

11.06.2024

# Research Data Management – The Basics

Cantini, Federico Felder, Fabian Förster, Christian Hauser, Stefanie, Nordén, Klara



#### These are your trainers today!



**Federico Cantini** 

- Software Developer
- Technical Lead at Lib4RI



**Fabian Felder** 

- Open Science specialist
- Group Leader IT services and Eresources at Lib4RI



Klara Nordén

Project manager
 Open Research Data
 and Research Data
 Management at
 Lib4RI



### Who are you and why are you here?

Copyright protected material.



https://www.pexels.com/photo/group-of-people-standing-indoors-3184396/



#### **Learning Aims**

- Life cycle of research data
- Adequate metadata documentation for your code and data
- Storing and publishing data
- Using OpenBIS (ELN) and writing Data Management Plans (DMP)



#### **Program**

Topic	Speaker	Time
Introduction	Fabian Felder	9.00 - 9.15
Why Open Science?	Klara Nordén	9.15 - 9.25
Policies and the Research Data Life Cycle	Fabian Felder	9.25 – 9.30
Collect & Store	Federico Cantini	9.30 - 10.00
Evaluate & Archive Share & Disseminate	Fabian Felder	10.00 - 10.10
Break		10.10 - 10.25
RDM Services & Support at Eawag	Christian Förster	10.25 - 10.45
RDM Services & Support at Empa	Stefanie Hauser	10.45 - 11.05
Plan & Design	Everyone	11.05 - 11.45



### Why Open Science?

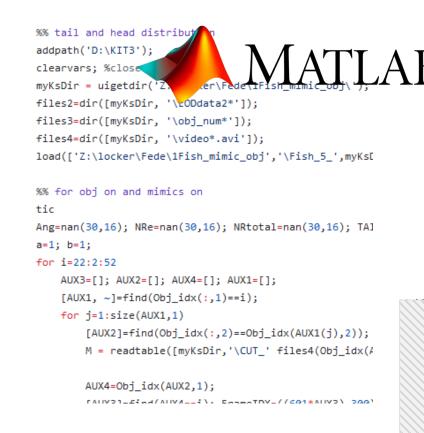


Copyright protected material.

Fast forward 320 years....

1704

2024



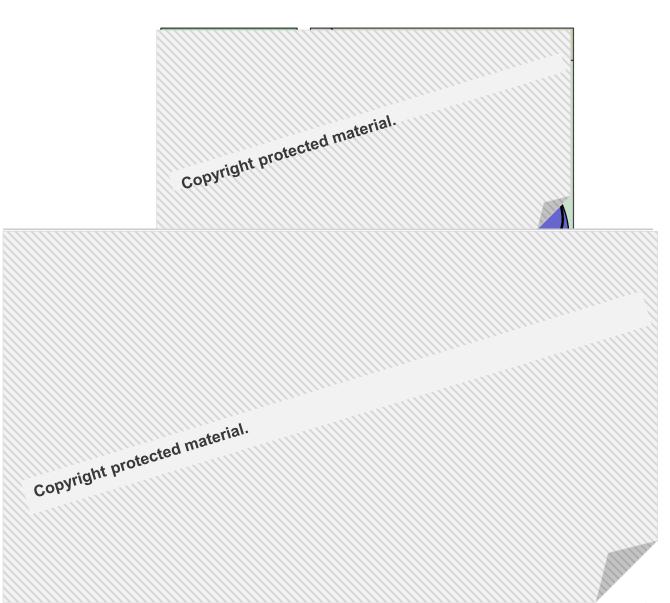
Copyright protected material.



#### "The study should be reproducible from the paper alone"

10-25 bugs per 1000 lines of code (Applications Division at Microsoft, Code complete, Steve McConnell)

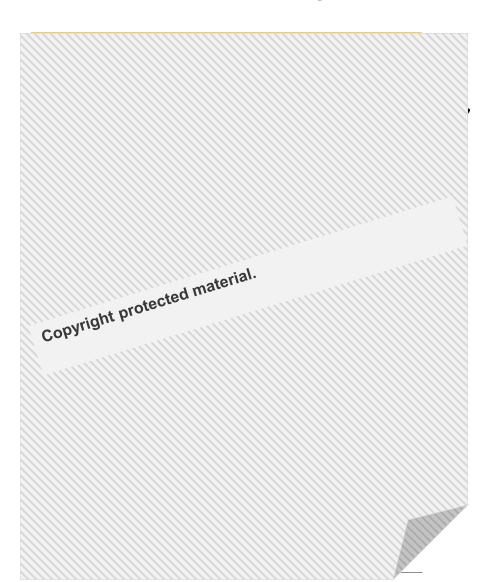
Spreadsheets show a typical error rate of 2-7% (Panko 2005)



Library for the Research Institutes within the ETH Domain: Eawag, Empa, PSI & WSL



#### Why care about open science?





#### **Data availability**

The data that support the findings of this study are available from the corresponding author upon reasonable request.

#### **Code availability**

All numerical codes are available from the corresponding authors on request





Illustration by Ainsley Seago, CC-by 4.0



2 months later....

Are your results different because you asked a different question

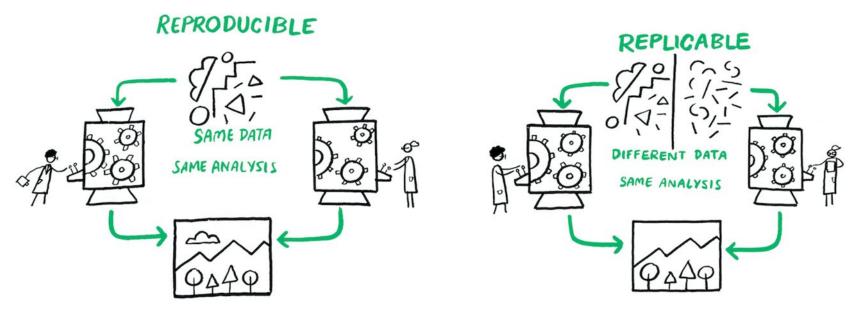
OR

#### because

- you used a different set-up in your experiment?
- you used a different software?
- you normalized your values differently?
- you've misunderstood the variables in the original data?
- the original study had errors?







The Turing Way project, CC-BY 4.0, DOI: 10.5281/zenodo.3332807

## "Non-replicable single occurrences are of no significance to science"

(Karl Popper, 1959). The Logic of Scientific Discovery

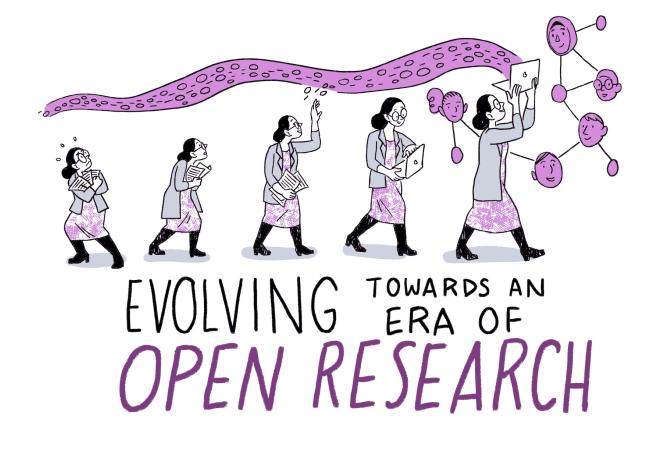


#### Why care about open science?

Open science is about making **your** contribution to the scientific project sustainable, lasting and impactful.

Science is a communal project, and open science practices creates building blocks that makes it easy for others to build on your results.

Your most likely future collaborator is... YOU



The Turing Way project. CC-BY 4.0. DOI: 10.5281/zenodo.3332807.



Open Access

Open Data

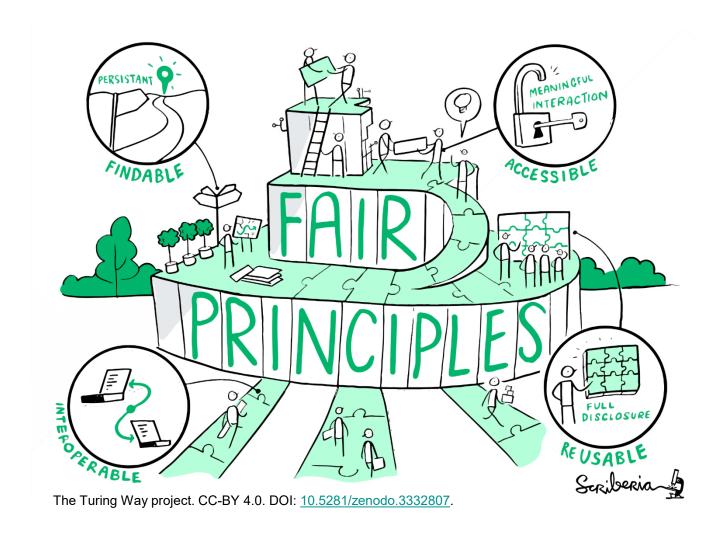
Open Source Software

Open Source Notebooks





#### The FAIR data principles





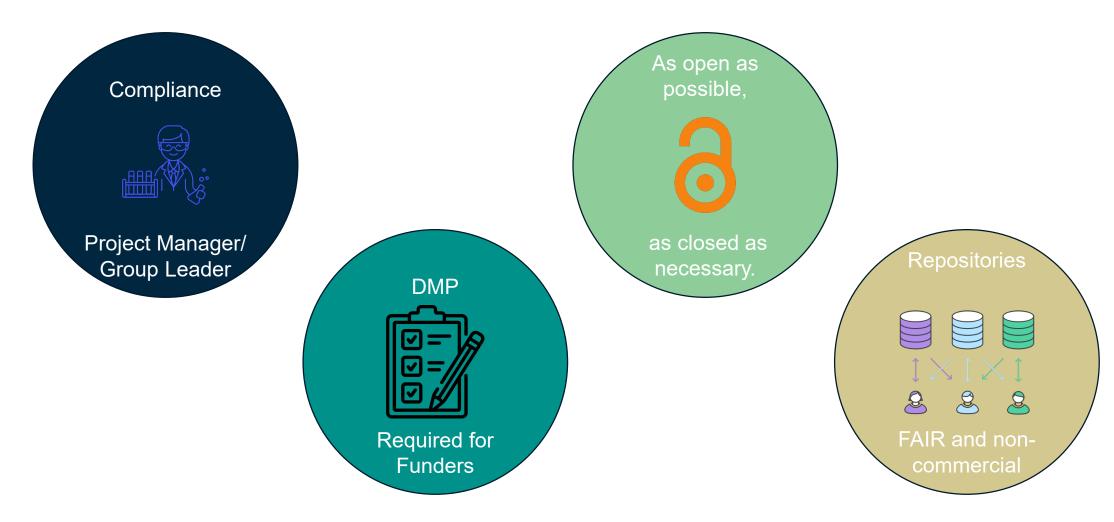
### **Policies**



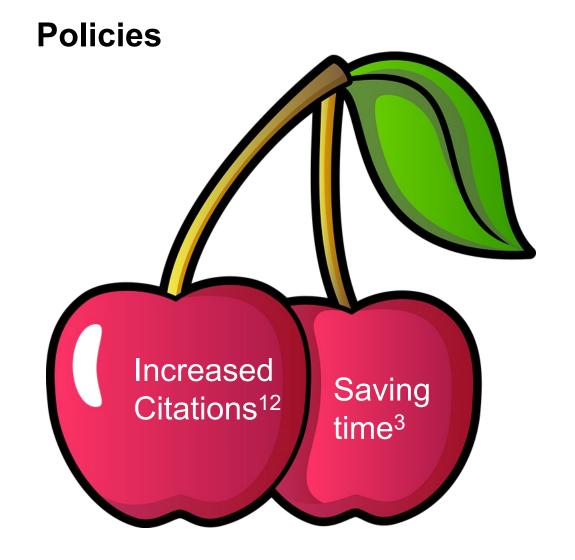
#### **Policies** Funder Policies (Horizon **Institutional Policies** Europe) **Eawag Empa** (internal) (internal) SNSF **WSL PSI** (internal) Journal and **Publisher Policies**

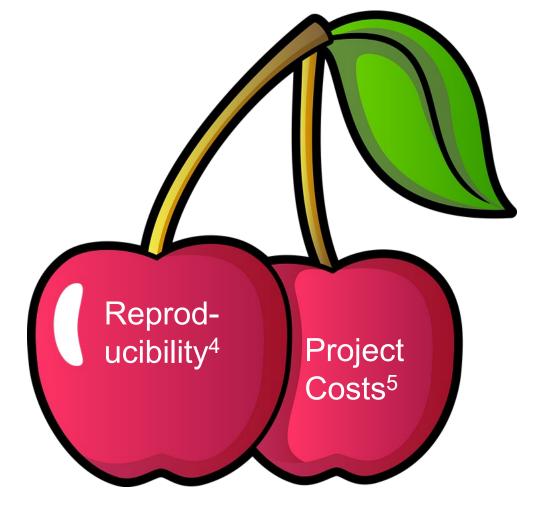


#### **Policies**





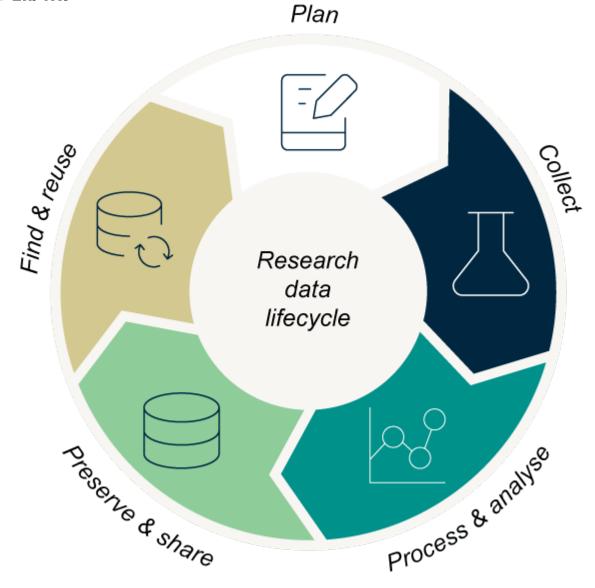






### Research Data Life Cycle





#### **Research Data Life Cycle**



### **Collect & Store**

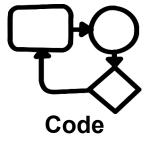


#### **Collect & Store**

01010100	01101000
01101001	01101110
01101011	00100000
01100100	01101001
01100110	01100110
01100101	01110010
01100101	01101110
01110100	00101110

#### Data

observational, experimental, simulation...



Applications, scripts...



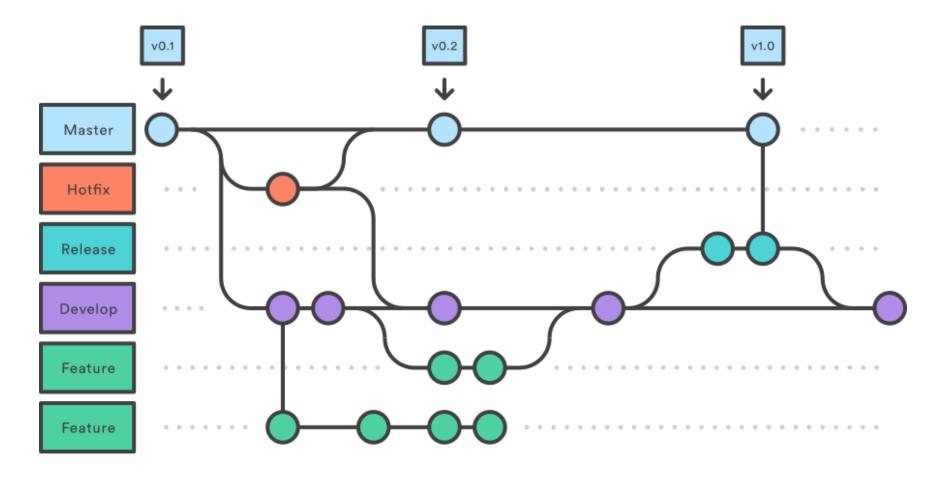
#### Metadata

Structured information associated with data (and code)

The Who, What, Where, Why & How of data

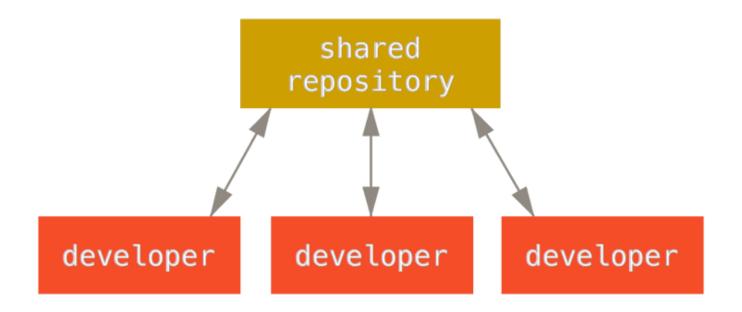


#### **Collect and Store: Software version control**





#### **Collect and Store: Software version control**





#### **Collect and Store: Software version control**





























- o CLI (Command Line interface)
- o GUIs (Graphical User Interfaces)
  https://git-scm.com/downloads/guis



#### **Collect and Store: Data versioning**

Raw rev. 0

Proc. lev. 1 rev. 0

Proc. lev. m rev. 0

Raw rev. 1

Proc. lev. 1 rev. 1

Proc. lev. m rev. 1

. . .

:

:

:

Raw rev. n Proc. lev. 1 rev. n

Proc. lev. m



#### **Collect and Store: Data versioning tools**



Renku (https://renku.readthedocs.io/en/stable/index.html)



Data Version Control (https://dvc.org)



Git Large File Storage (https://git-lfs.com)



Lake FS(https://docs.lakefs.io)



#### **Collect and Store: File Naming**

- Use unique names referencing content
- Limit to 42 characters (preferably less)
- o Use ASCII characters, no spaces, points or special characters, e.g. ~!@#\$%^&\*()[]{}<>';,'»/
- Include dates and label versions
- Use names to order files:
  - Either, use Dates YYYY-MM-DD or YYYYMMDD (according to ISO 8601) at the beginning to enable chronological order
  - Or, use Versioning with leading zeroes to enable numerical order (enables versions to go beyond 9 without disrupting order)
- o If you have started with your project use *Bulk Rename Utility* (Windows) or *Renamer 6* (Mac), *Rename/Thunar Bulk Rename* (GNU/Linux)



#### **Collect and Store: File Formats (recommendation)**

Data type	Recommended file formats
Text	<ul> <li>PDF/A</li> <li>Plain Text coded as ACII. UTF-8 or UTF-16</li> </ul>
	• XML
Spreadsheet	CSV (NEAD)
Images	<ul><li>TIFF (uncompressed or lossless compressed)</li><li>PNG</li></ul>
Code	Languages with free environments (e.g. Py or R UTF-8 format of ASCII text)
Audio	<ul><li>FLAC</li><li>Wav</li></ul>

Open and lossless formats

If you are using a proprietary format, think about adding an additional format



#### **Collect & Store: Metadata Standards**

- Definition: Structured data that contains information about other data, but is not the content of the data.
- o Metadata is very subject specific. The following directories are helpful:
  - o Digital Curation Centre (https://www.dcc.ac.uk/guidance/standards)
  - o RDA Metadata Standards (https://rdamsc.bath.ac.uk)
  - o Fairsharing (https://fairsharing.org)
- Recommendation: Stick to a list of defined terms (controlled vocabulary) and don't use synonyms to describe the same object (e.g. picture or image)



#### **Collect & Store: README File**

General information

- Title of the dataset
- Contact information principal investigator
- · Date of data collection
- Geographic location

Data and file overview

- · Short discription for each file name
- Date

Sharing and access informations

Licenses or restrictions

Methodological information

- Description of methods for data collection or generation
- · Description of methods used for data processing

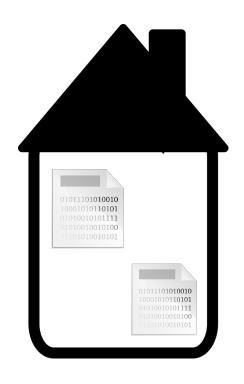
Data specific information (repeat for each dataset)

- Variable list, including names and definitions
- Units of measuments
- · Definition for codes or symbols to record missing data

Cornell University: Minimal viable content. For recommended visit: <a href="https://data.research.cornell.edu/content/readme">https://data.research.cornell.edu/content/readme</a>



#### Collect and Store: 3 - 2 - 1 backup







### **Evaluate & Archive**

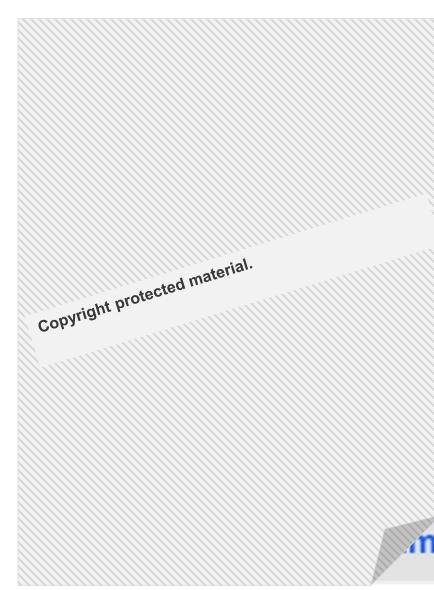


### **Evaluate & Archive: Data Protection**

- Relates to identified or identifiable person
- Solutions (<a href="https://dmlawtool.ccdigitallaw.ch/">https://dmlawtool.ccdigitallaw.ch/</a>) :
  - Identity irrelevant -> anonymisation
  - Identity relevant -> Ask for consent
    - -> Pseudoanomization
    - -> Manage access rights
    - -> Ability to address

subject's rights

 Always contact Data Protection Officers at your Research Institute if your research involves personal data





#### **Evaluate & Archive: Data Protection**

- Processed Data has copyright according to Swiss law
- Use CC licences when publishing factual data on data repositories (ideally CC 0)
- For software use licences specifically designed for software:
- Free Software (Open Source) licences like GPL, Apache, BSD and MIT.
- Exceptions! If you collaborated with external partners in your research project, you need to clarify together with them how and if data can be published.
- Contact the legal teams at your research institute if you feel lost.





### **Share & Disseminate**

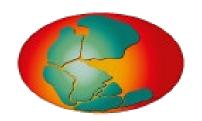


#### **Share & Disseminate: The Choice of Data Repository**

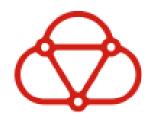














For alternatives: <a href="https://www.re3data.org/">https://www.re3data.org/</a>

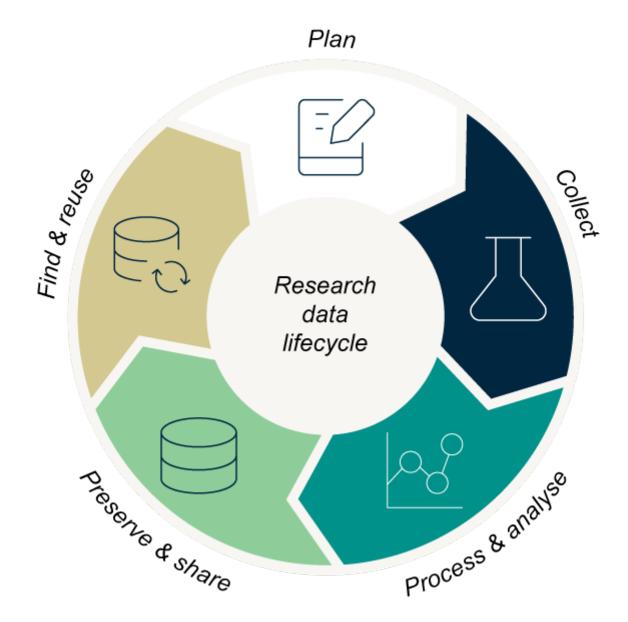


# RDM Services and Support at Eawag and Empa



# Plan & Design: Data Management Plan (DMP)





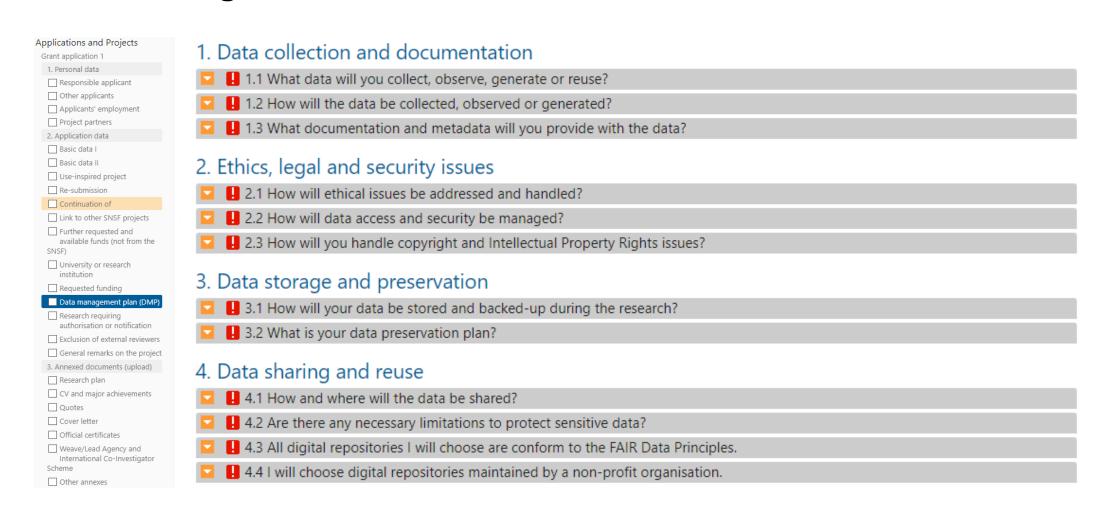
## **DMP**

## Covers the whole Research Data Life Cycle



- What types of data will be collected and which code (incl. software) will be created or used?
- How will you document the data used and code programmed?
- Where will data and code be stored?
- Who owns the data and code is responsible for security and backup?
- Which data and code will be shared and preserved?
- How will data be shared and with whom?









- Keep it short and simple
- Be stingy with words
- Have one idea per sentence
- Use the active form
- Use positive phrases
- Use concrete terms

«we used the method» not «the method was used»
«the results are different» not «the results are not the same»
«it will be published in Nature» not «it will be published in a reputable journal»



- Don't write in «sophisticated style»
- Save on adjectives and adverbs
- Avoid unnecessary constructions
- Don't nominalise
- Don't use empty modifiers
- Don't use tautologous modifiers

- e.g. «It is clear that», «the fact is that», «in an attempt to», «in order to»
  - «reduce» not «achieve a reduction in length»
- e.g. «basically», «indeed», «quite», «actually»
- e.g. «completely finish», «may potentially», «ultimate result», «blue in colour»



- 1. Organize yourselves in groups of two (5 minutes)
- 2. Each group will engage with the first section of the SNSF DMP (20 minutes)
  - Read requirements
  - Write answers and questions
  - Discuss with other group members
  - Designate presenter
- 3. Presentation and discussion of findings (20 minutes)



## Plan & Design: DMP - Data Collection and Documentation

## 1.1 What data will you collect, observe, generate or reuse?

Type, format (NEAD), content, volume of data, reference to data (if reused)

## 1.2 How will the data be collected, observed, generated?

- Standards methodology, quality assurance
- File organisation and versioning (folder structures, git, ELN/LIMS, etc.)

## 1.3 What documentation and metadata will you provide?

- Scientific Metadata (README, metadata standards)
- General Metadata (Depending on choice of data repository)



## Plan & Design: DMP - Ethics, Legal and security issues

#### 2.1 How will ethical issues be addressed and handled?

- Information and consent to using personal data, location of critical infrastructure ase well as rare and protected species
- Requirements for assessments by ethical review boards, premission by third parties
- Description of Pseudonymisation or Anonymisation Methods

#### 2.2 How will the data access and security be managed?

- Distinguish datasets according to the level of risk (cf. §2.1) and use an adverb to describe the level
  of risk («high», «medium», «low»)
- State Storage Location, secure transmission, access restruction, IT infrastructure

#### 2.3 How will you handle copyright and Intellectual Property Rights Issues?

- Consider non-dislosure agreements, potential patents, research collaborations accross institutions
- Recommendation to use CC0 where possible



## Plan & Design: DMP - Data Storage and Preservation

## 3.1 How will your data be stored and backed-up during the research?

 Backup strategy for work at all stages of research (amount of storage needed, frequency of updates, responsibilities, security measures)

## 3.2 What is your data preservation plan?

- Data formats
- Selection mode for data to be preserved (all relevant data related to reported results, long term preservation of unique datasets)



## Plan & Design: DMP - Data Sharing and Reuse

#### 4.1 How and where will the data be shared?

- Repository of choice (non-commercial preferred and required for contribution of up to 10'000 CHF for storage)
- Metadata Policy of said repository

#### 4.2 Are there necessary limitations to protect sensitive data?

Reasons data cannot be published at certain times (Section §2.1)

#### 4.3 All Digital Repositories I will choose conform to FAIR Data?

Check box

#### 4.4 All Digital Repository I will choos are maintained by a non-profit oranisation?

If no, provide justification (costs will not be covered)



## Thank you for your attention!

Feedback!

Please give us a short feedback

**Questions?** 

Presentation slides: lib4ri.ch > Learn

> Trainings



## **Appendix**



## **Appendix: Eawag**

- Four links under data.eawag.ch:
  - https://opendata.eawag.ch/eawagrdm/help/quickstart.html
  - https://opendata.eawag.ch/eawagrdm/help/opendata.html
  - https://doi.org/10.25678/000066
  - https://www.internal.eawag.ch/fileadmin/intranet/informatik/datenman/rdm/directive\_archiving\_o
     f researchdata.pdf
- Difference between ERIC/internal (data.eawag.ch) and ERIC/open (opendata.eawag.ch)
- Services are in the form of guides and consulting. Most notable guides in addition to the one mentioned above are
  - https://doi.org/10.25678/000033
  - https://opendata.eawag.ch/eawagrdm/software-licensing.html
- Finally the list of resources can be helpful:
  - https://opendata.eawag.ch/eawagrdm/resources.html



## **Appendix: Empa**

• General overview of topics:

https://www.empa.ch/web/s909/overview

•Support topics like DMP template of Empa:

https://www.empa.ch/web/s909/support1

## **OpenBIS**

- oGeneral overview: <a href="https://www.empa.ch/group/s909/openbis">https://www.empa.ch/group/s909/openbis</a>
- Documentation & trainings info:

https://www.empa.ch/group/s909/documentation-tutorials



## **Appendix: File Formats EPFL**

Bibliothèque de l'EPFL, Research Data, fast guide #4», 2019, https://bit.ly/3NFloYx

TYPE OF DATA	APPROPRIATE	ACCEPTABLE	DEPRECATED
Tabular (extensive metadata)	CSV — HDF5	TXT — HTML — TEX — FASTQ <sup>[3]</sup> — POR	
Tabular (minimal metadata)	CSV — TAB — ODS — SQL — TSV	XML (if appropriate DTD) – XLSX	XLS — XLSB
Textual / Presentation	$TXT - PDF - ODT - ODM - TEX - MD - HTM - XML - EXTXYZ^{[4]} - ODF$	PPTX — RTF — DOCX — PDF (with embedded forms) — EPS — IPF	DOC — PPT — DVI — PS
Code / Computation	M — R — PY — IYPNB — RSTUDIO — RMD — NETCDF — AIML	SDD	MAT — RDATA
Image & Spectroscopy	TIF — PNG — SVG — JPEG — FITS	JCAMP — JPG — JP2 — TIF — TIFF — PDF — GIF — BMP — DM3 — OIR — LSM <sup>[5]</sup>	INDD — AIT — PSD — SPC
Audio	FLAC — WAV — OGG — MXL — MIDI — MEI — HUMDRUM	MP3 – AIF	
Video	MP4 – MJ2 – AVI – MKV	OGM — MP4 — WEBM	WMV — MOV — QT
Geospatial	NETCDF – tabular GIS attribute data – SHP – SHX – DBF – PRJ – SBX – SBN – POSTGIS – TIF – TFW – GEOJSON	MDB — MIF	
3D structures & images	X3D – X3DV – X3DB – PDF3D – POV – PDBML	DWG — DXF — PDB	PXP
Generic	XML - JSON - RDF		



## **Appendix: File Formats ETH Zürich**

ETH-Library, File formats for archiving, 2022,

https://bit.ly/3DBqXmb

#### Assessment of various file formats

Table 1: Our assessment of future readability of some common file formats. (For more detailed information we refer to the recommendations of the Bundesarchiy (German) the KOST (German or French) the Memoriay the Forschungsdatenzentrums Archäologie & Altertumsvissenschaften IANUS (Germany) the Library of Congress and the Harvard Library).

File type	Recommended	Suitable to only a limited extent	Not suitable for archiving
Text	PDF/A (*.pdf, preferred subtypes 2b and 2u) Plain Text (*.bxt, *.asc, *.c, *.h, *.cpp, *.m, *.py, *.r etc.) coded as ASCII, UTF-8, or UTF-16 using byte order mark  XIML (inclusive XSD/XSL/XHTML etc.; with included or accessible schema and character encode explicitly specified)	PDF (*,pdf) with embedded fonts Plain text (*,bxt, *asc, *x_c *h, *,cpp, *m, *,py, *r etc.) (ISO 8859-1 coded) Rich Text Format (*,rtf) HTML and XML (The ASCII text is readable over long term; try to avoid external links.) Not accepted for publication, OK for supplementary materials: Word *.docx Word *.docx PowerPoint *.pptx LaTEX_TRC (The ASCII text is readable over long term; open source software required for formatting and the resulting PDF should be included.) OpenDocument formats (*.odm, *.odt, *.odg, *.odc, *.odf)	Word *.doc     PowerPoint *.ppt
Spreadsheet or table	Comma- or tab delimited text files (*.csv)	Excel *x/sx (container format)     OpenDocument spreadsheets (*.ods)	Excel *.xls, *.xlsb (binary formats)
Raw data and workspace		ASCII Text is suitable for long-term use, but the data import may be time-consuming. S-Plus files (*sdd) may be saved as text files. Matlab *.mat files may be saved in HDF Format. Saving nontrivial ASCII Matlab *.mat files should be avoided because they are not readable with the Matlab load command (see table 2). Network Common Data Format or NetCDF (*.nc, *.cdf) Hierarchical Data Format (HDF5) (*.h5, *.he5)	Binary files such as the standard Matlab files *.mat or the R files *.RData
Raster image (bitmap)	TIFF (*tif) (uncompressed, preferentially TIFF 6.0, Part 1: baseline TIFF). TIFF is preferred as compared to PNG or JPEG2000. Portable Network Graphics (*png, uncompressed) JPEG2000 (*jp2, lossless compression) Digital-Negative-Format (*dng) to keep raw data of digital fotos in addition to an second copy in TIFF format	TIFF (*.tif) (compressed) GIF (*.gif) BMP (*.bmp) JPEG/JFIF (*.jpg) JPEG2000 (lossy compression) (*.jp2)	
Vector graphics	SVG without JavaScript binding (*.svg)		Graphics InDesign (*.indd), Illustrator (*.ait) Encapsulated Postscript (*.eps) Photoshop (*.psd)
CAD	AutoCAD Drawing (*.dwg)     Drawing Interchange Format, AutoCAD (*.dxf)     Extensible 3D, X3D (*x3d, *x3dv, *x3db)		
Audio	WAV (*.wav) (uncompressed, pulse-code modulated)	Advanced Audio Coding (*.mp4)     MP3 (*.mp3)	
Video <sup>1</sup>	FFV1 codec (version 3 or later) in Matroska container (*.mkv)	MPEG-2 (".mpg,".mpeg) MP4, which is also called MPEG-4 Part 14 (".mp4) QuickTime Movie (".mov) Audio Video Interieave (".avi) Motion JPEG 2000 (".mj2, ".mjp2)	Windows Media Video (*.wmv)

#### ootnotes

<sup>&</sup>lt;sup>2</sup> In the Version of Nov 21, 2018 of the current document, the format QuickTime Movie was downgraded from "Recommended" to "Suitable to only a limited extent". Apple discontinued the support of Windows QuickTime Player in the year 2016. Windows Media Player thus only supports file format versions 2.0, or earlier, of QuickTime Movie files.



<sup>1</sup> In addition to the file format (or container format), also the codec and the compression method are important. See Janus, Memoriay and KOST for further information,



## **Appendix: References (Slide 18)**

- <sup>1</sup> SPARC Europe, «The Open Data Citation Advantage», 2017, <a href="https://sparceurope.org/open-data-citation-advantage/">https://sparceurope.org/open-data-citation-advantage/</a>.
- <sup>2</sup> Digital Science, «The state of Open Data Report», 2019, https://digitalscience.figshare.com/articles/report/The State of Open Data Report 2019/9980783/2
- <sup>3</sup> European Commission and PwC, «Cost-Benefit analysis fro FAIR research Data», 2019. https://op.europa.eu/en/publication-detail/-/publication/d375368c-1a0a-11e9-8d04-01aa75ed71a1
- <sup>4</sup> Baker, M., "1,500 scientists lift the lid on reproducibility". *Nature* 533, 452–454 (2016). https://doi.org/10.1038/533452a





## **Appendix: Icon References**

#### Slide 4:

- Le Moign, Vincent, «Lab Scientist Icon», <a href="https://icon-icons.com/icon/lab-scientist/101049">https://icon-icons.com/icon/lab-scientist/101049</a>,
   free for commercial use.
- Flaticon, «Checkliste», <a href="https://www.flaticon.com/de/kostenloses-icon/checkliste\_2666469">https://www.flaticon.com/de/kostenloses-icon/checkliste\_2666469</a>, free for personal and commercial use.
- PLoS, «Open Access logo», <u>https://de.wikipedia.org/wiki/Datei:Open Access logo PLoS white.svg</u>, CC-0.
- «Databases and People», <a href="https://freesvg.org/databases-and-people">https://freesvg.org/databases-and-people</a>, <a href="https://freesvg.org/databases-and-people">CC-0</a>.

#### Slide 8

Felixmh, «Krischen-Früchte-Natur-Symbol», free commercial use.