., Poisot, T., Woo, K. H., Zimmerman, N. B., & Hollister, J. W. (2016). Ten Simple Rules for Digital Data Storage. PLOS Computational Biology, 12(10), e1005097. <u>https://doi.org/10.1371/journal.pcbi.1005097</u>
- Wickham, H. (2014). Tidy Data. Journal of Statistical Software, 59(10), Article 10. https://doi.org/10.18637/jss.v059.i10

• Guidelines for Citing Data

- Colavizza, G., Hrynaszkiewicz, I., Staden, I., Whitaker, K., & McGillivray, B. (2020). The citation advantage of linking publications to research data. PLOS ONE, 15(4), e0230416. <u>https://doi.org/10.1371/journal.pone.0230416</u>
- Guidelines for Making Data More Reusable
 - White, E., Baldridge, E., Brym, Z., Locey, K., McGlinn, D., & Supp, S. (2013). Nine simple ways to make it easier to (re)use your data. Ideas in Ecology and Evolution, 6(2), Article 2. <u>https://doi.org/10.4033/iee.2013.6b.6.f</u>

• Guidelines for Selecting a Data Repository

 Sansone, S.-A., McQuilton, P., Cousijn, H., Cannon, M., et al (2020). Data Repository Selection: Criteria That Matter. Zenodo. <u>https://doi.org/10.5281/zenodo.4084763</u>

Data Management 101

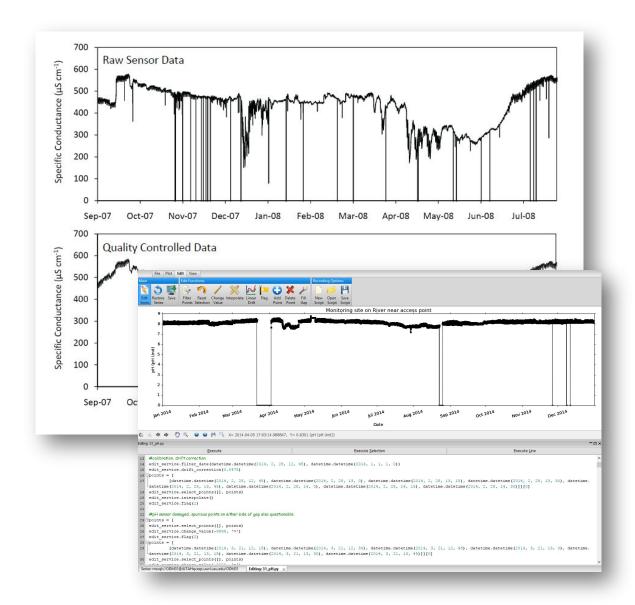
- Simple guidelines to improve data management
- Benefits
 - Improved data organization facilitates analysis
 - Improved reproducibility
 - Improved capacity for data re-use
 - Facilitates compliance with funding sources and publishers

An oldie – but a goodie!

Borer, E.T., E.W. Seabloom, M.B. Jones, and M. Schildhauer (2009). Some simple guidelines for effective data management, *ESA Bulletin*, 90(2):205-214, <u>https://doi.org/10.1890/0012-9623-90.2.205</u>

1. Don't mess with the raw data

- •Always store uncorrected data with all of its "bumps and warts"
 - You could change something that was actually correct
 - You could make mistakes while correcting other mistakes
- Script procedures and write results to a new file/copy of the data



2. Use descriptive file names

- Use only plain ASCII characters and avoid spaces
- Brief, but indicative of content
- Include a "readme" file when using many files in a directory

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3. Use descriptive headers in files/tables

- Standard convention for many software applications
- Encapsulate data and descriptive metadata together

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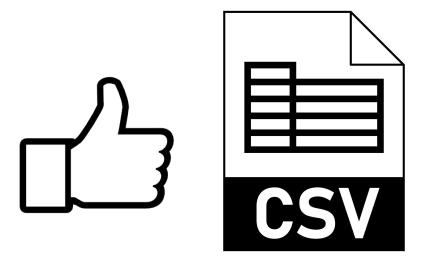
4. Archive data in non-proprietary formats

- •Microsoft Excel is widely available and used now, but what about in 10 years? 20 years?
- •How many other software programs can open your data?
- •Will your data disappear if the file format/software become obsolete?



What format to use?

- Store it in a file format that can be used by many different software programs
 - Text files e.g., comma separated values (CSV) for tabular data
- Use a standard file format accepted by your scientific community
- Consider:
 - Format the file type
 - Syntax the structure within the file
 - Semantics the values in the data



Best Practices For Tabular Data

- Each row should have a single observation
- Each column should represent a single variable/attribute
- Every cell should have a single value
- There should be only one column for each type of information
- Do not mix data types within a column
- Use standard formats within cells
 - Be consistent
 - Avoid special characters
 - Avoid using your column delimiter in the data
 - Use standard date formats (e.g., YYYY-MM-DD)
- Use null and NoData values correctly to represent empty or missing data values
- Do not repeat metadata set up separate table

ID	Site_ID	Name	Latitude	Longitude	City	State_or_Province	Country	ID2	Site_ID	d180	d2H	d180_sd	d2H_sd	Type [DEX	Site_ID
SLV-15-125	SLV-WS-001	Maverick	40.54414	-111.87157	Draper	Utah	USA	15-103	SLV-WS-001	-15.57159565	-117.0815005	0.026185373	0.086739176	Тар	7.4912647	SLV-WS-001
SLV-15-129	SLV-WS-003	Seven Eleven	40.5265	-111.87182	Draper	Utah	USA	15-103	SLV-WS-003	-15.58521063	-117.0362963	0.017747305	0.087391515	Тар	7.64538874	SLV-WS-003
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SLV-15-134	SLV-WS-007	Seven Eleven	40.48592	-111.88457	Draper	Utah	USA	15-103	SLV-WS-007	-15.59920887	-119.1033377	0.028137458	0.093218217	Тар	5.69033326	SLV-WS-007
SLV-15-079	SLV-WS-008	Spring View Farms Trail	40.48642	-111.92639	Bluffdale	Utah	USA	15-103	SLV-WS-008	-15.59811322	-117.2283092	0.028781583	0.17131442	Тар	7.55659656	SLV-WS-008
SLV-15-080	SLV-WS-009	Seven Eleven	40.50505	-111.89738	Draper	Utah	USA	15-103	SLV-WS-009	-15.65822932	-117.0422576	0.014637371	0.064054855	Тар	8.22357696	SLV-WS-009
SLV-15-132	SLV-WS-009	Seven Eleven	40.50505	-111.89738	Draper	Utah	USA	15-103	SLV-WS-009	-15.53472795	-117.1648488	0.03884896	0.206939051	Тар	7.1129748	SLV-WS-009
SLV-15-076	SLV-WS-010	Holiday	40.50714	-111.98578	Riverton	Utah	USA	15-103	SLV-WS-010	-14.49605205	-113.2791354	0.02547515	0.091029684	Тар	2.689281	SLV-WS-010
SLV-15-073	SLV-WS-011	McDonalds	40.50857	-112.01044	Herriman	Utah	USA	15-103	SLV-WS-011	-15.44874428	-119.1508446	0.020055622	0.073675097	Тар	4.43910964	SLV-WS-011

White, E.P, Baldridge, E., Brym, Z.T., Locey, K.J., McGlinn, D.J., and S.R. Supp (2013). Nine simple ways to make it easier to (re)use your data, PeerJ PrePrints, <u>http://dx.doi.org/10.7287/peerj.preprints.7v2</u>

5. Consider data entry

- All data collection involves some data entry
 - Recording observations and notes in a field notebook
 - Transcribing field notebooks and sheets into digital forms
 - Automated processing of sensor data streams into a database
- When you create data entry tools:
 - Use pre-designed forms or templates (electronic or paper)
 - Use lists of valid values rather than free form text entry
 - Example: "Temperature" versus "T", "Temp", "Tem"
 - Use validation checks (e.g., range checks)
 - Example: pH must be between 0 and 14. If it's not there is a problem!



6. Automate analyses

- Code creates reproducible results
- Code is a record of the steps involved in processing and analyzing data
- Code can be shared
- Code can be re-executed at any time

```
# Create a plot of the streamflow statistics
fig = plt.figure()
ax = fig.add subplot(1, 1, 1)
ax.plot(localDateTimes, dataValues, color='lightgrey', linestyle='solid', label='15-minute flows')
ax.plot(dailyFlows[0], dailyFlows[1], color='blue', linestyle='solid', marker='o', markersize=5, label = 'Daily min flows')
ax.plot(dailyFlows[0], dailyFlows[2], color='green', linestyle='solid', marker='o', markersize=5, label = 'Daily avg flows')
ax.plot(dailyFlows[0], dailyFlows[3], color='red', linestyle='solid', marker='o', markersize=5, label = 'Daily max flows')
ax.set_ylabel('Discharge, cubic feet per second')
ax.set_xlabel('Date')
ax.grid(True)
ax.set title('Daily Min, Max, and Avg Flows')
# Add a legend with some customizations
                                                                                 Daily Min, Max, and Avg Flows
legend = ax.legend(loc='upper left', shadow=True)
                                                                  15-minute flows
                                                               Daily min flows
# Create a frame around the legend.

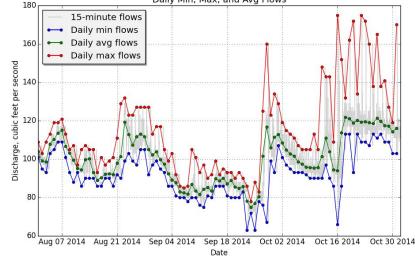
    Daily avg flows

                                                           160
frame = legend.get frame()
                                                               Daily max flows
frame.set_facecolor('0.95')
                                                         ğ 140
# Set the fontsize in the legend
for label in legend.get texts():
```

label.set_fontsize('large')

for label in legend.get_lines():
 label.set_linewidth(1.5) # the legend line width

```
fig.tight_layout()
plt.show()
```



The initial investment to learn pays off later!

7. Consider storage media

- CDs?
- DVDs?
- External hard drives?
- Don't strand your data!!!

Borer et al.: "As hard as it is to believe today, we can foresee the day when CD-ROMs might be difficult to read."













2000



1986

1994

Preservation/Backup Media How are you preserving your data now?

- Does your office look like this?
- What are the potential problems?
- What are some potential solutions?







Backups

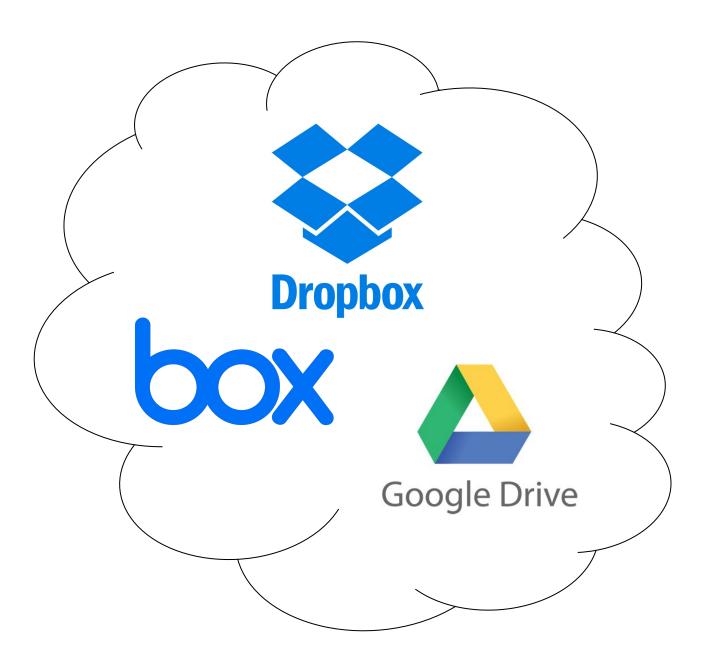
- 1. Have a plan
- 2. Stick to your plan
- **3.** <u>Test your plan</u> preferably under non-failure conditions!
- 4. Betty Rozum's 3-2-1 rule
 - 3 copies
 - 2 types of storage media (e.g., cloud, hard drive)
 - 1 copy offsite
- 5. Consider hard copy data lab notebooks, research notes, field notes, etc.
 - Don't trust/rely on hardware redundancy

Plan to Preserve

- What will be preserved?
- Where will it be preserved?
- Back ups?
- Version control?
- Policies for access, sharing, and reuse
 - Obligations for sharing
 - Security and access control
 - Sensitive data
 - How long?
 - Intellectual property issues
 - Responsible parties

To the Cloud!

- Convenience
- Accessibility anywhere
- Cross platform
- Enhanced sharing
- Low cost
- But...
 - Privacy?????
 - Delay (slow or non-existent internet)
 - Storage, but not much else
 - File formats and semantics still matter



Better Opportunities for Data Sharing and Preservation

- Data archives/repositories
- Functionality for collaboration and archival/preservation
- Still very much discipline specific
- Impact is higher if you choose carefully!



PANGAEA . Data Publisher for Earth & Environmental Science

















Which Repository to Use?

• For CZ Net – we are recommending some repositories

- For others:
 - Does your research sponsor stipulate a repository?
 - Does your scientific discipline have a repository?
 - Disciplinary data is best stored together where researchers are likely to find it
 - Code many use GitHub (and there are ways to make your code citable)

Repository Challenges

- How to best use the repository?
- How to avoid data misinterpretation?
- Size limitations for individual users
- Level of required metadata where to set the bar?
- Dataset review
- Ongoing curation

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thors: IUTAH GAMUT Working Group mers: IUTAH Data Manager source type: Generic statet: July 19, 2016, 10:03 p.m. tupdated: Nov. 18, 2016, 4:58 a.m. by IUTAH Data Manager			
bstract			
s dataset contains a stage-discharge relationship developed for the IUTAH GAMUT Na ssurements were collected by a SonTek FlowTracker. Measured stage and discharge ar h discharge measurements are documented in the README file. Files associated with r string curve was used to generate discharge data through 12/31/2015. New versions Jished in the IUTAH GAMUT operational databases and may be accessed via http://dat	nd the curve are contained in the Rating each measurement (e.g., output by the s of these files may be loaded when nev	g Curve file. Information on the site conditi FlowTracker instrument) are contained in	ions and any iss the .zip director
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8. Maintain effective metadata

• Borer et al.: *"Do not underestimate your ability to forget details about a study!"*

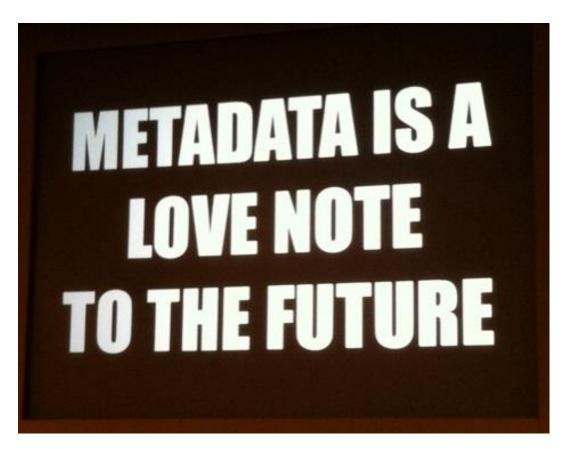
- When did the tree that was stuck in my stream cross section get removed????
- You may not analyze your data until years down the road
- Exact details of methods, names, files, etc. will become fuzzy

What is Metadata?

• Metadata is "Information about Data"

- WHO created the data?
- WHAT is the content of the data?
- WHEN were the data created?
- WHERE is it geographically?
- WHY were the data developed?
- **HOW** were the data developed?

Content, quality, condition, and other characteristics



Metadata Content and Format

- What metadata are needed?
 - Details that make data findable
 - Details that make data meaningful
- How will metadata be created?
 - Lab notebooks?
 - Curation by you or a data manager?
 - Automatically generated by a sensor or instrument?
- What format will be used for the metadata?
 - Standards may be chosen by community or dictated by an agency
 - May be dictated by the repository into which you deposit the data

Metadata Extend to Samples for Reuse & Reproducible Science (upcoming webinars!)

- Use of <u>globally unique and persistent identifiers</u> for samples
 - to support unambiguous citation
 - to support linking of information in distributed data systems and with publications
- <u>Standards for metadata</u> to document the diverse range of samples and collections to make sample Findable & Accessible
- <u>Best practices for sample and collection cataloguing</u>, including a broad range of issues from interoperability to persistence of catalogues
- <u>access policies</u> for sample metadata & samples/specimens

Slide from Kerstin Lehnert

Sharing Data: The Golden Rule

• When you *provide* data to someone else, what types of information are they going to need to understand the data?



 When you *receive* a dataset from an external source, what types of details do you want to know about the data?

Sharing Data

• Providing data:

- Why were the data created?
- What limitations do the data have?
- What does the data mean?
- How should the data be cited if it is re-used in a new study?

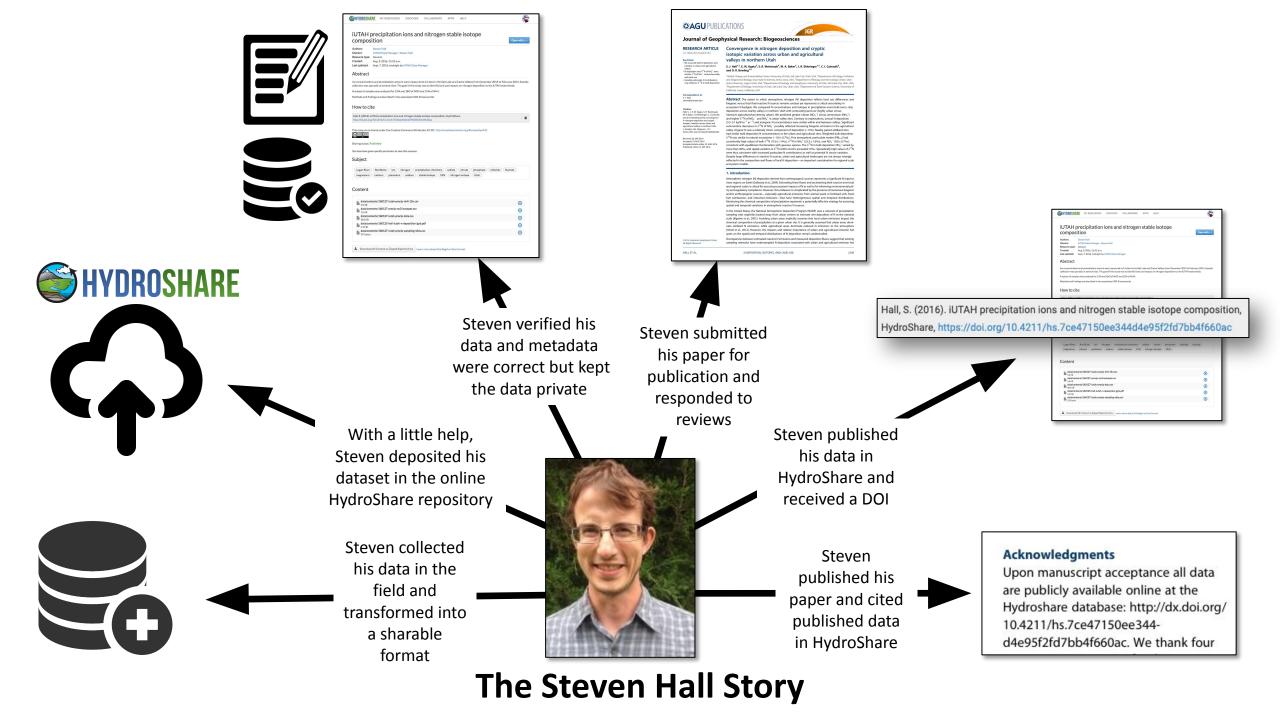
• Receiving data:

- What are the data gaps?
- What processes were used for creating the data?
- Are there any fees associated with the data?
- In what scale were the data created?
- What do the values in the tables mean?
- What software do I need in order to read the data?
- What projection are the data in?
- Can I give these data to someone else?

Data Sharing: Planning

- Address questions related to timing, organization, and authorship <u>up front</u>
- Considerations:
 - Which products will be generated and shared?
 - Are there sensitivities around any of the products?
 - How will data/files be organized?
 - Who is responsible for data/metadata creation and curation?





Summary

- 1. Don't mess with the raw data
- 2. Use descriptive file names
- 3. Use descriptive file headers
- 4. Archive data in non-proprietary data formats
- 5. Consider data entry
- 6. Automate analyses
- 7. Consider storage media
- 8. Maintain effective metadata

Following these steps help prepare datasets for deposit and sharing in a repository

Questions?

Contact us:

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Critical Zone Network