

02.11.2023

# Research Data Management – The Basics

Cantini, Federico Felder, Fabian Iosifescu, Ionut



#### 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



**Ionut Iosifescu** 

- Software Engineer
- Technical coordinator and product owner of EnviDat



# 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)

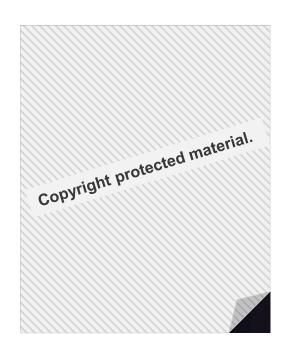


#### **Program**

Topic	Speaker	Time
Introduction	Fabian Felder	9.00 - 9.15
Policies, Incentives & the Research Data Life Cycle	Fabian Felder	9.15 - 9.30
Collect & Store	Federico Cantini	9.30 - 10.05
Evaluate & Archive Share & Disseminate	Fabian Felder	10.05 - 10.15
Break		10.20 - 10.30
RDM Services & Support at WSL	Ionut Iosifescu	10.30 - 11.00
Plan & Design	Everyone	11.00 - 11.45









«We kill people based on metadata» (2014), Michael V. Haden, director of CIA 2006-2009

Cham, J. G., «Scratch: A context-changing framework for contextualizing nano informatic structures» (2014), International Journal of Temporal Deflective Behaviour, 4 (1689), p. 432.



No clean metadata

=

Limited access to Data



Source: www.fosteropenscience.eu/project







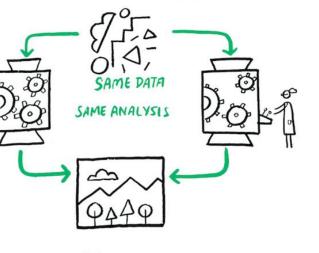
Proper metadata tagging and research description is time consuming



# Reproducibility

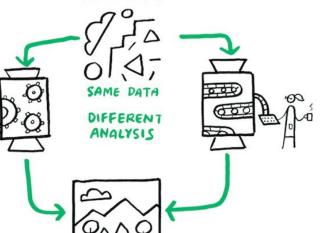


#### REPRODUCIBLE

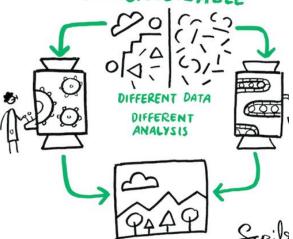


# PEPLICABLE DIFFERENT DATA SAME ANALYSIS PAPA

#### ROBUST



#### GENERALISABLE



#### Reproducibility

Scriberia, "Reproducible Research", *The Turing Way*, CC-BY, DOI:

10.5281/zenodo.3332807



A Handbook for Reproducible Data Science,

https://the-turingway.netlify.app/welcome.html



#### **LEGO®** Metadata for Reproducibility







**Group A builds Car** 

Group A documents build

Group B rebuilds the car

Donaldson, Mary and Matt Mahon, «Lego: Metadata for reproducibility», 10.5281/zenodo.3685685.



#### **LEGO® Metadata for Reproducibility**

What matters?

What will you need to record?

Is there a way to record it automatically?

Which structure do you use? Or do you rely on a narrative expression?

Which formats do you use?

How do you describe your materials?

Is there a standard?

Donaldson, Mary and Matt Mahon, «Lego: Metadata for reproducibility», 10.5281/zenodo.3685685.



#### FAIR principles – A lot of Metadata

Findable F1 (Meta)data are assigned a globally unique and persistent identifier

F2 Data are described with rich metadata

F3 Metadata clearly and explicitly includes the identifier

F4 (Meta)data are registered or indexed in a searchable resource

Accessible

A1 (Meta)data are retrievable by their identifier using a standardised communications protocol

A1.1 The protocol is open, free, and universally implementable

A1.2 The protocol allows for an authentication and authorisation procedure, when

necessary

A2. Metadata are accessible, even when the data are no longer available

nteroperale

I1 (Meta)data use formal, accessible, shared, and broadly applicable language for knowledge

representation

I2 (Meta)data use vocabularies that follow FAIR principles

13 (Meta)data include qualified references to other (meta)data

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

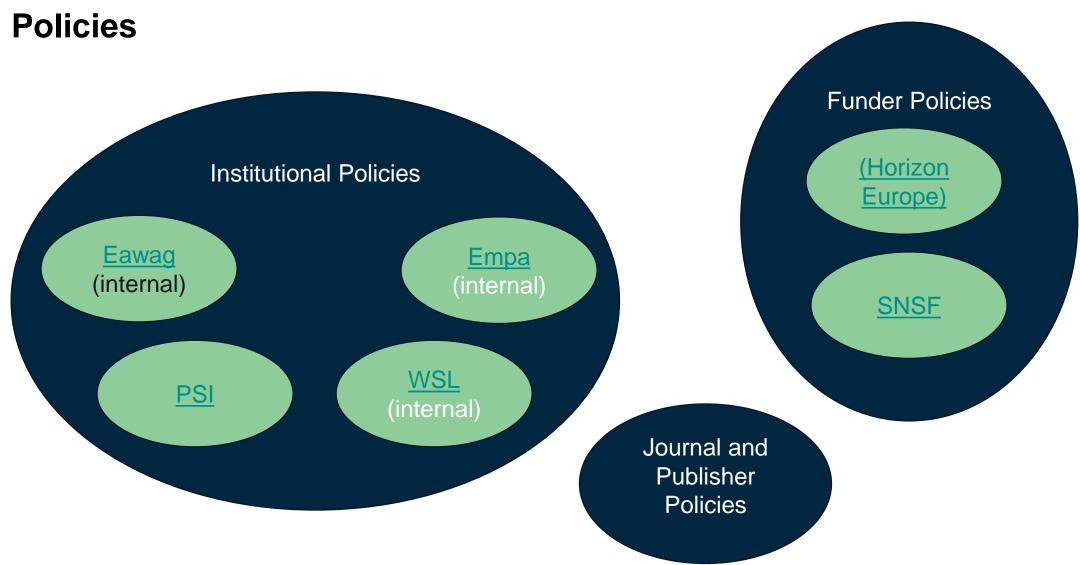
R1.2 (Meta)data are associated with a detailed provenance

R1.3 (Meta)data meet domain-relevant community standards



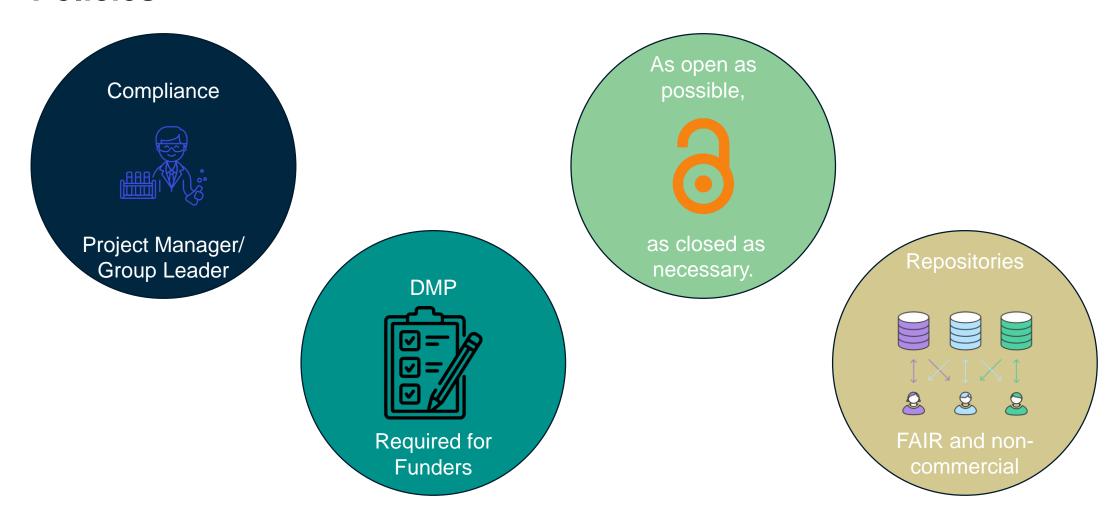
## **Policies**



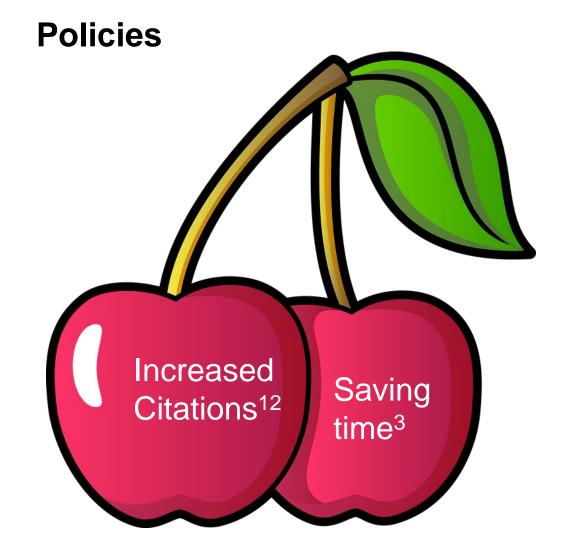


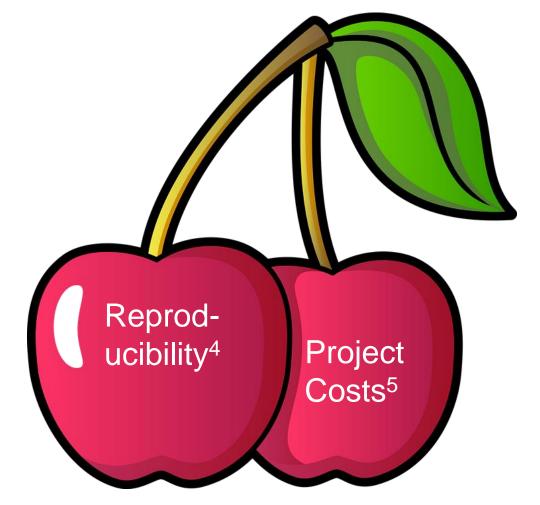


#### **Policies**





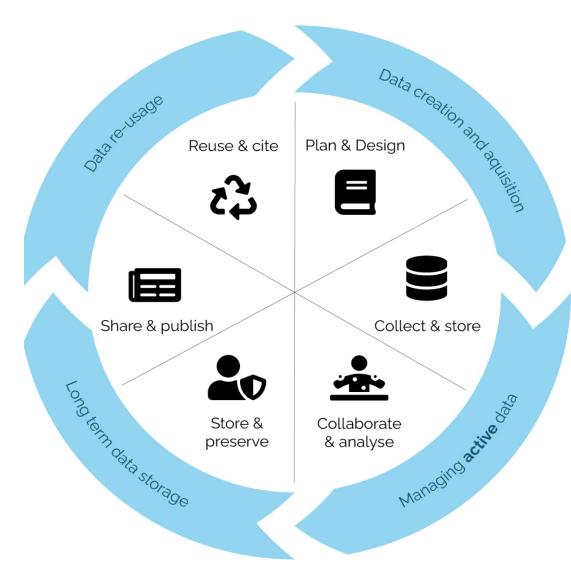






# Research Data Life Cycle





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



### **Collect & Store**

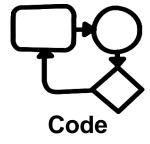


#### **Collect & Store**

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

#### Data

observational, experimental, simulation...



Applications, scripts...



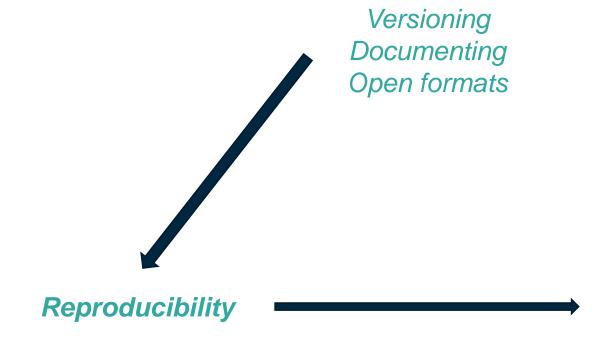
#### Metadata

Structured information associated with data (and code)

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



#### **Collect and Store**

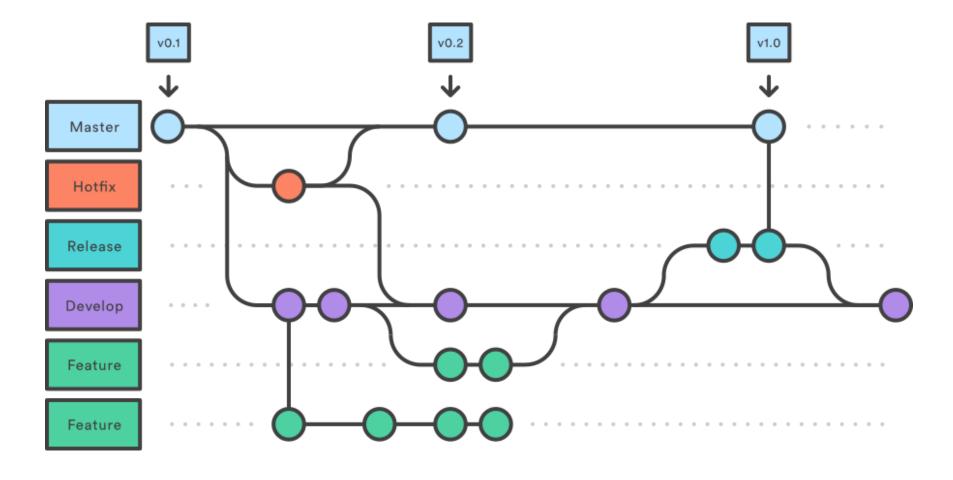


- o You can find it
- Your coworkers can find it
- You can easily share it
- o It's ready for archiving/publishing

Replicability

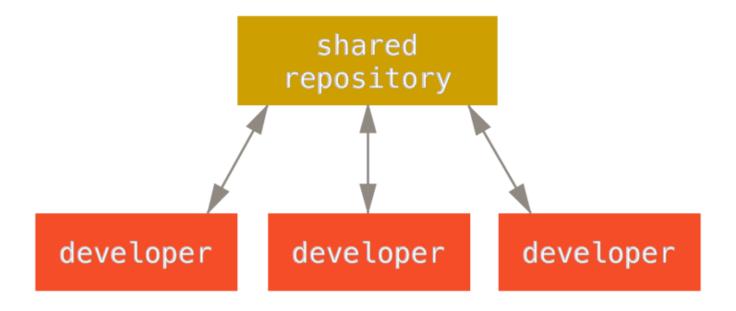


#### **Collect and Store: Software version control**





#### **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 rev. n



#### **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	• PDF/A
	Plain Text coded as ACII. UTF-8 or UTF-16
	• XML
Spreadsheet	CSV (NEAD)
Images	TIFF (uncompressed or lossless compressed)
	• PNG
Code	Languages with free environments (e.g. Py or R UTF-8 format of ASCII text)
Audio	• FLAC
	• Wav

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.
- 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)
- o 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

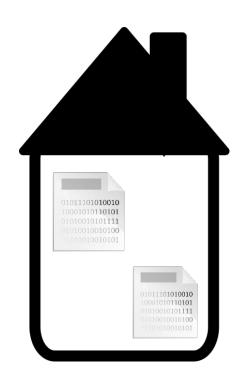
Data specific information (repeat for each dataset)

- 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: https://data.research.cornell.edu/content/readme



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







## **Evaluate & Archive**

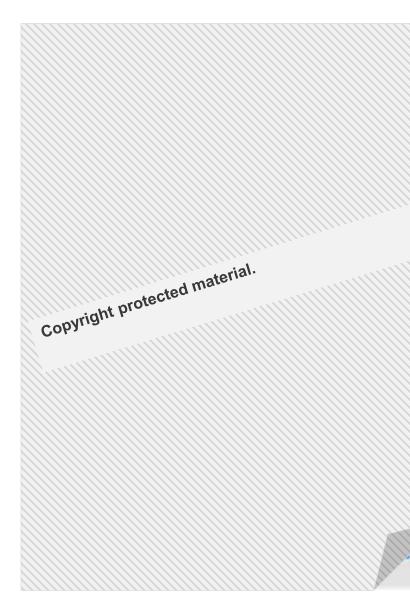


# **Evaluate & Archive: Data Protection**

- 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**















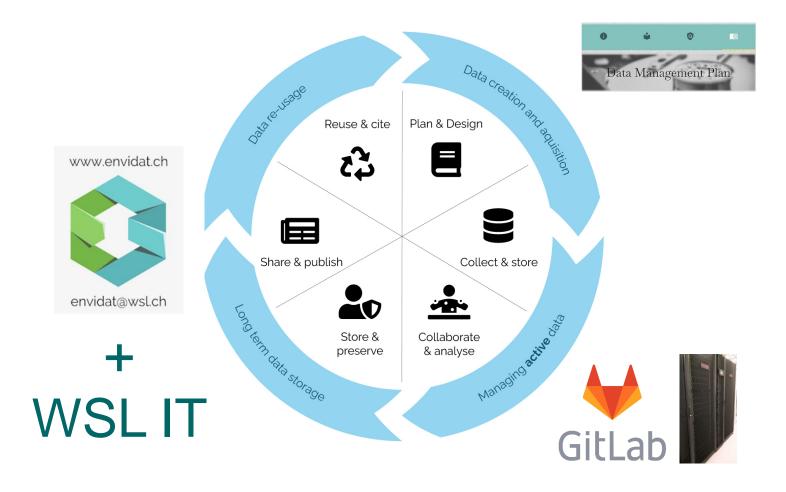
For alternatives: <a href="https://www.re3data.org/">https://www.re3data.org/</a>



# RDM Services and Support at WSL

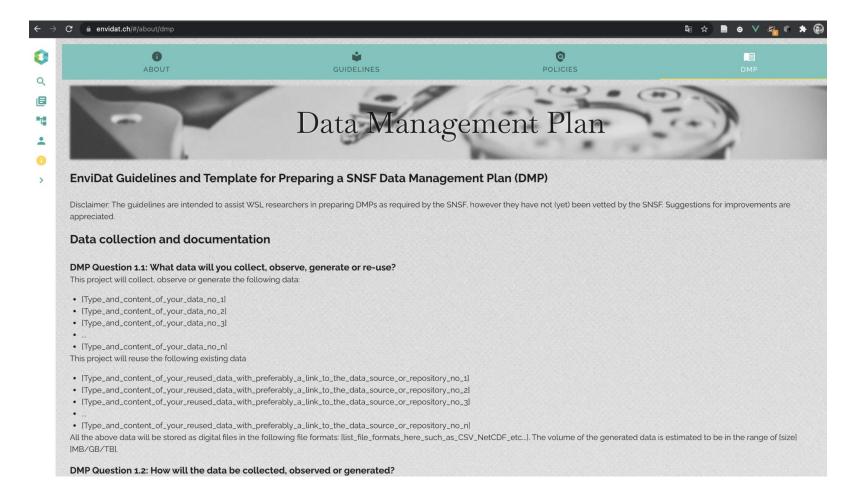


## **RDM Services and Support at WSL**



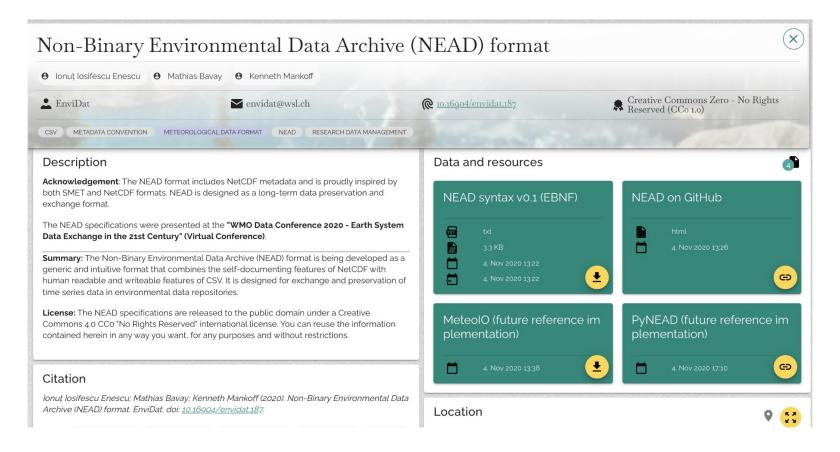


## **RDM Services and Support at WSL: DMP Template**





## **RDM Services and Support at WSL: NEAD Format**



https://www.doi.org/10.16904/envidat.187



## RDM Services and Support at WSL: GitLab

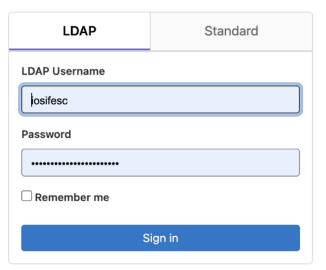


## Welcome to WSL/SLF GitLab repository!

You must sign up to use this GitLab instance. If you are new and not member of WSL/SLF please **register** first. Then contact the project leader to be approved.

LDAP login is only for WSL/SLF members. External users can sign in on the **Standard** tab.

For public GitLab projects please visit https://gitlabext.wsl.ch/public.

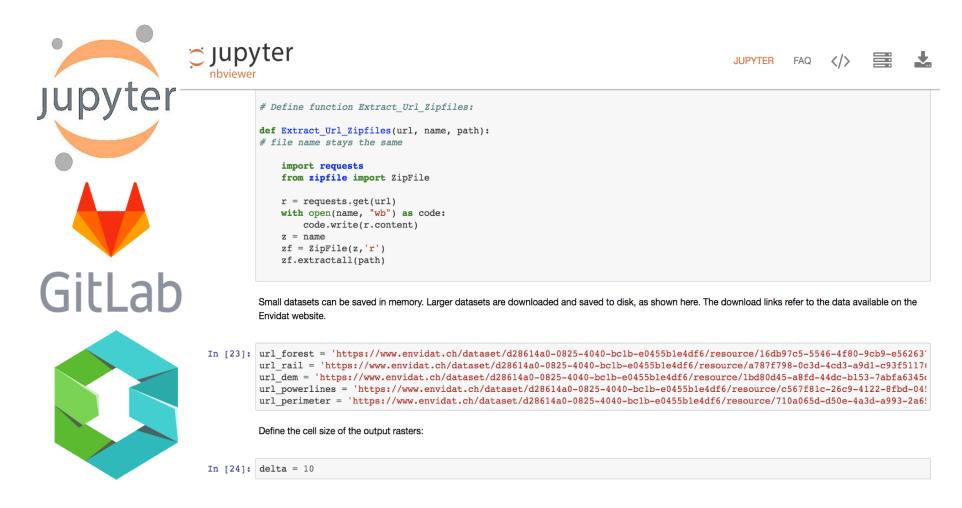


Don't have an account yet? Register now

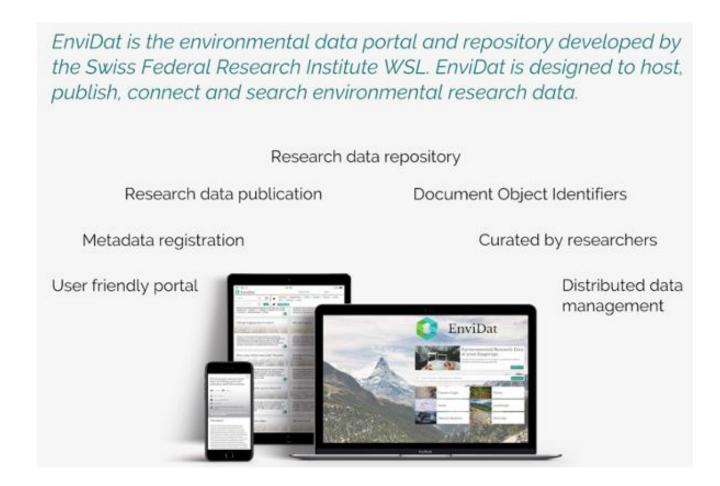




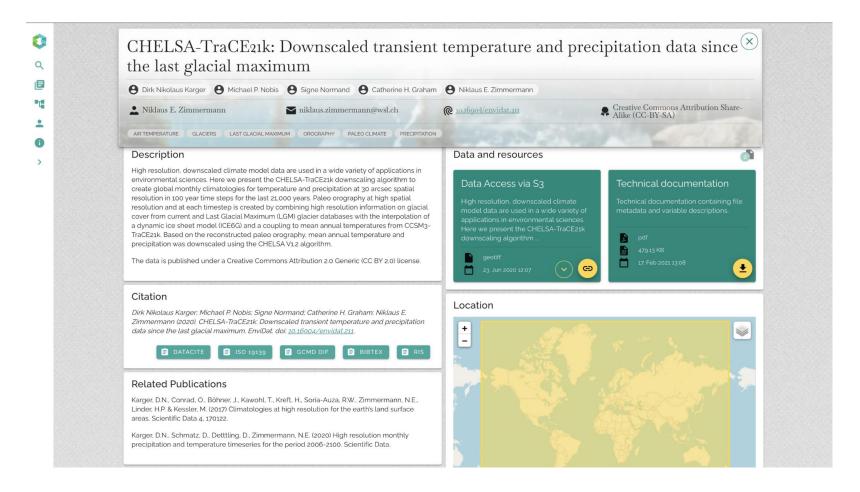
## **RDM Services and Support at WSL: Jupyter Notebooks**





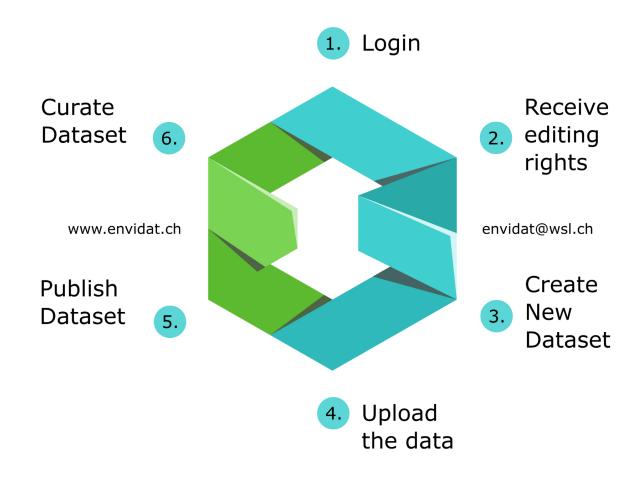




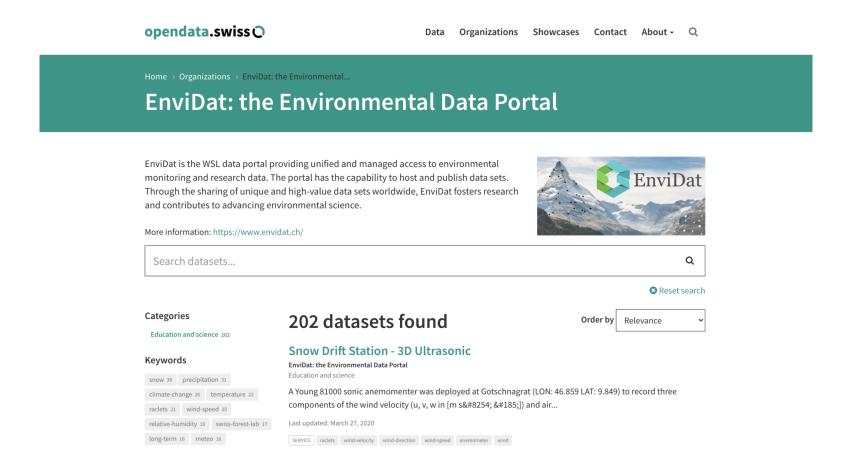


doi:10.16904/envidat.211







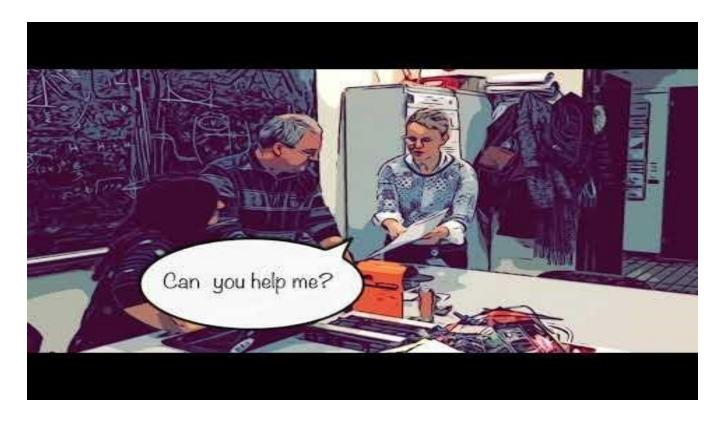




# Plan & Design: Data Management Plan (DMP)



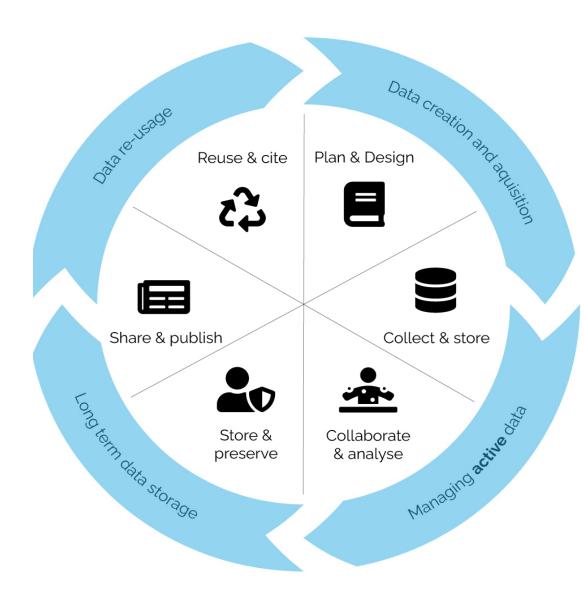
## Plan & Design: Why?



Bibliothèqe de l'EPFL, «RDM Horror stories | Episode 2 – Stranger Data Things», 11th February 2020.

https://bit.ly/3qPWMIS





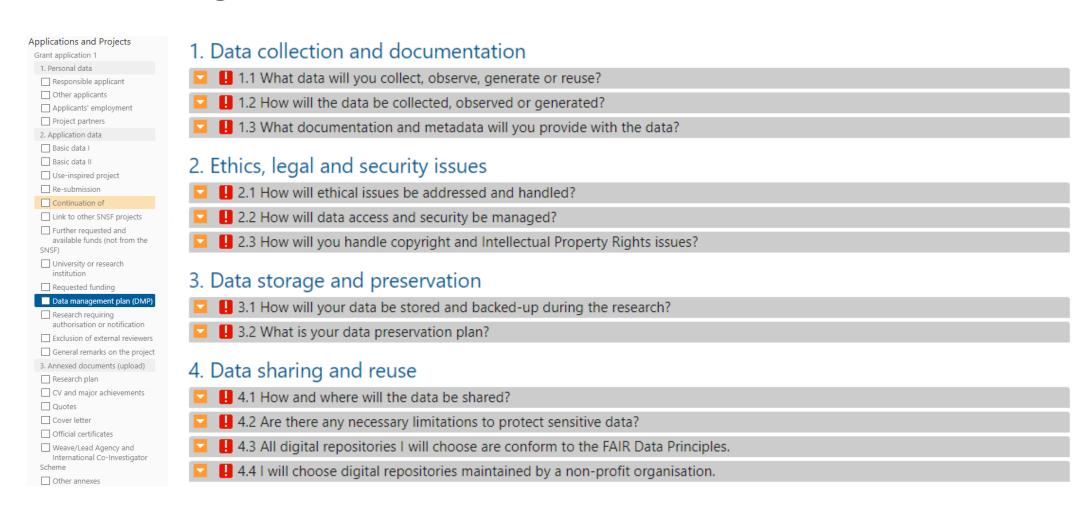
## **DMP**

# 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: WSL**

- RDM consulting services (contact <u>envidat@wsl.ch</u>)
- 2. DMP templates ( <a href="https://envidat.ch/#/dmp">https://envidat.ch/#/dmp</a> ) and consulting services (contact <a href="mailto:envidat@wsl.ch">envidat@wsl.ch</a> )
- 3. WSL/SLF GitLab repository: <a href="https://gitlabext.wsl.ch">https://gitlabext.wsl.ch</a> (allows collaboration with external partners)
- 4. WSL's Hyperion High-Performance Computing (HPC) Linux Cluster <a href="https://hyperion.wsl.ch/documentation-master/build/html/">https://hyperion.wsl.ch/documentation-master/build/html/</a> (only available inside the WSL Intranet!)
- 5. JupyterLab/JupyterHub interactive development environment to combine documentation, code and data <a href="https://hyperion.wsl.ch/documentation-master/build/html/">https://hyperion.wsl.ch/documentation-master/build/html/</a> (only available inside the WSL Intranet!)
- 6. Temporary data transfers to external partners for collaboration purposes:
- For data up to 300GBs SWITCHfilesender: <a href="https://filesender.switch.ch/">https://filesender.switch.ch/</a> (temporary for 10 days up to max. 60 days)
- For data above 300GBs and up to several TBs <a href="https://envicloud.wsl.ch/">https://envicloud.wsl.ch/</a> (contact <a href="envidat@wsl.ch">envidat@wsl.ch</a> temporary for max. 10 days)
- 7. EnviDat <a href="www.envidat.ch">www.envidat.ch</a> for final data publication with DOI assignment (datasets larger than 1 TB needs to be approved by the WSL directorate)



## **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 (*,bd, *,asc, *,c, *,h, *,cpp, *m, *,py, *r, etc.) coded as ASCII, UTF-8, or UTF-16 using byte order mark XML (inclusive XSD/XSL/XHTML etc.; with included or accessible schema and character encode explicitly specified)	PDF (*,pdf) with embedded fonts  Plain text (*,bxt, *asc, *ac, *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 *.doox  PowerPoint *,pptx  LaTeX_RC (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 *xisx (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 (".jpz. lossiess 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) BIMP (*.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) <sup>2</sup> Audio Video Interieave (*.avi) Motion JPEG 2000 (*.m)2, *.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»,
   <a href="https://de.wikipedia.org/wiki/Datei:Open\_Access\_logo\_PLoS\_white.svg">https://de.wikipedia.org/wiki/Datei:Open\_Access\_logo\_PLoS\_white.svg</a>, 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.