FAIR data principles, metadata and data standards, documentation and formatting tools

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The value of sharing data



Always think about being a data provider, but also a data consumer



- Support/expect transparency and open science
- Support/expect integration and reuse of data
- Support/expect visibility and recognition (both of the institute and the researchers)



The FAIR guiding principles

 To be Findable: F1. (meta)data are assigned a globally unique and persistent identifier 	 To be Interoperable: I1. (meta)data use a formal, accessible, shared, and broadly applicable language
• F2. data (defined) Remember:	on. Iaries that follow
 F3. meta identifier F4. (meta a search To be Access Don't take it as a MUST Don't take it as a MUST Something is better than noth You need to start somewhere Do as much as you can 	5
 A1. (met Be aware identifier commun.current protocol 	escribed with a evant attributes sed with a
 A1.1 the protocol is open, free, and universally implementable A1.2 the protocol allows for an authentication and authorization procedure, where necessary A2. metadata are accessible, even when the 	 clear and accessible data usage license R1.2. (meta)data are associated with detailed provenance R1.3. (meta)data meet domain-relevant community standards
data are no longer available	Wilkinson et al. 201

The FAIR guiding principles

- To be Findable:
 - F1. (meta)data are assigned a globally unique and persistent identifier
 - F2. data are described with **rich metadata** (defined by R1 below)
 - F3. metadata clearly and explicitly include the identifier of the data it describes
 - F4. (meta)data are registered or indexed in a searchable resource
- To be Accessible:
 - A1. (meta)data are retrievable by their identifier using a standardized communications protocol
 - A1.1 the protocol is open, free, and universally implementable
 - A1.2 the protocol allows for an authentication and authorization procedure, where necessary
 - A2. metadata are accessible, even when the data are no longer available

- To be Interoperable:
 - I1. (meta)data use a formal, accessible, shared, and broadly applicable language for knowledge representation.
 - I2. (meta)data **use vocabularies** that follow FAIR principles
 - I3. (meta)data include qualified references to other (meta)data
- To be Reusable:
 - R1. meta(data) are richly described with a plurality of accurate and relevant attributes
 - R1.1. (meta)data are released with a clear and accessible data usage license
 - R1.2. (meta)data are associated with detailed provenance
 - R1.3. (meta)data meet domain-relevant community standards

Data and Metadata

The concept of data and metadata can be at times unclear

- Data is a collection of information, such as observations, measurements, computations of models etc...
 - It can be used to analyze trends and patterns, to extract and visualize actual values of variables
- Metadata, on the other hands, is data about the data, i.e. they extensively provide description about the data they are attached to
 - It gives the necessary context to the user to be able to access, understand and use the data correctly
 - Several types of metadata can and should be used to describe the data

Types of metadata

Туре	Purpose	Description	Examples
Discovery metadata	Used to find relevant data	Discovery metadata are also called index metadata and are a digital version of the library index card. It describes who did what, where and when, how to access data and potential constraints on the data. It shall also link to further information on the data like site metadata. GCW is required to expose this information through WMO Information System as well. Discovery metadata are thus WIS metadata, although the GCW portal can translate to WIS for those not using WMO standards directly.	ISO19115 GCMD DIF ACDD
Use metadata	Used to understand data found	Use metadata are describing the actual content of a dataset and how it is encoded. The purpose is to enable the user to understand the data without any further communication. It describes content of variables using standardised vocabularies, units of variable, encoding of missing values, map projections etc.	Climate and Forecast Convention BUFR GRIB Darwin Core Archive
Configuration metadata	Used to tune portal services for datasets for users.	Configuration metadata are used to improve the services offered through a portal to the user community. This can be e.g. how to best visualise a product. This information is maintained by the GCW portal and is not covered by discovery or use metadata standards.	Used locally by data centres
Site metadata	Used to understand data found	Site metadata are used to describe the context of observational data. It describes the location of an observation, the instrumentation, procedures etc. To a certain extent it overlaps with discovery metadata, but more so it really extends discovery metadata. Site metadata can be used for observation network design.	WIGOS OGC O&M

What is in a metadata standard?



- A metadata standard is made up of defined elements, including the type of information the user should enter (e.g. text, numbers, date).
- Examples of elements include Title, Abstract, Keyword, Online Link
- Multiple standard exists and they are linked to the type of metadata they address and the communities they target
- Terminology for the same concepts may vary across standards (values of mapping)



Adopting standards

- Most projects (rightly so) focus on the **content** of their data files, you need to consider the format as well.
- Since you captured or created the data, and stored them in your own files, you know
 - how the data are **organized**,
 - how to **read** them,
 - how to **use** them,
 - characteristics of the data that could **constrain** their use.
- The goal of a good (meta)data format is to make it easier for **others** to read the data too.
- Many hours have gone into developing standards for formats try to learn from them.



Why using community standards?

- If you try to develop your data format from scratch, you will forget something.
- Build on the experience and improvements built into the community standards over years of use.
- Tools and analysis software natively support reading community standard data.
- Reduce development effort and support reuse.
- Positive feedback they are more likely to be adopted by others.



Why using community standards?

- Consider your **archive**:
 - Do they have any recommendations?
- Consider your **users**:
 - Who wants this data? Why do they want it?
 - What do they want to do with it?
 - Will they be using your data in concert with other data?
- Consider heritage:
 - What worked well for similar data in the past?
 - What could be done better for newly created data?
- Consider tools:
 - Try to use data formats supported by the software you intend to use it with.

Filling in Metadata Standards

I need to fill in a metadata element about:

Dataset Production Status: Describes the production status of the data set regarding its completeness.

What should I put in there?

Metadata file:

<Title>The title of the dataset</Title> <Abstract> This dataset collects...</Abstract> <Dataset_Production_Status>XXX</Dataset_Production_Status> <Start_Date>2020-01-20</Start_Date>

Filling in Metadata Standards

I need to fill in a metadata element about:

Dataset Production Status: Describes the production status of the data set regarding its completeness.

Data provider A can use:
"Not ready yet"
"Done"

"Still acquiring data" "Continuously updating" "???"

Data provider B can use:

"Not finished" "Finished and stored" "unknown" "Not started yet" "See www.mydataset.com"

They will all pass and we are left with unmanageable information

Controlled *vocabulary*

controlled vocabularies are a **source of authoritative terms** to be entered for values of certain elements

Label	Description
Planned	Refers to data sets to be collected in the future and are thus unavailable at the present time.
In Work	Refers to data sets currently undergoing production or data that is continuously being collected or updated.
Complete	Refers to data sets in which no updates or further data collection will be made.
Obsolete	A new version of the dataset has been generated. The new version should be used, this is kept for back tracing.

Discovery Metadata - ACDD Convention

When encoding data as netCDF/CF is good practise to include discovery metadata in the file using the <u>Attribute Convention</u> for dataset Discovery (ACDD).

Discovery metadata will then be directly connected to the data themselves and can be extracted for ingestion in the searchable catalogue.

Index by Attribute Name

- acknowledgement (Recommended)
- cdm_data_type (Suggested)
- comment (Recommended)
- contributor_name (Suggested)
- contributor_role (Suggested)
- Conventions (Highly Recommended)
- coverage_content_type (Highly Recommended)
 [Variable]
- creator_email (Recommended)
- creator_institution (Suggested)
- creator_name (Recommended)
- creator_type (Suggested)
- creator_url (Recommended)
- date_created (Recommended)
- date_issued (Suggested)
- date_metadata_modified (Suggested)
- date_modified (Suggested)
- geospatial_bounds (Recommended)
- geospatial_bounds_crs (Recommended)
- geospatial_bounds_vertical_crs (Recommended)
- geospatial_lat_max (Recommended)
- geospatial_lat_min (Recommended)
- geospatial_lat_resolution (Suggested)

- geospatial_lat_units (Suggested)
- geospatial_lon_max (Recommended)
- geospatial_lon_min (Recommended)
- geospatial_lon_resolution (Suggested)
- geospatial_lon_units (Suggested)
- geospatial_vertical_max
- (Recommended)
- geospatial_vertical_min (Recommended)
- geospatial_vertical_positive (Recommended)
- geospatial_vertical_resolution (Suggested)
- geospatial_vertical_units (Suggested)
- history (Recommended)
- id (Recommended)
- institution (Recommended)
- instrument (Suggested)
- instrument_vocabulary (Suggested)
- keywords (Highly Recommended)
- keywords_vocabulary (Suggested)
- license (Recommended)
- long_name (Highly Recommended) [Variable]
- metadata_link (Suggested)
- naming_authority (Recommended)
- platform (Suggested)

- platform_vocabulary (Suggested)
- processing_level (Recommended)
- product_version (Suggested)
- program (Suggested)
- project (Recommended)
- publisher_email (Recommended)
- publisher_institution (Suggested)
- publisher_name (Recommended)
- publisher_type (Suggested)
- publisher_url (Recommended)
- references (Suggested)
- source (Recommended)
- standard_name (Highly Recommended) [Variable]
- standard_name_vocabulary (Recommended)
- summary (Highly Recommended)
- time_coverage_duration (Recommended)
- time_coverage_end (Recommended)
- time_coverage_resolution (Recommended)
- time_coverage_start (Recommended)
- title (Highly Recommended)
- units (Highly Recommended) [Variable]

Use Metadata - Climate and Forecast (CF) convention

For proper interpretation of data

- Standardised naming of variables
- Units of variables
 - o date ISO8601
- Encoding of missing values

CF Standard Name Table

Version 78, 21 September 2021

Refer to the Guidelines for Construction of CF Standard Names for information on how the names are constructed and interpreted, and how new names could be derived.

A note about units

The canonical units associated with each standard name are usually the SI units for the quantity. <u>Section 3.3 of the CF conventions</u> states: "Unless it is dimensionless, a variable with a standard n units which are physically equivalent (not necessarily identical) to the canonical units, possibly modified by an operation specified by either the standard name modifier ... or by the cell methods of Section 1.3 of the CF conventions states: "The values of the units attributes are character strings that are recognized by UNIDATA's Udunits package [UDUNITS], (with exceptions allowed as disc "Units")." For example, a variable with the standard name of "air temperature" may have a units attribute of "degree_Celsius" because Celsius can be converted to Kelvin by Udunits. For the full: refer to section 6 of the <u>Udunits documentation</u>. Refer to the <u>CF conventions</u> for full details of the units attribute.

Search

AND O OR (separate search terms with spaces)
 Also search help text

View by Category

 Atmospheric Chemistry
 Atmosphere Dynamics
 Carbon Cycle
 Cloud
 Hydrology

 Ocean Dynamics
 Radiation
 Sea Ice
 Surface

Standard Name	Canoni Unit:
acoustic signal roundtrip travel time in sea water	S
aerodynamic particle diameter	m
aerodynamic resistance	m-1 s
Age of sea ice	year
▶ age of stratospheric air	s
age of surface snow	day
▶ aggregate quality flag	1
▶ <u>air_density</u>	kg m-3
alias: equivalent_potential_temperature	К
air equivalent temperature alias: equivalent_temperature	К
▶ <u>air potential temperature</u>	K
▶ air pressure	Pa

Site Metadata - WIGOS WMO Integrated Global Observing System

#	Category	Description					
1	Observed variable	Specifies the basic		• • • • • • • • • • • • • • • • • • •		1450	
		datasets.	6-01	Name Sampling procedures	Definition Procedures involved in obtaining a sample	O MCO	Phase
•	Dumana of channetics	On a sifing the masin	6-02	Sample treatment	Chemical or physical treatment of sample prior to analysis	0	10
2	Purpose of observation	Specifies the main	6-03	Sampling strategy	The strategy used to generate the observed variable	0*	1
		programme(s) and	6-04	Sampling time period	The period of time over which a measurement is taken	M ^e	10
3	Station/platform	Specifies the environ 6. Sampling equipment or remove	6-05	Spatial sampling resolution Temporal sampling interval	Spatial resolution refers to the size of the smallest observable object. The intrinsic resolution of an imaging system is determined primarily by the instantaneous field of view of the sensor, which is a measure of the ground area viewed by a single detector element in a given instance in time Time period between the beginning of consecutive sampling periods	M [#]	11
	Environment	Describes the second	6-07	Diurnal base time	Time to which diurnal statistics are referenced	C#	1
4	Environment	Describes the geog It also provides an unstructure	6-08	Schedule of observation	Schedule of observation	M♯	1
		considered relevant for adequ anywhere else in this standard	1.		his not captured		
5	Instruments and methods of observation	Specifies the method of obser instrument(s) used to make th generate the observation, the	e obs	ervation. If mu cod category shou	le table: 6-03 de table title: Sampling strategy Name Definition		
6	Sampling	Specifies how sampling and/o observation or how a specime			Integrating, i.e., none of the medium escapes observations. Sampling is done at regular time intervals for certain sampling periods the time interval. Sampling is not integrating, i.e., parts of the medium escapes of the time interval. Sampling is not integrating to the medium escapes of the medium	at are sma	aller than
7	Data processing and reporting	Specifies how raw data are trate to the users.	nsfer	red into the observea	variable and reported		
8	Data quality	Specifies the data quality and	tracea	ability of the observati	on.		
9	Ownership and data policy	Specifies who is responsible f	or the	observation and own	s it.		
10	Contact	Specifies where information a	bout t	he observation or data	aset can be obtained.		

File formats

- Always choose open file formats
 - Remember that data are to be handled in a 50-100 year perspective
- Use self-describing formats
 - You will not be around to answer questions forever
 - Well accepted way of archiving and disseminating scientific data.
 - Information describing the data contents of the file are embedded within the data file itself
- NetCDF Network Common Data Form
 - Widely used by agencies (NASA and NOAA)
 - Climate and forecast (CF) metadata conventions help standardize some things into NetCDF in a common manner.

On spreadsheets

- Spreadsheet for computer readability and computability
 - Extra information is often lost in translation
- Avoid extra formatting
 - Merged cells, bold/italic, colors
 - Anything that has to do with visual formatting is not computer-readable.
- Aim at one table (one row for variables, the other for data points)
 - This helps computing the data
 - While a human can see the layout and interpret the tables as separate, the computer doesn't have eyes and won't understand that these are separate
 - Get rid of extra information (graphs/figures)

Example: Poor Data Entry

	A	B	C	n	E	F	G	Н		J	K	L	M	M
	Site	Date	Plot	Species	Weight	Acult		Rodent Trappin	ng 3/15/2010					
2	DeepWell	2/13/2010	1	DIPU	12.1	j		Site	Plot	Adult	RodentSp	Weight		
	Deep Wel	Feb-10		Pero	13.22	j		DW	1	У	Pero	12		
4	rioSalado	2/13/2010	la	pero	16	N		RS	2	j	PERO	escaped <15		
5	riuSladu	"	1*	CleGap	18.92	gul away		RS	3	ri 🛛	Clegap	91		
6			f	Mean1	15.06									
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8			-						_					
9														_
10														
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			A dealt	Species	grams	Comments		event	°C					
13	Site	Plot	Adult					CVCIII	13					
13 14	deep well	1	у	woodrat	13									
13 14 15	deep well riosalado	1	у У	woodrat PERO	13 24.5					of da	ite info	rmation		
13 14 15 16	deep well	1	у У	woodrat	13			• Lo	cation					
13 14 15 16 17	deep well riosalado	1	у У	woodrat PERO	13 24.5			• Lo	cation		ite info late for			
13 14 15 16 17 18	deep well riosalado	1	у У	woodrat PERO	13 24.5			• Lo • Inc	cation consist	ent o	ate for			
13 14 15 16 17	deep well riosalado	1	у У	woodrat PERO	13 24.5			• Lo • Inc	cation	ent o	ate for			



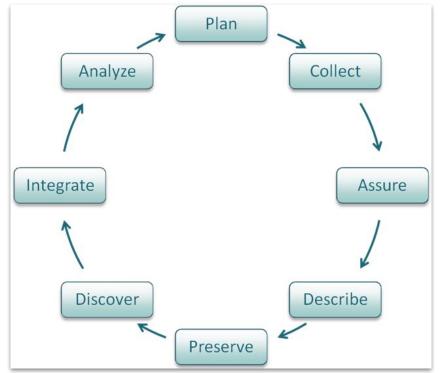
Format conversion: Rosetta tool

- Web-based application
- Can read metadata from header(s), and add user defined metadata
- Profiles, time series, trajectory
- Saves "setup" as templates for future use
- Open source tool, written in Java
- http://tomcat.nersc.no/rosetta/



Data Life Cycle and its relation to the researchers workflow

- Plan
- Generate or collect data
- Quality control and document data
- Analyse data
- Prepare and publish data through a mandated archive
 - Remember to get a DOI!!
- Write a data paper
 - Cite your datasets using the provided DOI
- Write your scientific paper
 - Cite your data paper describing the context of the data



Data Citation

- Data authors get credit for the data publication and subsequent citations
- Can be used to show the impact of research projects
- Shows the scientific impact of data center

Goal: citations become a normal part of the scientific process

- Publishing data products is recognized as a part of scholarly research
- Authors cite the data products they use
- Journals require data to be published when related papers are published

Scientist overview:

- Develop appropriate citations for your data
- Assign identifiers to data
- Find citations for existing data
- Make citing data a regular practice

Data License

A license is an official permission or permit to do, use, or own something (as well as the document of that permission or permit). (Cambridge English Dictionary)

Make sure to use standards when you declare your license.

- Include the license in your metadata
- Whenever possible use machine readable licenses
- Pick from the creative commons license list (or spdx)
- Avoid using free text

Research data: "as open as possible, as close as necessary" to ensure transparency and openness.

- FAIR data does not mean Open Data
 - Embargo
 - Sensitive data



CC BY 4.0: This license lets others distribute, remix, adapt, and build upon your work, even commercially, as long as they credit you for the original creation. This is the most accommodating of licenses offered. Recommended for maximum dissemination and use of licensed materials.

Resources

- https://commons.esipfed.org/
- https://dmtclearinghouse.esipfed.org/browse
- DataONE Education: https://dataoneorg.github.io/Education/
- https://www.youtube.com/watch?v=r29LTAR1-vg
- https://ecorepsci.github.io/reproducible-science/spreadsheets.html
- https://datacite.org/
- https://support.datacite.org/docs/doi-basics
- https://www.doi.org/faq.html
- https://commons.esipfed.org/node/726
- https://commons.esipfed.org/node/1428
- https://dataoneorg.github.io/Education/lessons/08_citation/index.html
- https://creativecommons.org/licenses/

Example: Poor Data Entry

1	Δ	В	C	D	E	F	G	Н	1	J	K	L	M	N
1	Site	Date	Plot	Species	Weight	Acult		Rodent Trappin	g 3/15/2010					
2	DeepWell	2/13/2010	1	DIPO	12.1	i		Site	Plot	Adult	RodentSp	Weight		
3	Deep Well	Feb-10	2	Pero	13.22	j		DW	1		Pero	12		
4	rioSalado	2/13/2010	1a	pero	16	N		RS	2	j l	PERO	escaped <15		
5	riuSladu		1+	CleGau	18.92	gul away		RS	3	n	Cleyap	91		
6				Mean1	15.06									
7														
8	()													
9							l Ir	nconsiste	ncy be	etween	data	collection	า	
10							P	vents						
11		and a second second					Ŭ							5
_	Rodent Tra		MJK & ALN		Contractor and the second second		•	Differe	nt site	spellir	ngs. ca	apitalizati	on.	
	Site	Plot	Adult	Species	9	Ccmments					• •			
	deep well	1	У	woodrat	13			spaces	in site	name	$S = \Pi a$	rd to filte	:r	
15	riosalado		у	PERO	24.5		•	Codes	usod f	or sito	namo	s for som	0	
0	riosalado	3	У	Clegap	91								e	
16							-	data, b	ut spe	lled ou	t for	others		
17														
16 17 18 19								Mean1	2 . **					



and 91?

what is the meaning of 12, "escaped < 15",

Best practices

- Columns of data are consistent: only numbers, dates, or text
- Consistent names, codes, formats (date ISO8601) used in each column
- Data are all in one table, which is much easier for a statistical program to work with than multiple small tables which each require human intervention

	A	В	C	D	E	F	G	Н	
1	Date	Site	Plot	Species	Weight	Adult	Comments		
2	2/5/2010	Deep Well	1	DIPO	13.2	у			
3	2/4/2010	Deep Well	1	CLEGAP	11.6	j			
4	2/5/2010	Rio Salado	1	DIPO	14.2	у			
5	2/5/2010	Rio Salado	2	PERO	10.1	y			
6	3/15/2010	Deep Well	1	DIPO	15.2	у	plot burned	plot burned	
7	3/15/2010	Deep Well	2	DIPO	21.7	ý	pregnant		
8	3/15/2010	Rio Salado	1	CLEGAP	16.2	j			
9									
10									
11									
12									-
1		allMammalTi	. (-1	10 /				-	1



Best practices

- Identify missing values with dedicated code
- Indicate reason for missing value in code
- In numeric fields, use a distinct value such as 9999 to indicate a missing value
- In text fields, use NA ("Not Applicable" or "Not Available")

Date	Time	NO3_N_Conc	NO3_N_Conc_Flag	
20081011	1300	0.013		M1 = missing; no sample
20081011	1330	0.016		collected
20081011	1400		M1	E1 = estimated from
20081011	1430	0.018		grab sample
20081011	1500	0.001	E1]



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Vandation		[Retry] Cancel				
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7 BOSP BRAN				15		N
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12	Allow:	Ignore blank				
13		In-cell dropdown				
15	Decimal					
II I I I Sheet1 / Sheet2 / Sheet3 /	Date Time					
	Text length Custom					
	Apply these changes to all other cells with t	he same settings				
	Clear All	OK Cancel				
1						

