

Onboarding into Research Data Management

Training Course for Max Planck Early Career Researcher

Mainz, Max Planck Institute for Chemistry, 3th April 2024 https://hdl.handle.net/21.11116/0000-000E-194D-1 Michael Franke, <u>franke@mpdl.mpg.de</u> David Walter, <u>d.walter@mpdl.mpg.de</u> Dr. Yves Vincent Grossmann <u>grossmann@mpdl.mpg.de</u>



Introduction

Speakers

Michael Franke

- https://orcid.org/0000-0002-2661-8242
- Division Manager MPDL Collections
- 2011-2019: Alliance WG "Research Data"
- 2015-2018: Science Europe WG "Research Data"
- 2019-2023: Alliance WGs "Digital Tools" and "Federated IT Infrastructures"
- 2014-2020: RDM teaching position at HföD Bavaria
- franke@mpdl.mpg.de

David Walter

- https://orcid.org/0000-0001-6807-5007
- since 2024: Research Data Management Officer at the MPDL
- since 2021: Data management of S/Y Eugen Seibold, editor at PANGAEA
- 2014-2020: Greenhouse gas measurements and data management at ATTO
- 2013: PhD in Physics (DOAS technique onboard CARIBIC aircraft)
- <u>d.walter@mpdl.mpg.de</u>

Programme for Today

09:00-09:15	Welcome and introduction
09:15-09:30	Topic block 1: Digital research data
09:30-10:10	Topic block 2: Normative Frameworks
10:10-10:30	Topic block 3: Data management plans
10:30-10:50	Coffee break
10:50-11:15	Topic block 4: Order and Structure
11:15-11:45	Topic Block 5: Saving
11:45-12:00	Topic block 6: Access security

12:00-13:00	Lunch (self-pay basis) and photo
13:00-14:00	Topic block 7: MPG-internal services
14:00-14:20	Topic block 8: Metadata
14:20-15:15	Topic block 9: Publishing
15:15-15:45	Coffee break
15:45-16:05	Theme Block 10: Electronic Laboratory Notebook
16:05-16:25	Theme Block 11: New Horizons
16:25-16:30	Closing Remarks

Organisational Issues

- Questions:
 - Ask immediately
 - Ask after the thematic block
 - Ask in the break
 - Ask afterwards: <u>rdm@mpdl.mpg.de</u>
- Slides are available on MPG.PuRe



Objectives for Today

- 1. Develop basic understanding of Research Data Management
- 2. See that research data management is not rocket science (except in rocket science)
- 3. Insight into the various RDM topics
- 4. Exchange and clarify questions
- 5. Suggestions and communication of new topics



Questions to You via Slido

Join via slido.com and enter 1174667

- 1. How would you rate your level of experience in working with research data?
- 2. What do you expect from this course?

Digital Research Data

- Research Data Management
- Definition of research data
- Research data lifecycles
- Examples

Worum geht es?



What is Research Data Management?

Explicit handling of research data before, during and after the project



Why Research Data Management?

You **should** think about it, because:

- Re-use data, at least oneself, but also by others
- Scientific reputation increasing
- Acceptance of data as a separate publication is likely to increase in the future
- Because "fits somehow" has never won a Nobel Prize

•

Why Thinking about RDM?

- Time and resource savings through early RDM
 - Potential problems are identified earlier
 - Save time by organising so that less time is spent searching
- Easier project management for participating scientists
 - Less communication effort
- Reduction of project complexity through structured procedure
 - Easier processing for the oneself

Why Research Data Management?

You have to think about it, because:

- MPG Good Scientific Practice
- DFG Code of Conduct
- Funding Agencies, i.e. by DFG and Horizon Europe, ERC, Volkswagen Foundation
- Publishers

■ ...

Example RDM Tasks

- 1. Planning the handling of research data at the beginning of a research project and, if necessary, presenting the planned measures in funding applications
- 2. Defining a folder structure and file naming conventions
- 3. Documentation of research data and labelling with metadata
- 4. Backup and long-term archiving of research data
- 5. IT security and access rights for research data
- 6. Publication of research data
- 7. Finding and reusing existing research data
- 8. Consideration of data protection and copyright law when handling research data

Definition Attempts Data

"Research data include measurement data, laboratory values, audiovisual information, texts, survey data or observational data, methodological test procedures and questionnaires." DFG Checklist, 21st December 2021, p. 1, https://www.dfg.de/download/pdf/foerderung/grundlagen_dfg_foerderung/forschungsdaten/forschungsdaten_checkliste_en.pdf

Research data are "data generated in the course of scientific projects, e.g. through digitisation, source research, experiments, measurements, surveys or interviews." Allianz AG "Forschungsdaten", Forschungsdatenmanagement – Eine Handreichung, 2018, p. 4, <u>https://gfzpublic.gfz-potsdam.de/rest/items/item_3055893_5/component/file_3055894/content</u>

"Research data comprise all data generated in the scientific work process and processed in digital form."

Guideline on handling research data in the Leibniz Association, 2018, p. 1, <u>https://www.leibniz-gemeinschaft.de/fileadmin/user_upload/Bilder_und_Downloads/Forschung/Open_Science/Leitlinie_Forschungsdaten_2018.pdf</u>



* which only very schematically presents the handling of research data...



Short Audio Quiz

What is hidden behind this audio file of a research dataset?



Resolution: Cecilia Durojaye, 2020, "Recodings - Nigerian Talking drum", file D1s, Edmond, <u>https://doi.org/10.17617/3.IUMMLP</u>, CC BY 4.0.

Short Video Quiz



What is hidden behind this video file of a research dataset?

Chiavassa, R. Kudritzki, B. Davies, B. Freytag, & S. E. de Mink. (2022, March 16): Photo-center displacements for RSGs as seen by Gaia (Version v1), Max Planck Institute for Astrophysics, CC BY 4.0, Zenodo, https://doi.org/10.5281/zenodo.63630 11. Paper: https://www.aanda.org/articles/

aa/pdf/2022/05/aa43568-22.pdf

Short Video Quiz



What is hidden behind this video file of a research dataset?

Kaumudi Prabhakara (Max Planck Institute for Dynamics and Self-Organization), Spiralwaves, 2015, CC BY 4.0, https://www.youtube.com/watch?v=D mRZn073Uus.

Short Image Quiz



What is hidden behind this image file of a research dataset?

Prelic, Sinisa, 2021, "Functional interaction between Drosophila olfactory sensory neurons and their support cells", Max Planck Institute for Chemical Ecology, <u>https://doi.org/10.17617/3.7m</u>, Edmond, V1, CC BY 4.0, 20191021 image 4 ASE5-Gal4 GFP.tif.

Normative Frames

- What is an RD policy?
- New MPG-GWP rules
- Possible institutional policies
- Subject-specific policies
- Perspectives of the funders
- Perspectives of the publishers

What is a Research Data Policy?

A research data policy describes the guidelines for handling data.

There are different types of policies, for example:

- Journal and publisher policies
- Institutional policies
- Project-specific policies
- Subject-specific policies
- Policies of research funders



https://www.forschungsdaten.org/index.php/Data_Policies, CC BY 4.0

Normative Requirements

- Standard for "Good Scientific Practice" by institutions
- Research data policies of institutions
- Requirements of funding institutions
- Request from publishers





MPG "Good Scientific Practice"

"2.4 Securing and storing primary data – Documentation and archiving

[..] The Institute Management is <u>expected to provide</u> the usual storage media for the field concerned and to guarantee that information stored both digitally and in analogue format is secured and remains accessible. The framework conditions must be such that protection from unauthorized access, loss, destruction, theft, and manipulation can be guaranteed. [..]

Research Group Leaders and individual researchers are <u>obligated</u> to make use of the protection options provided by Institute Management and retain and store both research data and research results. It does not matter in this context whether the research results are published or not."

(<u>https://www.mpg.de/197494/rulesScientificPractice.pdf</u>, p. 41)

MPG "Good Scientific Practice"

"2.4 Securing and storing primary data – Documentation and archiving

[..] Cooperative research also requires continuous, long-term availability of research data. For this, corresponding research data management specific to the discipline must also be ensured. All Research Group Leaders involved bear joint <u>responsibility</u> for this."

(<u>https://www.mpg.de/197494/rulesScientificPractice.pdf</u>, p. 41)

"2.7 Accessibility of research data

For reasons of traceability, follow-on research and potential later use, scientists store the research data and central materials on which the publication is based <u>whenever possible</u> – <u>following the FAIR principles</u> (see I. 2.5 Publications – Authorships) – e.g. in accessible, commonly recognized archives and repositories."

(<u>https://www.mpg.de/197494/rulesScientificPractice.pdf</u>, p. 45)

FAIR Data Principles

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 they describe
- F4. (Meta)data are registered or indexed in a searchable resource

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

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

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

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

Data Culture in the Own Research Field

- Comparatively difficult to catch → more tacit knowledge
- Common understanding about "data"
- Community specific file formats
 - E.g. <u>NeXus</u> for neutron, X-ray and muon research (HDF5 format with specified metadata information)
- Established venues for data publication
 - e.g. subject-specific repository

DFG's Code of Conduct "Safeguarding Good Research Practice"

Guideline 13: Providing public access to research results

"[..] If it has been decided to make results available in the public domain, **researchers describe them clearly and in full**. Where possible and reasonable, this includes making the research data, materials and information on which the results are based, as well as the methods and software used, available and fully explaining the work processes. [..]" (<u>https://doi.org/10.5281/zenodo.3923601</u>, p. 17)

Guideline 17: Archiving

"When scientific and academic findings are made publicly available, the research data (generally raw data) on which they are based are generally archived in **an accessible and identifiable manner for a period of ten years at the institution** where the data were produced or in cross-location repositories." (<u>https://doi.org/10.5281/zenodo.3923601</u>, p. 20)

Deutsche Forschungsgemeinschaft (DFG)

"For this reason, the DFG expects research projects to include a description of how research data is handled. The description should be based on the checklist for handling research data (to the questionnaire)."

- "The recommendation is that contact should be established as early as possible during the project planning phase with a research data centre or repository where the research data can be deposited".
- "The description of how research data will be handled is included in the review and also forms part of the reporting obligation after completion of the project."

www.dfg.de/proposal_process/research_data



European Commission

ERC Work Programme 2021:

"Finally, as from 2021 it is no longer possible for applicants to opt out of the submission of Research Data Management plans." (European Commission Decision C(2021) 930 of 22/02/2021, p. 4)

Marie Skłodowska-Curie Actions:

"[..] data management plan submitted at mid-term and an update towards the end of the project if needed" (European Commission Decision C(2022)7550 of 6 December 2022, p. 88)

RDM as Career Development Activities

3. Career Development Activities

In line with the <u>European Charter for Researchers</u>, the MSCA put special emphasis on skills development and improving the career prospects of researchers.

Therefore you may undertake professional training and development activities during your fellowship, such as:

- Complementary training in transferable skills such as proposal writing, research management, open science, FAIR² data management, intellectual property rights, patent submission, innovation and entrepreneurship, communication, etc.
- Attendance of conferences and workshops to boost your competences and networking capacity
- Outreach and/or citizen engagement activities
- Teaching
- Language courses

Horizon Europe

"The beneficiaries must manage the digital research data generated in the action ('data') responsibly, in line with the FAIR principles and by taking all of the following actions:

- establish a data management plan ('DMP') (and regularly update it)
- as soon as possible and within the deadlines set out in the DMP, deposit the data in a trusted repository [...].
- as soon as possible and within the deadlines set out in the DMP, ensure open access - via the repository - to the deposited data [plus CC0, CC BY or equivalent]".

Horizon Europe and Euratom: General Model Grant Agreement, Version 1.0, 1st June 2021, p. 109, https://ec.europa.eu/info/funding-tenders/opportunities/docs/2021-2027/common/agr-contr/generalmga_horizon-euratom_en.pdf

Volkswagen Foundation

- Open Science Policy since 2021
 - "The Volkswagen Foundation encourages researchers to store the data generated within funded projects in public, noncommercial repositories [..]" (p. 4)
 - "In the application process, data generating and data using projects working in disciplines lacking a clear data workflow are asked to upload a digital concept with a <u>data</u> <u>management plan</u>". (pp. 4-5)
 - "In the application process, the applicants are asked to mark separately the <u>already generated Open Data</u> in the CV for the review and decision process." (p. 5)
- Funding opportunity: "Data Reuse Additional Funding for the Preparation and Storage of Research Data (Open Science)"



Schon 2003 hat die VolkswagenStiftung die "Berlin Declaration on Open Access to Knowledge in the Sciences in the Humanities⁻¹ unterschrieben. Der kurze Text formuliert eine, vision of a global and accessible representation of knowledge", die mit Hilfe des Internet als neuem Kommunikationsmedium in den Wissenschaften umgesetzt werden könne. Zwei Jahrzehnte später ist Open Access eingebettet in ein Gesamktonzept Open Science, das der digitalen Revolution mit der Wechselwirkung von immer effizienteren Speichermedien, immer größeren Datenmengen und immer wirkmächtigeren Softwareprogrammen in allen Bereichen der Wissenschaft Rechnung trägt und gleichzeitig die Forderung formuliert, dass Wissen als Gemeingut der Menschheit zur Verfügung stehen sollte. Innerhalb der Wissenschaft ist Open Science wiederum die Voraussetzung für die Reproduzierbarkeit von wissenschaftlichen Ergebnissen, die ihrerseits ein Grundpfeller für die Vertrauenswürdigkeit von Forschung, letztlich Voraussetzung für Wissenschaft an und für sich, ist.

Die VolkswagenStiftung verfolgt in ihrer im November 2021 verabschiedeten Policy das Ziel, das Konzept von Open Sciene positiv fördernd zu unterstützen. Die Stiftung sicht sich hier an der Setle "ihrer Wissenschafterinnen im laterforden sehr dynamischen Transformationsprozess der datenintensiven Wissenschaft. Sie wird ihre Position auch sukzessive anpassen, denn bei einer Vielzahl von technischen, rechtlichen, institutionellen wie auch politischen Rahmenbedingungen von Open Science steht noch eine Klärung aus.

OPEN SCIENCE

Die VolkswagenStiftung unterstützt das Konzept von Open Solence in ihrem Förderhandeln. Sie legt dabei die Begriffsdefinition der UNESCO zugrunde: Open Solence wird definiert als inclusive construct that combines various movements and practices aiming to make multilingual solentific knowledge openly available, accessible and reusable for everyone, to increase solentific collaborations and sharing of information for the benefits of science and society, and to open the processes of scientific knowledge creation, evaluation and communication to societal actors beyond the traditional scientific community.¹² Den Umfang des Gesamtkonzepts macht die Open Science Taxonomy deutlich:

¹¹ https://openaccess.mpg.de/Berliner-Erklaerung [25.2.2022]
² UNESCO Recommendation on Open Science 11/2021.
(https://unesdoc.unesco.org/ark/48223/pf0000379949.locale=en) [25.2.2022]

Questions to You via Slido

Join via slido.com and enter 1174667

- 1. Have you already received an RDM training?
- 2. Are you currently writing an application with data reference?

20 minutes Coffee Break
Data Management Plans

- What is a DMP
- DMP components
- Tools and templates
- DMP examples

Data Management Plan (DMP)

- A DMP structures the handling of research data in a scientific project.
- It describes how to deal with the data used during and after the project.

The DMPs usually cover the following aspects:

- 1. Description and collection of data
- 2. Documentation and metadata
- 3. Storage and backup
- 4. Legal and ethical requirements
- 5. Data sharing and long-term storage
- 6. Responsibilities and resources

Why a DMP?

- Increasingly required by funding organisations (e.g. Horizon Europe)
- Costs for data management (software, hardware, technical expertise) are often eligible for funding
- Making your own handling of research data explicit
- Own project management
- Quality management



Write a DMP

How Do You Write a DMP?

- 1. Brainstorm yourself
- 2. Use a template
- 3. Use digital tools

Tools to Write DMPs

- Argos (https://argos.openaire.eu)
- Data Stewardship Wizard (<u>https://ds-wizard.org</u>)
- DMPTool (<u>https://dmptool.org</u>)
- DMPOnline
 <u>(https://dmponline.dcc.ac.uk)</u>
- RDMO (<u>https://rdmo.mpdl.mpg.de</u>)

Use existing DMPs

Templates for DMPs:

- Horizon Europe DMP Template by the European Commission, 2021
- Horizon 2020 DMP Template by the European Commission, 2018
- ERC Grants DMP Template by the European Research Council, 2021
- <u>DMP Template by the Swiss</u>
 <u>National Science Foundation, 2017</u>

Examples of Published DMPs:

- <u>Digital Curation Centre Example</u>
 <u>DMPs and Guidance</u>
- LIBER Europe DMP Catalogue
- Examples for Horizon 2020 DMPs by the University of Vienna

Get Feedback on DMP

- Ask your own supervisors and colleagues
- Ask science support staff at your own institute
 - e.g. IT regarding storage, library regarding publication and metadata, etc.
- Use centralised DMP service within the MPG
 - e.g. RDM Support by MPDL for cross-checking DMPs



Questions to You via Slido

Join via slido.com and enter 1174667

- 1. Have you already written an DMP?
- 2. If so, for which foundation or funding programm?

Order and Structure

- Directory structures
- File naming
- Version control
- File formats

File Naming – Good Practice

- Include relevant information in file names. This may include project, investigator (initials), experiment, location, date, parameter, status of data (raw, processed etc.), file version, or anything else.
- Use YYYY-MM-DD for dates (e.g. 2016-08-02) like ISO 8601 and put date at the beginning or end of file names, both to facilitate chronological sorting.
- Use leading zeros for other numbers as needed (001, 002, 011, 114 rather than 1, 2, 11, 114) depending on the expected amount of files, and also to allow files to be properly sorted.
- Use **dashes** (file-name.xxx) or **underscores** (file_name.xxx) to separate parts of a filename.
- Generate a README file explaining file nomenclature (including the meaning of acronyms or abbreviations), file organization and versioning. Store this file on top of a folder structure for easy access.
- Good example: 20140618_exp08_co2data_raw_v01.csv

File Naming – Avoid

- Using special characters such as ~!/\@#\$%^&*()`;<>?,[]{}'"| as they may have specific meanings in certain operating environments. Also avoid ä ö ü ß å ø ñ or similar.
- Using dots other than before the file extension.
- Using spaces in file names they might end up being truncated during file transfer (with the file extension also lost and files potentially becoming unreadable).
- Making file names overly long (a maximum of 32 characters is suggested) this may involve compromises regarding the recommendation above.
 - In Windows 255 characters is the maximum for a file name (without being in a folder)

File Naming – Examples

Untitles 138.00CX
Untitled 241.doc
Untitled 138 copy docx
Hatitled 139 car 7 days
Untilled 100 COPY 2.00CX
Untitled 139. docx
Untitled 40 MOM ADDRESS, Jpg
Untitled 242 day
Untitled 212.000
Untitled 243.00C
Untitled 243 IMPORTANT. Joc
Llotitlah 41; man
42
GT OH MY GOD.
H)
- O'
2 2 20 1

PROTIP: NEVER LOOK IN SOMEONE. ELSE'S DOCUMENTS FOLDER. xkcd. "Documents.", https://xkcd.com/1459/, CC-BY-NC 2.5.

To prefer	To avoid
website-texts-2020-05- v15.docx	Website-Texts-May- finalFinal2_new.docx
Digitized_XY-ZZ_E-2_HT- 493887.tiff	Image0001.tiff
Digitized_XY-ZZ_M-5_LS- 345-c.tiff	Image0002.tiff
Digitized_XY-ZZ_E-1_M- 296778.tiff	Image0003.tiff
Survey_OpenAccess_Clean ed_v04.csv	OA-Results-clean-4.csv

File Organization Structure

- Before you start collecting files or data, you should definitely define a convention to avoid a backlog of unorganised content.
- In general, for the **naming** of folders, the same rules apply as for files.
- Depending on the structure of your data and documentation, you have to decide on how to arrange your files and folders.
- This may also require judgment and compromises: a very deep folder structure (subsubsubsubsubfolders) can be as inconvenient as one folder with 100 or more individual files.
- In case different project members should have various access restrictions to files, this could be represented by your folder structure.

Example Directory Structures

Project Folder	Project1. Project ManagementFolder	 Proposals Finance Reports
	2. Ethics and Governance	 Ethical Approvals Consent Forms
	3. Experiment 01	1. Inputs
		3. Data Analysis
		4. Outputs
	4. Dissemination	1. Presentations
		2. Publications
		3. Publicity

After Suse Prejawa (2021). I think I have really good data ... except I cannot find it anywhere: Organising research data in a structured way. Talk presented at Human Research Data in Practice, Virtual Workshop. 2021-04-20, <u>https://hdl.handle.net/21.11116/0000-0008-662A-7</u>.

Example Directory Structures

Organized by File type

DatasetA.tar.gz

| - Data/

- |- Processed/
- |- Raw/
- |- Results/
 - |- Figure1.tif |- Figure2.tif
 - |- Models/

Organized by Analysis



Example from https://datadryad.org/stash/best_practices#organize

Example README Template

Title of Dataset

[Access this dataset on XYZ] (Dataset DOI link)

Give a brief summary of dataset contents, contextualized in experimental procedures and results.

Description of the data and file structure

This is a freeform section for you to describe how the data are structured and how a potential consumer might use them. Be as descriptive as necessary. Keep in mind that users of your data might be new to the field and unfamiliar with common terminology, metrics, etc.

Describe relationships between data files, missing data codes, other abbreviations used. Be as descriptive as possible.

Sharing/Access information

This is a section for linking to other ways to access the data, and for linking to sources the data is derived from, if any.

Links to other publicly accessible locations of the data:

```
- [http://...] (http://...)
```

Data was derived from the following sources:

- []()

Code/Software

This is an optional, freeform section for describing any code in your submission and the software used to run it

Describe any scripts, code, or notebooks (e.g., R, Python, Mathematica, MatLab) as well as the software versions (including loaded packages) that you used to run those files. If your repository contains more than one file whose relationship to other scripts is not obvious, provide information about the workflow that you used to run those scripts and notebooks.

From https://datadryad.org/docs/README.md

Brief own work

Question: Take a look at the files and folders in your current project. What problems do you see?

Method: Individual work

Time: 5 minutes

Securing knowledge: Exchange afterwards within the course

Version Control

Documents may evolve over time, several people may be involved in sequential changes. For data (of any kind, e.g. numeric or images) and text documents alike, file versioning serves two purposes:

- You can revert to earlier versions if needed.
- You can keep track of changes, including documentation on the underlying rationale and people involved.
- Version control can be done either manually by using naming conventions or by using a version control system.



Manual Version Control

- When working with a manual control system, versions should be numbered consecutively; major changes (v1, v2, v3, ...) can be distinguished from minor ones (v1-1, v1-2, v1-3 or 1a, 1b, 1c). Use leading zeros if you expect more than nine versions.
- However, do not apply such numbering when using version control software, as it will interfere with automatic versioning.
- Qualifiers such as "raw" or "processed" for data, or "draft" or "internal" for documents are useful.
- But terms such as "final2", "final-revised", "final-changed_again", "final_ready" can be confusing. In other words: Avoid "final" naming



https://doi.org/10.5281/zenodo.3674561

Version Control Systems

- A prominent example for a version control system is Git, as a distributed version-control system for tracking changes. It is widely used in the field of software development. Also a version control for research data with Git is possible as well.
- There may even be a local Git instance at your own Max Planck Institute? Ask for it!
- If not, there are a couple of central Git systems within the Max Planck Society, which can be used. For example the MPCDF is hosting a <u>GitLab</u> <u>instance</u>. The GWDG is offering a <u>GitLab system</u> as well.
- A tutorial for using Git is given by <u>Data Carpentry</u> or at <u>GitHub Education</u>.
- An helpful overview on tools for version controlling data is given by <u>The</u> <u>Turing Way</u>.



File Formats

Proprietary Data Formats vs. Open Data Formats

- Proprietary data formats often are not readable without the corresponding (commercial) software and may become obsolete in the future.
- An Open Data Format is a format with, "a freely available published specification which places no restrictions, monetary or otherwise, upon its use". (see <u>https://opendefinition.org/ofd/</u>)
- Conversion from proprietary to open formats is often possible, but may result in some loss of data.

More on https://rdm.mpdl.mpg.de/before-research/file-formats/

56 https://doi.org/10.5281/zenodo.5608845

Recommended File Formats I

Type of data	Recommended formats
Text	Plain text (.txt) Rich Text Format (.rtf) Open Document Text (.odt; ISO 26300) PDF (PDF/A-1)
Tabular data (minimal metadata)	Comma-separated values (.csv) Open Document Spreadsheet (.ods; ISO 26300) Tab-delimited (.tab)
Tabular data (extensive metadata)	SPSS portable format (.por) NetCDF HDF5

This list is a guidance and non-binding.

Recommended File Formats II

Type of data	Recommended formats
Images	TIFF6.0 uncompressed (.tif) JPEG2000 (.jp2) JPEG (.jpg) GIF (.gif) Scalable Vector Graphics (.svg) FITS (.fits) PNG (.png)
Video	MPEG-4 (.mp4) OGG video (.ogv, .ogg)
Audio This list is a guidance and non-bind	Free Lossless Audio Codec (.flac) _{in} Waveform Audio File Format (.wav)

File Standards

- Every standard is better than no standard
- Need to balance: More generic standards vs. community specific standard (i.e. DublinCore vs. DataCite metadata schemas)



More Specific File Standards

- Digital Imaging and Communications in Medicine (DICOM, <u>https://www.dicomstandard.org</u>), for medical imaging
- FITS (Flexible Image Transport System, <u>https://fits.gsfc.nasa.gov/fits_standard.html</u>), image data file format for astronomical data
- International Image Interoperability Framework (IIIF, <u>https://iiif.io</u>), for images i.e. art history
- NeXus Data Format

(<u>https://www.nexusformat.org</u>), for neutron, x-ray, and muon science

https://doi.org/10.5281/zenodo.3674561

Saving

- Storage and storage locations
- Backup strategies
- Sustainable file formats
- Long-term archiving

Storage and Storage Locations

- Own laptop
- Local institute
- Share systems like ownCloud, Keeper etc.
- Ask your local IT!

•



Backups to Ensure your Data

- Backups are an instrument to ensure that your data can be restored in case of damage or losses.
- The data backup strategy is usually already set in your DMP.
- Nevertheless, it is necessary to carry out your planned backup strategy continuously.
- Similarly, the restoring of data, for example, must really be tested for effectiveness. It is your task.
- Keep in mind, that your data is invaluable, in comparison to storage space.

Backup Strategies

3 - 2 - 1 rule

- 3 copies of your data
- On 2 different media
- 1 copy off side

Other concepts:

- 10 steps by CESSDA
- Checklist by OpenAIRE



Check if it works

- A data backup is only helpful if the recovery of the data is guaranteed
- It is advisable to check the data recovery at the start of the backup and at regular intervals to prevent data loss
- Sometimes files are corrupted and are faulty
- Occasionally the copying process of files itself causes errors



Sustainable File Formats

The US Library of Congress defines seven "sustainability factors for digital formats":

- 1. **Disclosure**: Do complete specifications and tools for validating technical integrity exist?
- 2. Adoption: A widely used format is less likely to become (rapidly) obsolete.
- **3. Transparency**: Are file formats open to direct analysis with basic tools?
- **4. Self-documentation**: Are metadata included within the file?
- **5.** (Limited) external dependencies: Minimize the degree to which a format depends on specific hardware, software, or operating systems.
- 6. Impact of patents: Patents related to a digital format may inhibit the ability of archival institutions to sustain content in that format.
- **7. Technical protection mechanisms:** Encryption poses problems for long-term archival and dissemination, migration to new formats, transfer to new storage media.

https://www.loc.gov/preservation/digital/formats/sustain/sustain.shtml

Long-Term Archiving

- "Long-term" is an auxiliary term used to describe an unspecified period of time in which technological and socio-cultural changes can occur that can influence the preservation, access to, research in and subsequent use of digital research data.
- Digital long-term archiving therefore comprises a series of measures that need to be planned, controlled and implemented.
- Ten years, as mentioned in the good scientific practice, or even beyond?

Frequent Problems

Probleme	Possible solution
Loss of bits	Check the checksums of the data
Delete or overwrite data	Backups and versioning
Defect data storage medium	Backups on external storage
Stolen data carrier	Encryption of your own data and backups on external storage media
Fire, flooding, etc.	Backups on external storage
Loss of compatibility of file formats	Use suitable, non-proprietary file formats (additionally)
Virus and Trojan	Backups on external storage and IT security concept of its own MPI

Secure!

- Encryption
- Checking the usability
- Password protection and access rights

Secure Research Data

- Research data are among the most valuable resources in science
- That is why there is great importance to their security
- The security and access rights aspects of data management should consist of measures to protect against data loss on the one hand and measures to prevent misuse of the data on the other



Encryption

- Physical access to a computer can enable unauthorised access to data, so it may be necessary to encrypt the data
- This measure only makes sense if all affected data is encrypted, especially copies and backups
- All involved parties must be aware of the need for encryption and the storage locations



https://doi.org/10.5281/zenodo.5608845

Password Protection and Access Rights

- Working with sensitive data, secure passwords should be assigned and access be restricted to the circle of persons directly involved.
- The assignment of authorisations determines which persons or groups of persons are allowed to access certain directories and files and with which rights.
- It is possible to assign graduated read and write authorisations as well as execution rights → some users can only view data, while others are granted full access
- It is important to assign permissions carefully not to hinder the workflow



Bundesamt für Sicherheit in der Informationstechnik,

https://www.bsi.bund.de/S haredDocs/Downloads/DE/ BSI/Checklisten/sichere_pa sswoerter_faktenblatt.pdf

Lunch break until 1 pm
Max Planck Data Services

- MPG Data Services: From local via central to external
- Data services: GWDG, MPCDF, DKRZ and MPDL

Which RDM Services Are Best To Use?

- It depends!
- Most important thing is to understand which data are generated and used
- Recommendation: A conscious approach to the management of data
- Procedure:
 - 1. Write a small specification with all the requirements for data and management
 - 2. Search for different service providers
 - 3. Choose the best for your research and in accordance with institute's practice
- The fastest first solution does not always have to be the best one



More Max Planck Data Services

- 1. Gesellschaft für wissenschaftliche Datenverarbeitung mbH Göttingen (GWDG)
- 2. Max Planck Computing and Data Facility (MPCDF)
- 3. Deutsches Klimarechenzentrum GmbH (DKRZ)
- 4. Max Planck Digital Library (MPDL)



Data Services of the GWDG



The GWDG



- Founded 1970
- Stakeholder
 - Max-Planck-Gesellschaft zur Förderung der Wissenschaften e.V.
 - Georg-August-Universität Göttingen Stiftung öffentlichen Rechts
- Mission
 - Computing and IT competence centre for the Max Planck Society
 - University Computer Centre for the Georg-August-Universität Göttingen



GWDG Service-Architecture





Data Services

File Services

- File-based storage of data via standard protocols (NFS, CIFS, CephFS)
- Different features available depending on the platform:
 - Snapshots
 - Sync. Mirroring
 - Storage efficiency process (Dedup, Compression)
 - HSM (transparent storage on tape)
- Differeit Performance Tiers: Cold-, Warm-, Hot-Storage

5



NetApp

StorNext. @ceph

ownCloud/Nextcloud



- File synchronisation service with Office collaboration function
- Central instance based on the ownCloud product
- Hosting of Nextcloud instances for individual institutes or crossinstitute projects/groups (on request)







Cryptshare

- share files with your web browser
- data will be transferred in encrypted form and
- stored encrypted on the server
- no additional user account necessary
- user-friendly web interface
- Password protected download



S3 Object Storage

- Amazon S3 compatible object storage
- Worldwide access to data via HTTPS
- Rapid growth in use cases (data lakes, Kubernetes, cloud-native architectures)
- Cost-effective and scalable
- Different performance tiers: cold / hot storage
- Support for advanced features: Bucket-Policies, Lifecycle-Policies, Encryption, Online-Compression, Replication, S3-Select, etc.





Backup auf Tape (TSM/ISP)

- Use of TSM / ISP as cost-effective backup software
- Focus on security (ransomware) and cost efficiency
- MPI-specific setups, e.g. :

 Replication of backups to the MPCDF (geo-redundant second copy)
 - Backups to HDDs for fast restores





Veeam Cloud Connect

- Backup-as-a-Service
- Simple integration into different infrastructures
- Georedundant backups
- Fulfilment of compliance requirements
- Very favourable data storage
- Encryption of the backups
- Tape integration in development



VeeaM

Long-term archiving (archive server)

- Secure and cost-effective long-term archiving of large amounts of data (10+ years)
- Storage of two copies in dedicated, geo-redundant tape libraries
- SSD-based file system (150+ TB) for easy access to the archive
- Flexible access via NFS, SMB or SCP / SFTP



StorNext_®

Scientific Compute Cluster -Supplement to the MPCDF offer



- Close integration with other GWDG services
 - Platform for various BioScience applications
 - Private cloud enables front ends for scalable HPC applications
 - Data sharing and publication services
- Offers
 - Test environments stepping stone to MPCDF and national offers
 - Exploration of alternative hardware
 - Future Technology Platform (Graphcore, ARM, RISC-V, ...)
 - Training offer (also locally at MPIs)
 - Maximum data protection (protection class D) and ISO27001 certification

Data Lakes



- Support for scientific projects and institutes with customised solutions
- Specially secured services for processing sensitive data (e.g. health data)
- Highly scalable mass storage
 Connection to HPC service
 Indexing of (sensitive) metadata



Version Control with GIT

- GWDG Gitlab
 - start a private repo
 - invite colleagues
 - use continuous integration CI/CD







JupyterNotebook



https://jupyter-cloud.gwdg.de https://jupyter-hpc.gwdg.de

- Python, R, Haskell, Julia ... environment to be used in the browser
- support interactive data science and scientific computing across all programming languages
 create and share documents that contain live code, equations,

visualizations and narrative text



Persistent Identifiers



- Elementary component of the FAIR criteria
- Supports the data management processes
- PIDs based on the Handle System
- GWDG is MPA on DONA (namespace 21.)
- Following the ePIC policies for namespace registration
 - allows also for test namespaces
- Fast provisioning time



How to connect



Visit: www.gwdg.de

Requests: support@gwdg.de









Overview of the MPCDF



Some MPCDF Data Services



GitLab

The MPCDF GitLab instance is available to all MPCDF users and their external collaborators. Continous Integration can be done on central hosted shared GitLab Runners, building a bridge to the MPCDF HPC clusters

CKAN Instances

For data publishing, the MPCDF offers hosting of CKAN-based data repositories. CKAN is a software framework which allows to manage metadata as well as object data. Beside a web-based interface, CKAN offers a REST API for automation of common workflows.

CKAN instances at the MPCDF are meant for Max Planck Institutes, groups or projects and not for individual users.

HPC Cloud

The HPC Cloud enables scientists to combine batch and cloudbased computing within the same pipeline, taking advantage of both massive HPC cluster resources and highly flexible software environments. The system offers standard cloud computing "building blocks", including virtual machines based on common Linux operating systems, software-defined networks, routers, firewalls, and load balancers, as well as integrated block and S3compatible object storage services.

Globus Online

Globus Online is a third party transfer service which enables fireand-forget data transfer at TB or multi-TB scale. Globus Online is well established and widely used with many computing centres and research institutes, as well as Universities, having Globus Services installed for their users.

Further Information





Homepage:

www.mpcdf.mpg.de

Email:

support@mpcdf.mpg.de

Deutsches Klimarechenzentrum GmbH (DKRZ)

Services for Climate Research Data

Andrea Lammert

Deutsches Klimarechenzentrum GmbH

The German Climate Computing Center (Deutsches Klimarechenzentrum, DKRZ) is a central service organisation for German climate and earth system research. Its high performance computer, data storage and services form the central research infrastructure for simulation-based climate science in Germany.

DKRZ is a **non-profit and non-commercial limited company** with four shareholders:

- the Max Planck Society
- the Freie und Hansestadt Hamburg, represented by the University of Hamburg
- the Alfred Wegener Institute Helmholtz Centre for Polar and Marine Research
- the Helmholtz Zentrum Hereon











UNIVERSITAT HAMBURG

MAX-PLANCK-GESELLSCHAF

FDM-Onboarding

Andrea Lammert

03.04.2024

Portfolio - Global Simulations



Portfolio - Regional Simulations



Portfolio - HighRes Simulations



FDM-Onboarding

DKRZ Data Management







Andrea Lammert

FDM-Onboarding

Contact:

Deutsches Klimarechenzentrum GmbH Bundesstraße 45a D-20146 Hamburg



User Support: <u>support@dkrz.de</u> Data Support: <u>data@dkrz.de</u>

Max Planck Digital Library

- Landsberger Straße 346, 80687 Munich
- Information services since 2007, independent service unit since 2012
- MPDL sees itself as
 - one of the four central IT service centres of the Max Planck Society (together with MPCDF, IKT and GWDG)
 - together with the institute libraries, MPDL forms the library system of the Max Planck Society
- Around 80 employees from software development, library, science management and administration
- www.mpdl.mpg.de
- Collections department for the topic of research data






RDM Support

- Consultancy for data management plans
- Support with data transformation
- Handling of metadata
- Identification of suitable data repositories
- Searching for the right repository/archiving software
- and much more
- Contact us via <u>rdm@mpdl.mpg.de</u>





RDM Information Platform



- Introduction
- Before Research
- During Research
- After Research
- MPDL Services
- News
- Contact
- <u>https://rdm.mpdl.mpg.de</u>



Introduction

Digital data are the basis of nearly all scientific research. The increasing amount and complexity of scientific data pose challenges to keeping data organized, documented, and available for verification of research and new analyses leading to new insights.

The purpose of this website is to provide **data management guidance** throughout the research process, introducing <u>Max Planck Digital Library(MPDL</u>) services to **support researchers of the Max Planck Society**.

This website is a guide for initial orientation and has used for this a simplified representation for the purpose of clarity and quick, easy readability. This includes, of course, no obligation for Max Planck researchers. And this also implies that the presented content not only corresponds to current practice within the Max Planck Society.

Edmond



- Open Research Data Repository of the Max Planck Society
- Serves the publication of research data from all disciplines
- Offers scientists the ability to create citable research objects
- Enables secure preservation: provision, describing, documentation, linking, publishing and archiving of all kinds of data
- Supports standardized metadata profiles

https://edmond.mpdl.mpg.de edmond@mpdl.mpg.de



RDMO for MPG



- RDMO stands for Research Data Management Organiser
- You can use it to write Data Management Plans (DMPs)
- You can also organise the data management for a project, e.g. a dissertation
- Collaboration with other users (also external to the MPG)
- Versioning
- Export and import functions

RDMO for MPG

https://rdmo.mpdl.mpg.de rdmo@mpdl.mpg.de

RDMO for MPG

Special Catalogues:

- Horizon Europe
- VW-Stiftung Science Europe
- DFG
- Software Management
- NFDI4Ing
- •••



RDMO for MPG Management - Admin

Writing a New DMP

Description This is a data management plan for demonstration purposes.				
Catalog	Horizon Europe This catalogue is for creating data management plans for projects in Horizon Europe and at the European Research Council.			

Tasks

Tasks are generated automatically from the answers given in the project. On the page of each task you can see which of your answers lead to the activation of the task.

No active tasks found.

Views

Views are created using the answers given in the project and can then be exported in various formats. Initially, all views are empty. Please answer some questions by visiting **Answer Questions** (at the top of the sidebar).

View	Description	ø
Cost overview	Overview of the personnel and non_personnel costs	۲
Cost Overview	Overview of the personnel and non-personnel costs	۲
DMPonline template	Template from DMPonline, online https://dmponline.dcc.ac.uk	۲
DMPTool template	Template from DMPtool, based on "NSF-GEN: Generic", online: https://dmptool.org	۲
Horizon 2020 FAIR Data Management Plan template	Template for Horizon 2020, from "Guidelines on FAIR Data Management in Horizon 2020", online: http://ec.europa.eu/research/participants/data/ref /h2020/grants_manual/hi/oa_pilot/h2020-hi-oa-data-mgt_en.pdf	۲

ø

Keeper



- 1 TB storage space
- Long-term archiving of the completed data set, 10 years
- Synchronises local projects
- File sharing with individuals and groups
- Cared Data certificate that confirms good scientific practice
- Digital object identifier (DOI)



https://keeper.mpdl.mpg.de keeper@mpdl.mpg.de

Labfolder



- Electronic laboratory notebook (ELN) for recording, integrating and managing experimental research data
- Two utilization scenarios:
 - In-house service at the respective institute
 - Central MPG Labfolder installation



Software Licensing Service

- Basic software supply
- Open source software solutions
- Preparation of an offer for support and maintenance contracts
- Applications for funding for open source software development projects



MAX

PLANCK

LIBRARY

DIGITAL

DOI Service



- Assign DOIs to scientific output, e.g. MPG.PuRe, Edmond and Keeper
- Self-service within MPG-IP
- Use for local data repositories possible (MoU needed)



https://doi.mpdl.mpg.de doi@mpdl.mpg.de

Metadata

- Metadata standards
- Identifiers

Metadata Standards

Rich metadata is good, using standards is even better

Example: <u>Virtual observatory</u>

Find your standard e.g. at <u>bartoc.org</u>, <u>University of Bath</u>

Identifiers

Digital Object Identifier (DOI)

- For digital objects
- https://www.doi.org



Open Researcher and Contributor ID (ORCID)

- For persons
- <u>https://orcid.org</u>



Public domain, CC0

Research Organization Registry (ROR)

- For organisations
- <u>https://ror.org</u>



Identifier Network



Max Planck Institute for Evolutionary Biology:

- https://ror.org/0534re684
- <u>https://commons.datacite.org/ror.or</u> <u>g/0534re684</u>



Questions to You via Slido

Join via slido.com and enter 1174667

- 1. Do you know your ORCID?
- 2. Do you know the ROR of your institute?

Publishing

- Data (and software) as a new genre of publication
- Legal aspects of publishing
- Data repositories and journals
- Publish or share data (Open Research Data)
- Reuse data

Three Pillars of Research Results?



Legal Aspects of Data Publishing

- Who owns the data?
 - The scientist, the supervisor, the Max Planck Institute, the Max Planck Society?
 - There is no universally valid statement on this!
 - Talk to your supervisor. Have a look at your employment contract and local research guidelines. The publication approval process must be clarified.
 - Find out more! It's better to clarify things earlier rather than after the data publication (= too late).



Legal Aspects of Data Publishing

- What type of data aggregation should actually be published?
 - That highly dependents!
 - Raw data, (pre-)processed data and analysed data are published. It always depends on the context, the specialised culture and the objectives.
 - Discuss this with your supervisor and team colleagues at an early stage.



Licenses Data Publishing

 A licence for a data publication can only be granted by the owner (see above)

Common (Data) License:

- Creative Commons
 (https://creativecommons.org)
 - CC 0
 - CC BY
- Open Data Commons
 (https://opendatacommons.org)
 - ODC-By
 - PDDL

Recommendation:

- 1. CC0 or 2. CC BY
- Any license is better than no license!



Contracts for Data Collection and Submission

Sample contract for data recording			Mustervertrag Datennutzung			
5b Working Par 2023	ber KonsortSWD Kensortium für die Sozial- Verhaltens, Bildungs- und Wirtschaftswissenschaften					
			Mustervertrag Datennutzung KonsortSWD: Erläuterungen und rechtliche Fragen			
	Erläuterungen zur Datenaufnahme in Forschungsdatenzentren Begleitdokument zum Mustervertrag Datenaufnahme KonsortSWD		Version 2.0.0., Stand: 19.07.2023			
	Dr. Till Kreutzer, Jan Schallaböck, Ute Hoffstätter, Daniel Buck ⁴ März 2023	Schallaböck, J., Kreutzer, T., Hoffstätter, U., & Buck, D. (2023). Mustervertrag Datenaufnahme KonsortSWD,		Schallaböck, J., Hoffstätter, U., Buck, D., & Linne, M. (2023). Mustervertrag Datennutzung		
	www.konsortswd.de	Zenodo, CC BY 4.0, https://doi.org/10.5281/zenod o.10406480.	Das Dokument steht unter folgender Lizenz: <u>CC0 1.0 Universell (CC0 1.0) Public Domain Dedication</u>	KonsortSWD, Zenodo, CC BY 4.0, https://doi.org/10.5281/zenodo. 10409864.		

Foreign Trade Law and Dual Use of Data

- The publication of research data is also subject to foreign trade law.
- Not only the physical exchange of goods is a relevant process, but also the pure (electronic or non-physical) exchange of data, information and knowledge/know-how.
- These aspects must be taken into account when publishing data.
- If you have any questions about foreign trade law, please ask your local export control officer at your Max Planck Institute.
- If this is not possible, please contact <u>the team at the Administrative</u> <u>Headquarters</u> at <u>aussenwirtschaft@mpg.de</u>.

VII.2.01 Außenwirtschaftsrecht – Aufbau einer MPG-weiten Exportkontrolle, https://ohb.mpg.de/Policies/MPG%20VII.201%20de%203.1/VII.2.01_Aufbau %20einer%20MPG-weiten%20Exportkontrolle_de.pdf.

Research Data Repositories

- Repositories for research data are specialised services for the (free/restricted) publication of research data.
- They are designed for publishing research data, to ensure the specified publication specifications and processes are automatically adhered to (e.g. FAIR principles).
- Depending on the culture of the discipline and its usage different repositories may be appropriate.



Recommendation for the Selection of a Research Data Repository



Find a (Open) Research Repository

- Registry of Research Data Repositories (= re3data)
- https://www.re3data.org
- Best starting point for finding a suitable place for data publication



re3data: Search by Subject, CC BY 4.0, https://www.re3data.org.

F-Uji

- Web service to programmatically assess FAIRness of published research data sets
- <u>https://www.f-uji.net</u>
- Identifier from research data repository in F-Uji assessment:
 - i.e. <u>https://doi.org/10.5281/</u> zenodo.6483002

F-UJI Home Assess About Methods Docs Code	
F-UII Home Assess About Methods Docs Code FAIR assessment F-UJI is a web service to programatically assess FAIRness of research data objects (aka data sets) based on metrics developed by the FAIRsFAIR project. Please use the form below to enter an identifier (e.g. DOI, URL) of the data set you wish to assess. Optionally you also can enter a metadata service (OAI- PUH, SPARQL, CSW) endpoint URI which F-UJI can use to identify additional information. Present Data Object URI./PID/* [Enter a wald PID or URL of the dataset's landing page (e.g. a DOI) [Start FAIR Assessment] About Feedback Privacy Policy Terms of Use Legal Notice	Z
r-Un is a result of the <u>partyparts</u> restering this units infactores in Europe project which received funding from the European Union's Horizon 2020 project can Houzo-HerrokeUSU. 2018-2020 (grant agreement 831558).	•
Anusuriya Devaraju, & Robert Huber. (2020). F-UJI - An Automated FAIR Data	

Assessment Tool, MIT license, https://doi.org/10.5281/zenodo.4063720

Questions to You via Slido

Join via slido.com and enter 1174667

- 1. Do you know of a community-specific repository for your discipline?
- 2. Have you ever published research data in a community-specific repository?

Data Journals

Examples:

- Generic:
 - <u>Scientific Data</u>
- Engineering
 - Journal of Chemical & Engineering Data
- Humanities
 - Journal of Open Humanities Data
 - <u>Research Data Journal for the Humanities</u> and Social Sciences
- Life Sciences
 - <u>Gigascience</u>
 - <u>Biodiversity Data Journal</u>
 - Open Health Data

WAVE	INTERVIEW- MODE	DIRECT ASSESSMENTS OF CHILD AND HOME LEARNING ENVIRONMENT (HLE)	YEAR	CHILD (TARGET) AGE	PARTICI- PATING FAMILIES	CHILDCARE			SUF
						EDU- CATOR	INSTITU- TION MANAGER	CHILD- MINDER	RELEASE
1	CAPI	Standardized and semi- standardized observational measures (Incl. HLE)	Aug-2012- Mar 2013	7 months	3,481				2015
2	CATI, PAPI		Apr-Oct 2013	14 months	2,862	171		73	2015
	CAPI (half sample)	Standardized and semi- standardized observational measures (incl. HLE)	July-Dec 2013	17 months	1,510				2015
3	CAPI, PAPI	Semi-standardized observational measures (Incl. HLE)	Apr-Nov 2014	25 months	2,609	449		110	2016
4	CAPI, PAPI	Tabled-based competence tests	Apr-Nov 2015	3 years	2,478	625	571		2017
5	CAPI, PAPI	Tabled-based competence tests	Apr–Sep 2016	4 years	2,381	628	521		2018
6	CAPI, PAPI	Tabled-based competence tests	Mar-Aug 2017	5 years	2,209	683	543		2019
7	CAPI, PAPI	Tabled-based competence tests	Apr-Sep 2018	6 years	2,116	546	444		2020
8	CAPI, PAPI	Tabled-based competence tests	Mar-Aug 2019	7 years (mainly grade 1)	2,070				2021
9	CATI-Remote ¹ / CAPI by phone ^{2,1}	Online Tests	June ¹ -Sep 2020	8 years (mainly arade 2)	1,848				2022

Table 1. Deviewer of all works, used modes, target age of the china, participanty annual sond childcore installution. Mores: CAPI = Compater-axisted personal interview, CAII = Computer assisted tetephone interview, PAPI = Paper and panci-Questionnite; SLF = Scientific use file; HE = Home tearning environment; Each year, beginning with wave 3, there was also a small CAII - fead for all trainise wind all not dee part in the CAII[®] Due to the Coxid-19 panatemic, in wave 9 nearly all interviews with the parents were administered via telephone from the regular CAPI-interviewers from their homes. "The competence tests for the children were administered online with support of an interviewer by telephone. The field of the oniginal CAPI started in March 2020 before it stopped due to the pandemic. The field was re-opened in June 2020 with telephone interviews and the online testing.

Hence, across the waves, for 1,563 children of the SC1 information from early child care personnel are available (at least one questionnaire available from childminders, educators, or head of institution).

2.2 TIME OF DATA COLLECTION

The first assessment wave started in August 2012, the sofor latest assessment included in this paper took place in 2020 (assessments in the SC1 are still continued). Table 1 gives an overview of the duration of the field for each wave.

For further information see study overview https://www. neps-data.de/Data-Center/Data-and-Documentation/Start-Cohort-Newborns/Documentation.

2.3 LOCATION OF DATA COLLECTION Overall, Data was collected at various sample points in Germany (see also 2.4.). In most waves, data collection took place in the households of the formilies. (2016).1 (2016).1

2.4 SAMPLING, SAMPLE, AND DATA COLLECTION

The targets of SC1 are the children. As already mentioned, the first wave was intended to take place when the infants were 6 to 8 months of age. As context persons, one parent (respondent, in most cases the molher) as well as child care personnel were interviewed.

wee as chaia care personnel were interviewed. The sample was drawn via a register-based sample of addresses available at the level of municipalities. A two-stage dispropartional structure sample of the newborn population in Germany. Overall, 84 German municipalities were considered as primary sampling units (Warbach et al., 2016). As a secondary step, addresses out of these municipalities were drawn. Overall, 8,483 addresses from 90 sampling points in 44 municipalities were used. A detailed description of the sampling strategy can be found in Warbach et al. (2016). Due to the food developmental prozenses of infants Attig, M., Vogelbacher, M. and Weinert, S., 2023. Education from the crib on: The potential of the Newborn Cohort of the German National Educational Panel Study. Journal of Open Psychology Data, 11(1), p.13.DOI: https://doi.org/10.5334/j opd.81, p. 4. CC BY 4.0.

Open Research Data

EU Directive 2019/1024: "Open data as a concept is generally understood to denote data in an open format that can be freely used, re-used and shared by anyone for any purpose." (http://data.europa.eu/eli/dir/201 9/1024/oj) "Knowledge is open if anyone is free to access, use, modify, and share it subject, at most, to measures that preserve provenance and openness."



Open Knowledge Foundation, https://opendefinition.org/od/2.1/en/, CC BY 4.0

5 ★ Model for Open Data by Tim Berners-Lee

★ Data online

★★ Data online available as structured data

 $\star \star \star$ Data online available in a nonproprietary open format

 $\star \star \star \star$ Use identifiers to denote things, so that people can point at your data

 $\star \star \star \star \star$ Link your data to other data to provide context



https://5stardata.info/en/, CC0.

https://5stardata.info

Open Research Data Dashboards

Charité Dashboard on Responsible Research (<u>https://quest-</u> <u>dashboard.charite.de</u>)



French Open Science Monitor (https://frenchopensciencemonitor. esr.gouv.fr)



OPEN LICENCE 2.0/LICENCE OUVERTE 2.0, <u>https://github.com/etalab/</u> licence-ouverte/blob/master/open-licence.md

Re-Use of Research Data

- The re-use of research data is a common, legitimate practice. There are rules for it.
- If in doubt, discuss the (subsequent) use of data with your supervisor.
- A licence for data can easily ensure legally compliant subsequent use.
- In the spirit of good scientific practice, you are obliged to cite your sources correctly; also re-used data.



https://doi.org/10.5281/zenodo.5608845

Questions to You via Slido

Join via slido.com and enter 1174667

- 1. Have you already published research data?
- 2. Have you re-used research data for your projects?

30 minutes Coffee break

Electronic Laboratory Notebooks

- Concept and use
- Selection
- Concrete examples

Aspects of a Laboratory Notebooks

- Permanent records of research ideas, concepts, data and observations
- A laboratory notebook is a legal record (i.e. evidence at applying for a patent)
- Protection of your intellectual property rights
- But only, if the laboratory notebook is used correctly

Mende, Michael (2021): Notebook Origins - why document? Talk presented at Digital Workshop "Living with Electronic Laboratory Notebooks", Munich, 21st September 2021, <u>http://hdl.handle.net/21.11116/0000-0009-3F16-9</u>.



Laboratory notebook from Hans Stocker, Kaiser Wilhelm Institute for Medical Research, 1930, folio 97, Copyright: Archive of the Max Planck Society, Berlin.

Usage of a Laboratory Notebooks

- Never remove pages
- Do not write outside the document
- Never use non-permanent pen/ink
- Use sequentially numbered pages
- Cross out blank spaces
- Do not start a new page until the previous one is full
- Never remove entries (errors must still be visible)

Mende, Michael (2021): Notebook Origins - why document? Talk presented at Digital Workshop "Living with Electronic Laboratory Notebooks", Munich, 21st September 2021, <u>http://hdl.handle.net/21.11116/0000-0009-3F16-9</u>.

Hindrag in total up algo fullouilet. 500 ag tille school in the algo fullouilet. 500 ag tille school in the algo fullouilet. Standaug (19 (102(100)) - 1 is filed (100)) 5.00 The 500 the filed 1: 35 none is filed (100) 5.00 The 500 the school of a standard (100) (100) 5.00 The 500 the school of a standard (100) (100) 5.00 The 500 the school of a standard (100) of a standard 15.00 the school of a standard (100) of a standard 15.00 the school of a standard (100) the school of a standard 15.00 ang the last school of a standard (100) s a standard 100 the school of a standard (100) the school of a standard 100 the school of a standard (100) the school of a standard 100 ang the last school of a standard (100) the school of a standard 100 ang to the last school of a sta	Burghung wir greigenten auf gen gehange har so yften herf 200 ger - 10° T/dec mig i plaft (10bT the birthing gid Under 10° 10° 60° 60° 00° 00° / min. 12 Under 10° 10° 60° 60° 00° 00° / min. 12 Under how de (10° 12° 40° 60° 60° 70° 60° 70° 60° 60° 60° 60° 60° 60° 60° 60° 60° 6
Burness adding to the state	

Laboratory notebook from Magdalena Wiedemann, Kaiser Wilhelm Institute for Chemistry, folio 13, Copyright: Archive of the Max Planck Society, Berlin.
From Analogue to Digital

- Normally no delete-function in an ELN available
- Tracking down changes etc. to one real user
- Only one account per user
- ELN continues to be a legal document
- Makes sense if the whole team works with the same medium and system

 Analog lab notebook is supposedly more error-tolerant, with an ELN errors are quickly noticed (because things like pulling out pages are not possible)

Bake a Cake with ELNs: Teaching tutorial by Heike Böhm in 2021 https://hdl.handle.net/21.11116/0000-0009-2D85-F

Lists of ELN Software Systems

- ELN Finder (<u>https://eln-finder.ulb.tu-darmstadt.de</u>)
- Harvard Medical School (<u>https://datamanagement.hms.harvard.ed</u> <u>u/analyze/electronic-lab-notebooks</u>)
- University of Cambridge

 (https://www.data.cam.ac.uk/datamanagement-guide/electronic-researchnotebooks/electronic-research-notebookproducts)



Schablone zum Zeichnen chemischer Gerätschaften, <u>https://commons.wikimedia.org</u>/wiki/File:Schablone_Logarex_25525-S,_Chemie_III.jpg, CC0.

Selection of an ELN: Example MPI-CEC

- Selection process for an MPI-CEC-wide ELN
- Pre-selection of ten ELN systems
- Three ELN systems for testing in the departments
 - eLabJournal, eLabFTW, Labstep

Greiner & Vaid (2021): Challenges in choosing a full-featured ELN/LIMS for a multi-disciplinary research organization. Talk presented at Digital Workshop "Living with Electronic Laboratory Notebooks", Munich, 20th September 2021, <u>https://hdl.handle.net/21.11116/0000-0009-3EE9-C</u>.



Example: JoplinApp

- Website: <u>https://joplinapp.org</u>
- Demo Video: <u>https://www.youtube.com/watch?</u> <u>v=VAAA6uNPxec</u>
- Software Type: Open Source
- Offline functions with Nextcloud, WebDAV etc.
- E2EE encryption



Screenshot of Joplin 1.0.218 on GNOME Desktop Environment on Fedora Linux 32, by Tonica, 2020-06-08, <u>https://en.wikipedia.org/wiki/File:Joplin-1.0.218-on-fedora-32-20200608.png</u>, Public domain.

Ampuero Ruiz (2021): Can 'electronic library notebooks' (ELN) become the new field diary?. Talk presented at Digital Workshop "Living with Electronic Laboratory Notebooks", Munich, 20th September, https://hdl.handle.net/21.11116/0000-0009-3F06-B.

Example: eLabFTW

- Website: <u>https://www.elabftw.net</u>
- Demo: <u>https://demo.elabftw.net</u>
- Software Type: Open Source
- Some LIMS possibilities



Logo eLabFTW, CC BY-SA 4.0.

See more: Niels Cautaerts. (2021): Using eLabFTW for materials science. FOSDEM21, <u>https://doi.org/10.5281/zenodo.4707352</u>, Max-Planck-Institut für Eisenforschung.

Example: Chemotion

- Website: <u>https://chemotion.net</u>
- Demo:

https://demo.chemotion.ibcs.kit.ed u/home

- Software Type: Open Source
- Developed at KIT
- Specialised in chemical research
- Lively community, e.g. NFDI4Chem
- Extensive "ecosystem"

E Chemotion -	Al- IUPAC, inchi, SMILES, Rink 🖊 🗴 🕂 😂 K 🕹 🕹 🖉 K 💿 🖌	Paggy Huang - C+
Collections	Q2(0) ₹0(0) =0(0) ⊕0(0) ∰0(0)	38
All		🗂 From To Sample 🕑 💙
Chemotion_net +	C10H9CIN2 2-chloro-6.7-dimethylquinoxaline	© * ^
Collection +		
Demo	CHI-279	Č
 My shared collections 		
Shared with me	C ₆ H ₆	€ □ •
 Synchronized with me 	benzene	
🗅 Inbox 🕕 🕽	*	
	CHI-278	■1-0-€
	Columnation Columnatio Columnation Columnation Columnation Columnation Columna	©-& © ×
	CHI-277	(III 1 - 0 -4) +
		Show 15

Copyright © 2024 Chemotion - KIT, https://chemotion.net/docs/eln/ui/first_steps.

Example: OpenBIS

- Website: <u>https://openbis.ch</u>
- Demo: <u>https://openbis-eln-</u> <u>lims.ethz.ch/openbis/webapp/eln-</u> <u>lims/</u>
- Software-Type: Open Source
- Development: Mainly at ETH Zurich
- ELN + LIMS

FAIRDOM-SEEK

- Web-based resource for sharing heterogeneous scientific research datasets
- FAIRDOM-SEEK and OpenBIS can be combined well → a "seamless" data flow
- Example at the Max Planck Institute for Evolutionary Biology:
 - see slides from ELN workshop 2021 <u>Ullrich</u> and <u>Fortmann-Grote</u>

Example: Labfolder

- Website: <u>https://labfolder.com</u>
- MPG-wide license through the MPDL
- MPDL instance or local instance possible
- https://labfolder.mpdl.mpg.de
- Software type: Proprietary
- Labregister as LIMS included



Questions to You via Slido

Join via slido.com and enter 1174667

- 1. Do you use an ELN in your working group?
- 2. Which ELN exactly do you use?
- 3. Is there a LIMS (Laboratory Inventory Management System) in use as well?

New Horizons

- Research software
- Open Science

Understanding Research Software

- In-house developed research software
- Software applications for research
- Infrastructure software/services

In discussion: Is it really helpful to distinguish between research software and "non-research software" (i.e. MS Word etc.)?



The Turing Way Community, & Scriberia. (2022). Illustrations from The Turing Way: Shared under CC-BY 4.0 for reuse. Zenodo. https://doi.org/10.5281/zenodo.6821117.

Researchers Writing Research Software

Observations:

- Usually not thoroughly trained but autodidactic developers
- Functionality over documentation over sustainability
- After the first publication, nothing happens for a long time, and then maybe data publication and software publication
- Research software is often handed over from one PhD student to the next





The Turing Way Community, & Scriberia. (2022). Illustrations from The Turing Way: Shared under CC-BY 4.0 for reuse. Zenodo. https://doi.org/10.5281/zenodo.6821117.

Questions to You via Slido

Join via slido.com and enter 1174667

- 1. Are you programming software?
- 2. Have you attended a code training course?

Reproducibility and Accessibility

- Software is often needed to reproduce research results
- It should be accessible according to good scientific practice
- Internal policies, funders, journals require or recommend the publication of software
 - "Software programmed by researchers themselves is made publicly available along with the source code."

<u>Guideline 13: Providing public access to</u> research results in the code of condauct of the <u>DFG</u>



The Turing Way Community, & Scriberia. (2022). Illustrations from The Turing Way: Shared under CC-BY 4.0 for reuse. Zenodo. <u>https://doi.org/10.5281/zenodo.6821117</u>.

Re-Usability of Research Software

Conscious handling is increasing the likeliness of re-use:

- Increased probability of publication
- Explicit licensing

•

- Clear code structure and reflected use of third-party libraries
- A targeted approach to archiving



The Turing Way Community, & Scriberia. (2022). Illustrations from The Turing Way: Shared under CC-BY 4.0 for reuse. Zenodo. <u>https://doi.org/10.5281/zenodo.6821117</u>.

Recognition of Research Software

- Disciplinary credits for software publication
- Credits/funding by funders
- Institution-wide credits for development
- Policies needed
 - Normative framework for software publication
 - Endorsement of software publication



Scriberia -

The Turing Way Community, & Scriberia. (2022). Illustrations from The Turing Way: Shared under CC-BY 4.0 for reuse. Zenodo. <u>https://doi.org/10.5281/zenodo.6821117</u>.

Examples for Software Policies

Software Policy



CODE @ MPI-M

Software Licensing and Copyright Policy for Research Software CODE @ MPI-M

1. Preamble

The Max Planck society is determined to promote Open Access to research data, and Open Science (Berliner Erklärung¹).

MPI for Meteorology in Hamburg (MPI-M) has developed, partly on its own, partly in collaboration with partners, various Research Software, for example the ICON Model Code², the Climate Data Operators cdos³, and others.

MPI-M believes that for the benefit of science such Research Software should be released as Open-Source Software.

2. Rules

This policy treats the issues of copyright and licensing. It is applicable and restricted to Research Software Source Code developed at MPI-M (CODE). CODE must either be copyright of MPI-M alone (i.e. new code for, or code developed earlier at MPI-M under the copyright of the institute) or code contributed by third parties to MPI-M code which has been licensed to MPI-M under a permissive license like MIT/X11, (2- or 3-Clause) BSD or Apache 2.0 under the Contributor License Agreement (CLA⁴) or where unlimited copyrights have been transferred to MPI-M by other means under similar conditions.

a. Contributor License Agreement (CLA)

Every developer of CODE at MPI-M, being an employee or in any other connection to MPI-M (freelancer, guest, post-doc, scholarship etc.) (CONTRIBUTOR) must sign a CLA to be allowed to contribute to an MPI-M project in the field of Research Software development. To clarify: MPI-M can agree upon co-operations with other institutions where this policy is not applicable.

b. License

CODE shall be licensed under the BSD-3-Clause License⁵, also see attachment. For any other open source license, you must consult with the MPI-M person responsible for licenses⁶.

1 https://openaccess.mpg.de/Berliner-Erklaerung

² https://mpimet.mpg.de/en/science/models

³ https://code.mpimet.mpg.de/projects/cdo

⁴ Link t.h.d. on MPL-Met Internet site

⁵ See https://opensource.org/licenses/BSD-3-Clause , SPDX short identifier: BSD-3-Clause

⁶ Currently: The person responsible for strategic IT partnerships, or the head of the MPI-M administration. mailto: licenses@mpimet.mpg.de

Authors: Reinhard Budich, MPI-M: Maximilian Funk, MPS 1 / 7

Version: V3.8.2. Date: 2022-07-04: License: CCBV4.0

Reinhard Budich und Maximilian Funk: Software Licensing and **Copyright Policy for** Research Software CODE @ MPI-M, v3.8.2 vom 4. Juli 2022. https://hdl.handle.net/21. 11116/0000-000C-80B1-A , CC BY 4.0.

TU Delft Guidelines on **Research** Software

Licensing, Registration and **Commercialisation**



Bazuine et al. (2021): TU Delft Guidelines on Research Software: Licensing, Registration and Commercialization, CC BY 4.0, https://doi.org/10.5281/zenod 0.4629635.

German Aerospace Center (DLR)

- Support for developed software in terms of good software development and documentation practices
- Focus of the recommendations is on knowledge preservation and the promotion of sustainable software development in research
- Categorization according to application classes 0 to 3, depending on the scope and use of the software



Schlauch, Meinel & Haupt (2018): DLR Software Engineering Guidelines (1.0.0), CC BY 4.0, https://doi.org/10.5281/zeno do.1344612.

Use of Software Repositories

- Differing publication patterns between software and data
- Our observation: software that is mentioned in a publication is often directly linked to GitHub, GitLab, ...

"In 2021, one out of five publications in the arXiv corpus included a URI to GitHub" (p. 1)



Why Should I Write a Software Management Plan?

- For myself!
- Together with IT/Scientific Computing Unit/... to better design a software project
- For funding applications
- For internal planning
- For sustainability and a possible publication/archiving (good scientific practice)
- Quality assurance
- …

Publish Software

- Checks before publication:
 - Legal considerations (e.g. integration of external library with restrictive license, dual use ...)
 - Commitment of the supervisor(s)
- Software repository, i.e. <u>https://github.com</u>, <u>https://gitlab.mpcdf.mpg.de</u>, <u>https://gitlab.gwdg.de</u>, ...
- Data repository, i.e. <u>Edmond</u> or <u>Zenodo</u>
 - manual publication
 - Automated from GitHub as push with GitHub Action towards repository
- Journal, i.e. Journal of Open Source Software (JOSS)
- <u>https://research-software-directory.org</u>
- Search repositories via <u>re3data</u>



Archiving Software

1. Decision on Archival Value:

- Yes or no?
- Intention of archiving
- Resources and responsibilities
- Duration (10 years or more?)

2. Essential Elements:

- Description (e.g. documentation or detailed readme)
- (machine-readable) metadata (e.g. .cff file) on authors, affiliation, date, etc.
- License

3. Decision Conservation Status:

- Bitstream-only preservation
- Preservation of functionality
- Continuous development

4. Decision on Archiving Location:

- At the own institute in a computer center
- In a subject repository
- Archiving of public software via <u>Software</u> <u>Heritage</u>

Research Data and AI

- AI use still new in the area of research data
- There are many possible applications for AI in research data...
 - Collect
 - Prepare
 - Search and find
 - Analyse
- ...and vice cersa: be aware of what and where your research data is passed on to (external) AI providers such as OpenAI

Discoveries in old data sets using neural networks



Map of the particularly metal-poor giant stars that could be identified thanks to the Gaia-DR3 dataset, image: H.-W. Rix / MPIA,

https://www.mpia.de/aktuelles/wissenschaft/2022-19-ancient-heart.

Open Science

- Better access to and participation in scientific research and its results and methods
- Enable fairer access to science worldwide and thus also better contributions to solving global problems
- Improve efficiency, transparency and comprehensibility within science



UNESCO, <u>https://www.unesco.de/wissen/</u> wissenschaft/open-science, CC BY 4.0.

Hypothesis: Open Science is a Reaction



UNESCO Recommendation on Open Science

- Adopted in November 2021
- <u>https://www.unesco.org/en/open-science</u>
- Increases scientific collaborations and sharing of information for the benefits of science and society
- Makes multilingual scientific knowledge openly available, accessible and reusable for everyone
- Opens the processes of scientific knowledge creation, evaluation and communication to societal actors beyond the traditional scientific community



UNESCO, https://unesdoc.unesco.org /ark:/48223/pf0000379949. locale=en, CC BY-SA 3.0.

G6 Statement on Open Science

"We share a common commitment to the principle of making research data **"as open as possible and as closed as necessary"**."

- Co-signed among others by the Max Planck Society in 2021
- Commitment to FAIR and open data



G6 statement on Open Science

Brussels, December 2021

EXCELLENT RESEARCH NEEDS OPEN SCIENCE

The growing momentum for Open Science is in line with our mission to foster research excellence and to accelerate the advancement of science. Open Science principles and approaches were developed from within the scientific community itself, out of genuine self-interest and to further develop key scientific principles - the transparency of research practises, reproducibility of results, and the sharing of knowledge. By opening up publications, data, processes, codes, methods and protocols, it also offers new ways for scientific practices. G6, as Research Performing Organizations (RPO), are committed to excellence in research and Open Science is definitely agood approach to foster excellent research.

G6 institutions actively support the transition to Open Science. This transition requires a concerted effort to reform cultural and technological practices. G6 institutions intend to contribute to this transition by jointly addressing the following priorities:

OPEN ACCESS PUBLICATIONS

Open Access to scientific publications is a cornerstone in the broader field of Open Science. We are committed to accelerating the transition to Open Access as the default mode of academic publishing. Open Access to publications improves the pace, efficiency and efficacy of research, and strengthens the authors' visibility, and thus the potential impact of their work.

Reaching 100% of Open Access is a main goal for all of our institutions but researchers cannot freely share and build on the results they publish if publishers hold copyrights of their articles and monographs. Therefore, we are committed to support our researchers to retain sufficient rights to publish their scholarly articles and monographs openly and we encourage them to publish their results (i.e. final version and/or manuscript) under an open license, preferably the Creative Commons Artivituon License CB W.

FAIR DATA

We share a common commitment to the principle of making research data "as open as possible and as closed as necessary". A balanced and flexible approach to data sharing is essential for an efficient science, research and innovation ecosystem, fostering collaboration, knowledge transfer and preserving scientific freedom.

Our institutions are committed to the sharing of data as guided by the FAIR principles (Findable, Accessible, Interoperable, Reusable). Applying FAIR criteria will guarantee discovery, access and reuse of research outputs by humans and machines. Because the cost of not having FAIR data for research is high, strict adherence to FAIR principles to resure sustainability of research data and software as well as data preservation are major challenges.

G6 statement on Open Science, 2021, https://www.cnrs.fr/sites/d efault/files/downloadfile/G6%20statement%20on %200pen%20Science.pdf

Open Science within Max Planck

Open Science @ Max Planck Society!

- Open Science Group within PhDnet
- Open Science Ambassadors
- Open Science in Practice by MPDL
 - Open Science Days

- Local initiatives at MPIs
 - <u>CBS Open Science</u>
 - ...

•

Max Planck Open Science Ambassadors





ambassadors

https://osambassadors.mpdl.mpg.de

If you still haven't had enough...

Carpentries



Software Carpentry

- <u>https://software-carpentry.org</u>
- Teaching basic knowledge for research software
- Participate: <u>https://software-</u> carpentry.org/workshops/
- Request workshop: <u>https://software-carpentry.org/workshops/request/</u>

Data Carpentry

- <u>https://datacarpentry.org</u>
- Data skills in a scientific context
- Example: "Data Analysis and Visualization with Python for Social Scientists" <u>https://datacarpentry.org/python-</u> <u>socialsci/</u>

Your final questions?



https://doi.org/10.5281/zenodo.3674561

Feedback

- Here directly and/or
- via slido.com and enter 1174667