FAIR Software Management

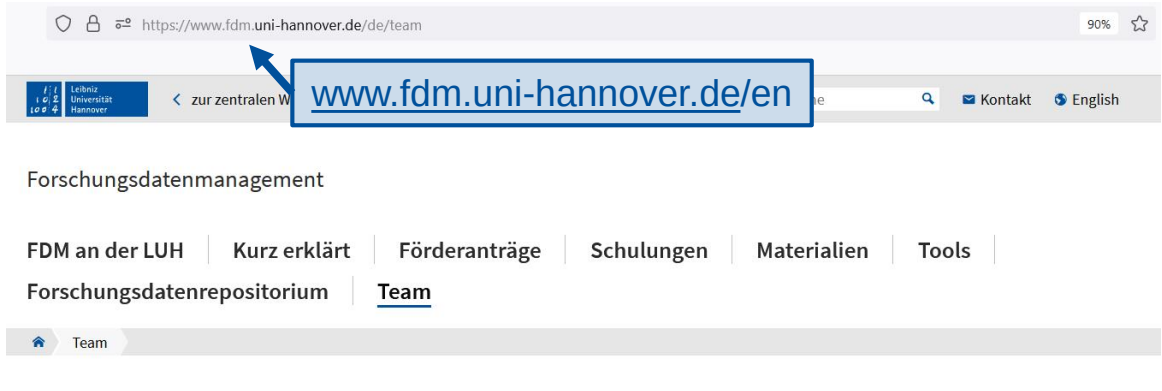
How to handle research software

Yvana Glasenapp, LUH Research Service

Anna-Karina Renziehausen, TIB Publication Services

18.07.2024

Welcome!



Anna-Karina Renziehausen

TIB - Leibniz-Informations-zentrum Technik und Naturwissenschaften und Universitätsbibliothek

Publikationsdienste

Yvana Glasenapp

Gottfried Wilhelm Leibniz Universität Hannover

Dezernat Forschung und EU-Hochschulbüro, Technologietransfer

visit the website of the Research Data Support Team

Content of this course

- Introduction to Research Data Management
- How to make research software re-usable
- How to publish research software and code
- Supporting services and initiatives

Introduction

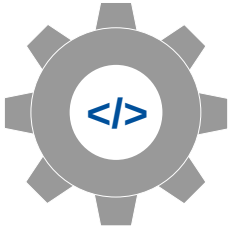
- What are research data?
- What is research data management (RDM)?
- Why is data management important?
- The FAIR principles
- RDM is good scientific practice!
- Guidelines for handling research data at LUH
- LUIS services for data storage and backup

What are research data?

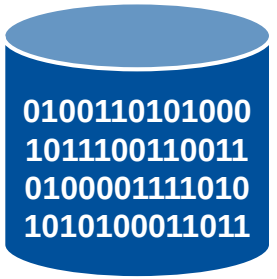
Documentation

Raw data

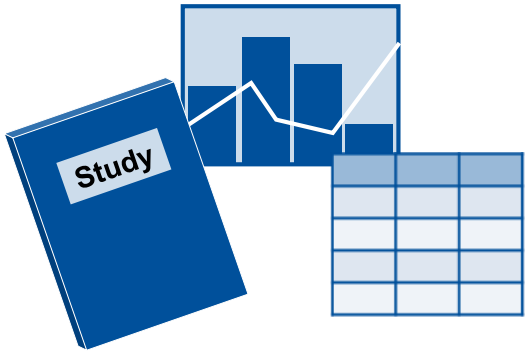
Software code



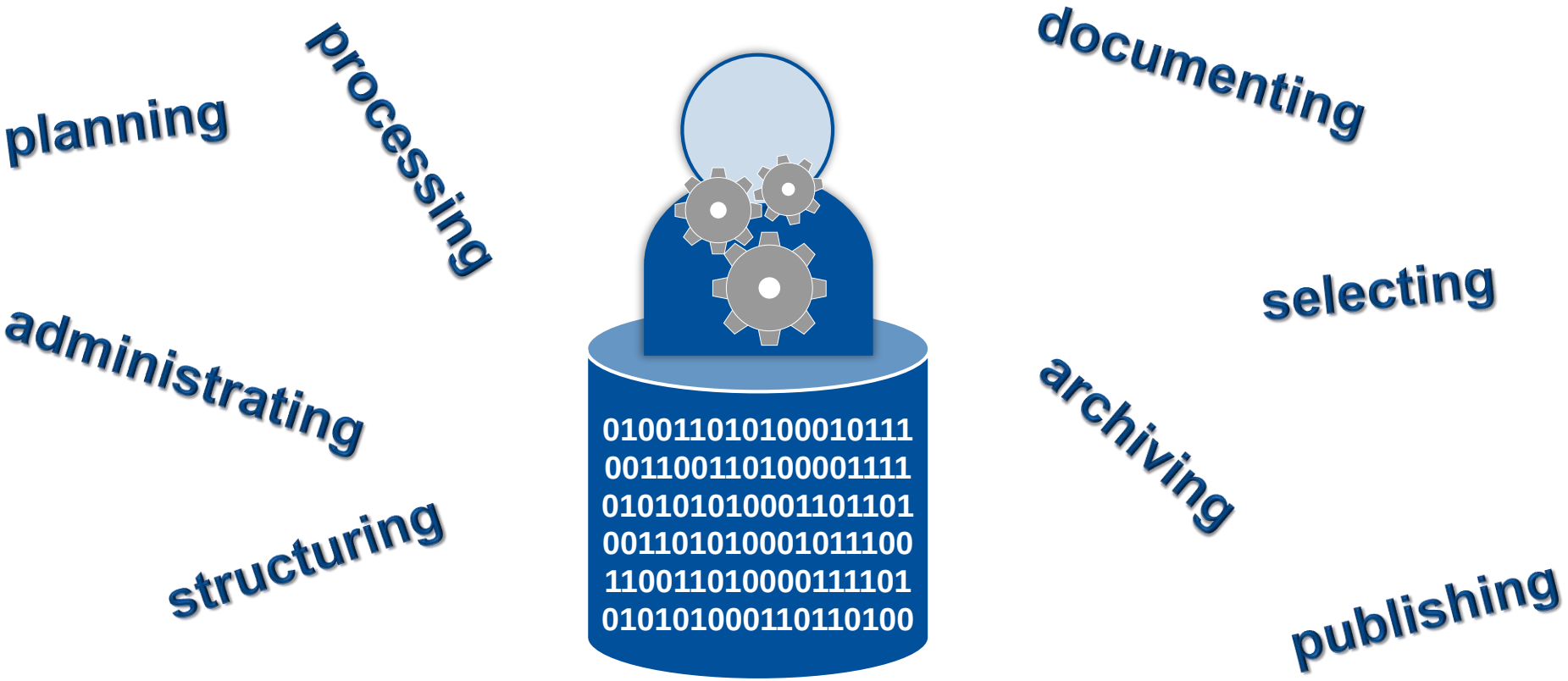
Processed data



Results



What is research data management (RDM)?



i RDM: Conscious and systematic handling of data from the planning stage until the end of a project and perhaps even beyond.

Why is data management important?

- ✓ you keep an overview
- ✓ team work is easier
- ✓ you can safeguard high quality standards in research
- ✓ you save time and avoid stress
- ✓ you comply with official requirements
- ✓ Data management is the basis for Open Science
- ✓ You gain recognition for published data and software

further reading

The Thuringian Competence Network for Research Data Management compiled some “Research Data Scarytales”. These are true stories about data management failures and their consequences.

go to the „Scarytales“

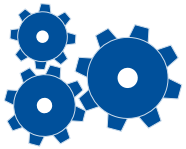
The FAIR Principles

Findable

- Unique and unambiguous identifier (e.g. DOI)
- Rich metadata (containing the DOI)
- Indexing in searchable directories (e.g. data repo)

Accessible

- Accessible via a standardized, open, free, universal communication protocol
- Transparent access (authentication)
- Metadata accessible even if data is not



Interoperable

- Standardized and widely applicable language for knowledge representation
- Vocabulary that follows FAIR principles
- References to related data

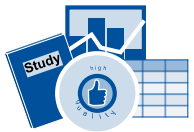
Re-usable

- Good documentation and precise attributes
- Clear license
- Detailed provenance
- Community standards

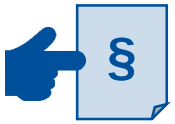
GO FAIR Website

RDM is good scientific practice!

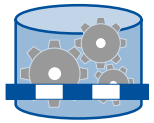
RDM is especially relevant for these 6 out of 19 guidelines:



Guideline 7: Cross-phase quality assurance



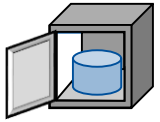
Guideline 10: Legal and ethical frameworks, usage rights



Guideline 11: Methods and standards

Guideline 12: Documentation

Guideline 13: Providing public access to research results



Guideline 17: Archiving

i

You can read the guidelines themselves and accompanying disciplinary comments in the DFG portal “Research Integrity” (English version not finished, yet).

to the DFG portal

!

Please note as well:

- DFG guidelines on the handling of research data
- disciplinary guidelines, requirements, policy papers etc.

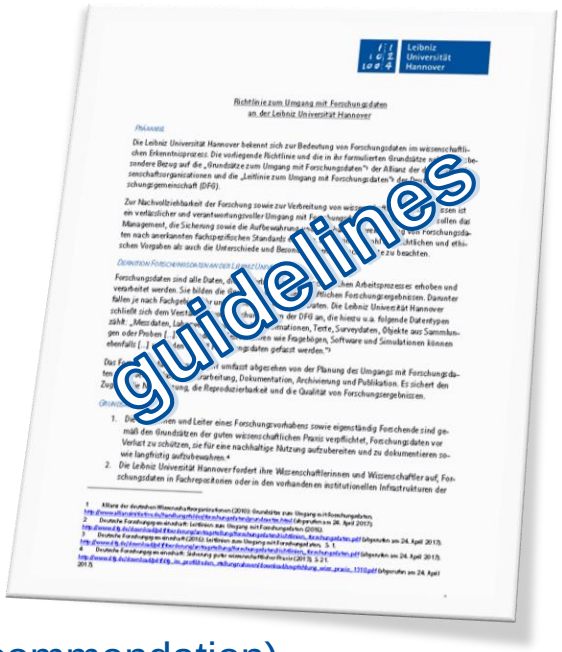
You can find both on this website:

to the DFG website „Handling of Research Data“

Guidelines for handling research data at LUH

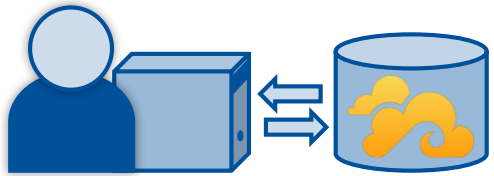
The four principles:

- Data management:
  - protect against losses
  - process for sustainable (re-)use
  - document
  - archive (long-term)
- publish research data according to the FAIR principles in (disciplinary) repositories
- develop project-internal RDM policies and data management plans (recommendation)
- integrate RDM into teaching (recommendation)



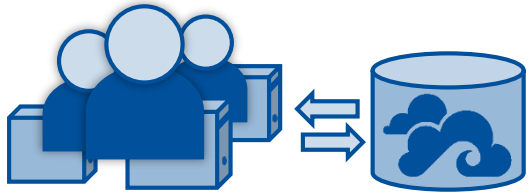
→ These principles do not include specific advice on research software (yet). But they do apply for software, as it is listed as a type of research data in the definition

LUIS services for data storage and backup



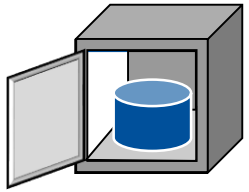
personal “Cloud-Seafile”
(storage + data synchronisation)

go to service description (German)



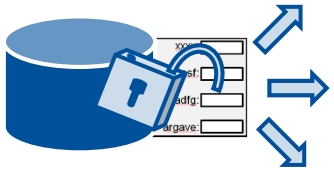
“Projekt-Seafile”
(storage + data synchronisation)

go to service description (German)



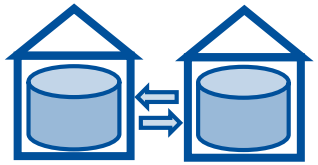
LUH data archive

go to service description (German)



LUH data repository

go to service description (German)



Backup & Restore
(for servers of institutes)

go to service description (German)

How to create re-usable research software

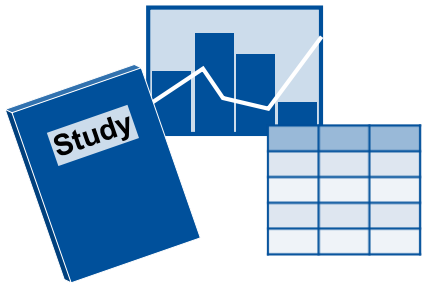
- Documentation of software projects
- The FAIR principles for research software
- Developing a software management plan (SMP)
- Services and infrastructure at LUH
- Foundation: How to set up a project
- Best practices of software projects
  - Tests and Test-driven development (TDD)
  - Refactoring
  - Clean code
  - Error messages
  - README

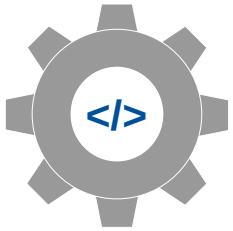
Documentation of software projects

Data

is not independent from

Research software



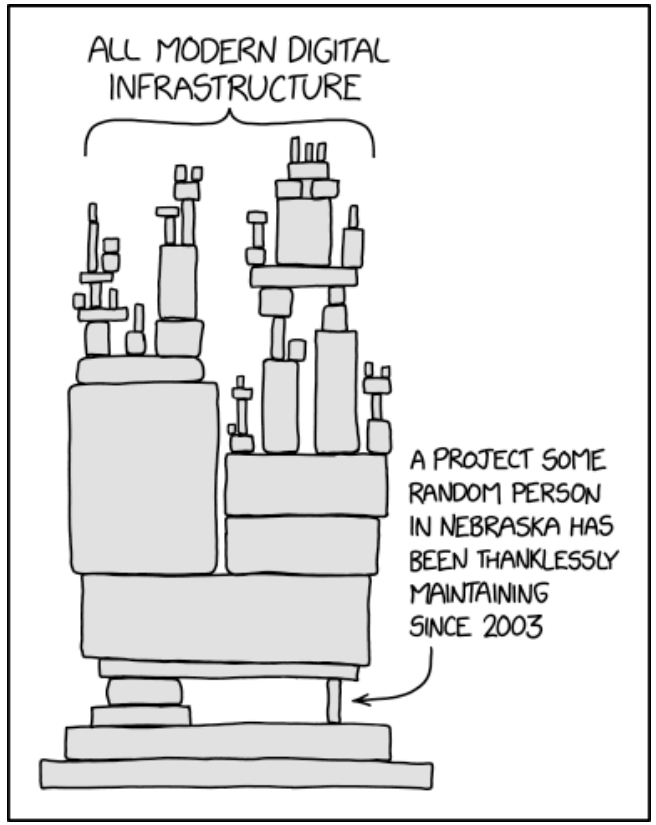


But most researchers

≠

Are no software developers

"Data without software are just numbers"
(Davenport & Grant, 2020)



https://xkcd.com/2347

The FAIR Principles for research software

F: Findable

This means that the software and all important related information can be easily found by both humans and machines.

F1. The software, individual important components of the software and the different versions of the software all receive persistent and unique identifiers (PID), e.g. DOI.

F2. The software is described in detail with metadata, which means that all important information for use and subsequent use is included.

F3. Metadata clearly and explicitly include the PID of the software they describe.

F4. Metadata is also FAIR, searchable and can be found and used by metasearch engines.

✓ Use persistent identifiers and rich metadata

Findable

The FAIR Principles for research software

A: Accessible

Which means that the software and its metadata is retrievable via standardized protocols

A1. For this, the protocol should fulfil some requirements, it should be open and free as well as universally implementable. It should also enable an authentication and authorisation procedure, if necessary.

A2. In addition the metadata are accessible, even when the Software is no longer available.

✓ Make software and metadata retrievable

Accessible

The FAIR Principles for research software

I: Interoperable

For software, being interoperable means the possibility to exchange data between independent software. (It differs from data in the way that independent software can not be combined like data to form a new data set.)

I1. When software interacts to exchange data, the exchange protocol need to be clearly described. Domain-relevant standards should be used and APIs should be documented in human and machine readable form.

I2. Software should include references to external data, software or objects, which are required to execute the software. Example: software X is implemented using software A (a programming language)

✓ Use APIs, standards and references

Interoperable

The FAIR Principles for research software

R: Reusable

This means that you can not only use the software as it is, but have further information to understand, modify and built new versions upon this software.

R1. The software is described with relevant attributes.

R1.1. A license is given and should be as unrestrictive as possible.

R1.2. Software is associated with detailed provenance: This is a metadata which includes the history of the software, how it came to be and who contributed to it.

R2. Include references to other software which is necessary to compile and run the software.

R3. Your software should meet domain-relevant community standards and coding practices. This can be the choice of programming language, testing methods or file formats.

✓ Document, licence, and follow community standards

Reusable

Developing a software management plan (SMP)

Can help to:

- Create a basis for establishing best practices
- Make the research software reusable and sustainable
- Plan for the necessary resources (financial, human, infrastructure)
- Make it easy to introduce new developers into the project

Ideally an SMP should be drafted at the beginning of a research project. The extent of information in the SMP varies with level of management intensity of the software (low, medium, high).

Software Management Plan (SMP)

A SMP does not need to be long. The following guide offers three templates adapted for different software management levels:

Practical guide to software management plans

The Max Planck Society has published a comprehensive SMP template, which can be integrated in RDMO:

MPG-Template “Software management plan for researcher”

Developing a software management plan (SMP) part I

- Purpose
- Version Control
- Repository
- User Documentation
- Software licensing and compatibility
- Deployment documentation

Figure 1. Software Management Plan requirements grouped by their focus.

Graphic from: Martinez-Ortiz, C. et al. (2022), Practical guide to Software Management Plans, p. 17. https://doi.org/10.5281/zenodo.7185371

Developing a software management plan (SMP) part II

- Citation
- Developer documentation
- Testing
- Software Engineering quality
- Packaging
- Maintenance
- Support
- Risk analysis

6.1.4. Summary of SMP templates developed for three management levels

Core requirement (Section 5.1)	Software management level (Section 6.1)		
	Management level: Low (6.1.1)	Management level: Medium (6.1.2)	Management level: High (6.1.3)
Purpose	×	×	×
Version control	×	×	×
Repository		×	×
User documentation		×	×
Software licencing and compatibility		×	×
Deployment documentation		×	×
Citation		×	×
Developer documentation		×	×
Testing		×	×
Software Engineering quality		×	×
Packaging		×	×
Maintenance		×	×
Support			×
Risk analysis			×

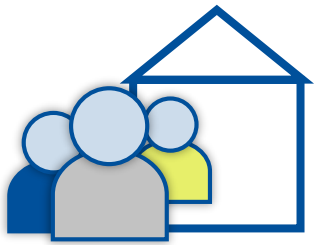
Table 4. Core requirements of an SMP for software grouped by management level.

Table from: Martinez-Ortiz, C. et al. (2022), Practical guide to Software Management Plans, p.29. https://doi.org/10.5281/zenodo.7185371

Services and infrastructure at LUH

For you

- Version control and software development: GitLab
- Courses for employees and students:
  - Statistics with R
  - Python: Introductory course, Object-oriented programming, Numerical calculation



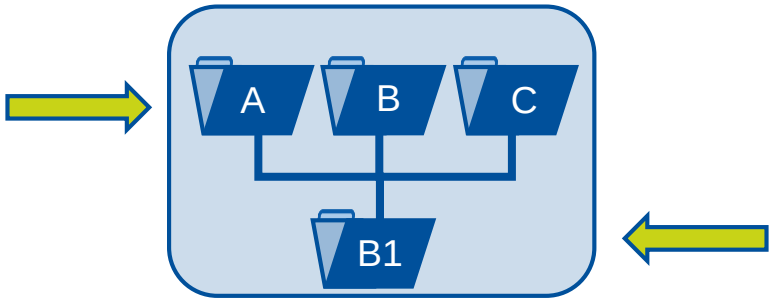
For your institution

- Research cluster housing service: The hardware of an institution can be integrated into the existing cluster system of LUIS
- Scientific Computing: For computationally intensive research project, LUIS provides a cluster system with massively parallel computer systems

Foundation: How to set up a project

Create a similar folder layout:

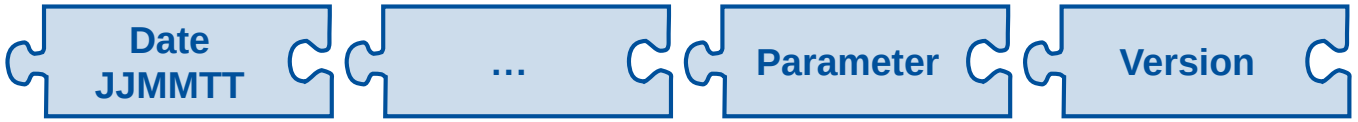
- Licence
- Readme
- Experiments (chronological)
- Provenance
- Scripts



Logical order in subfolders:

- Main script
- Data-generating scripts
- Raw data
- Post-processed data

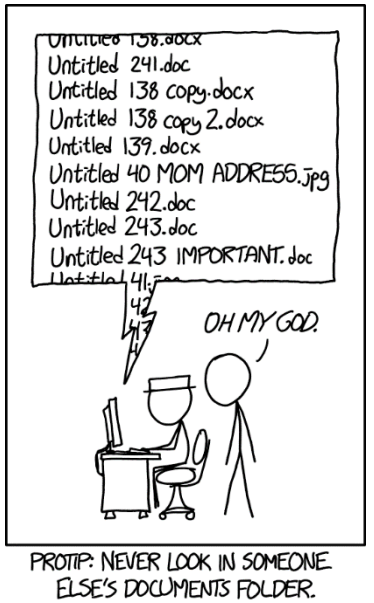
Modular naming scheme:



Example: 230701_PuppyCuteness_Treats_Cheese_Camembert_v03.fff

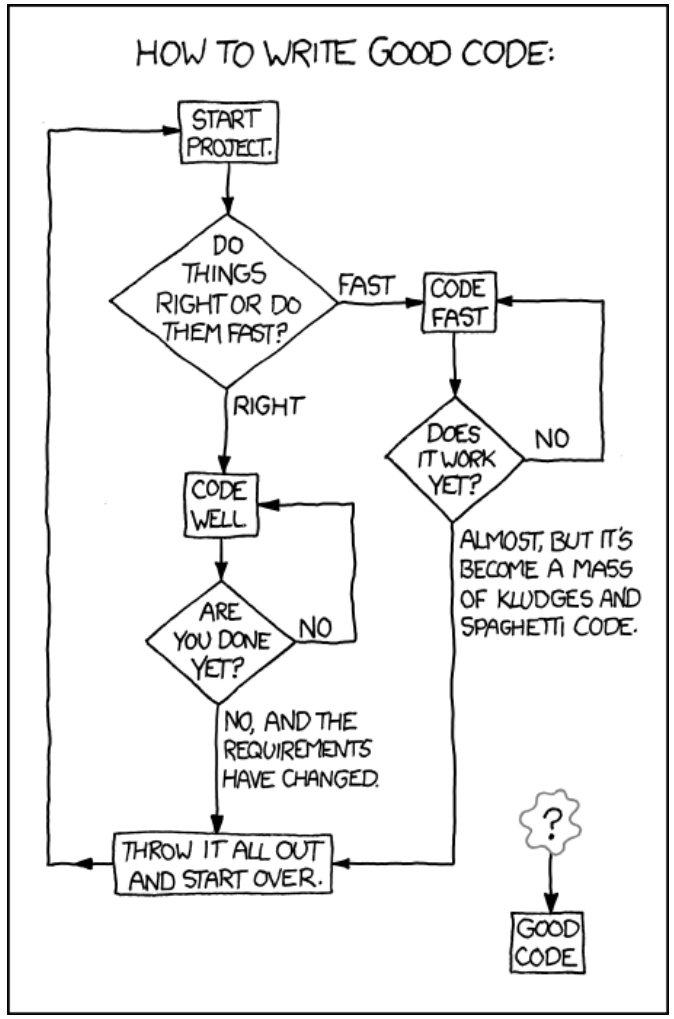
Data format: Better not choose "Fancy File Format"

Find a file format



https://xkcd.com/1459

Best practices of software projects



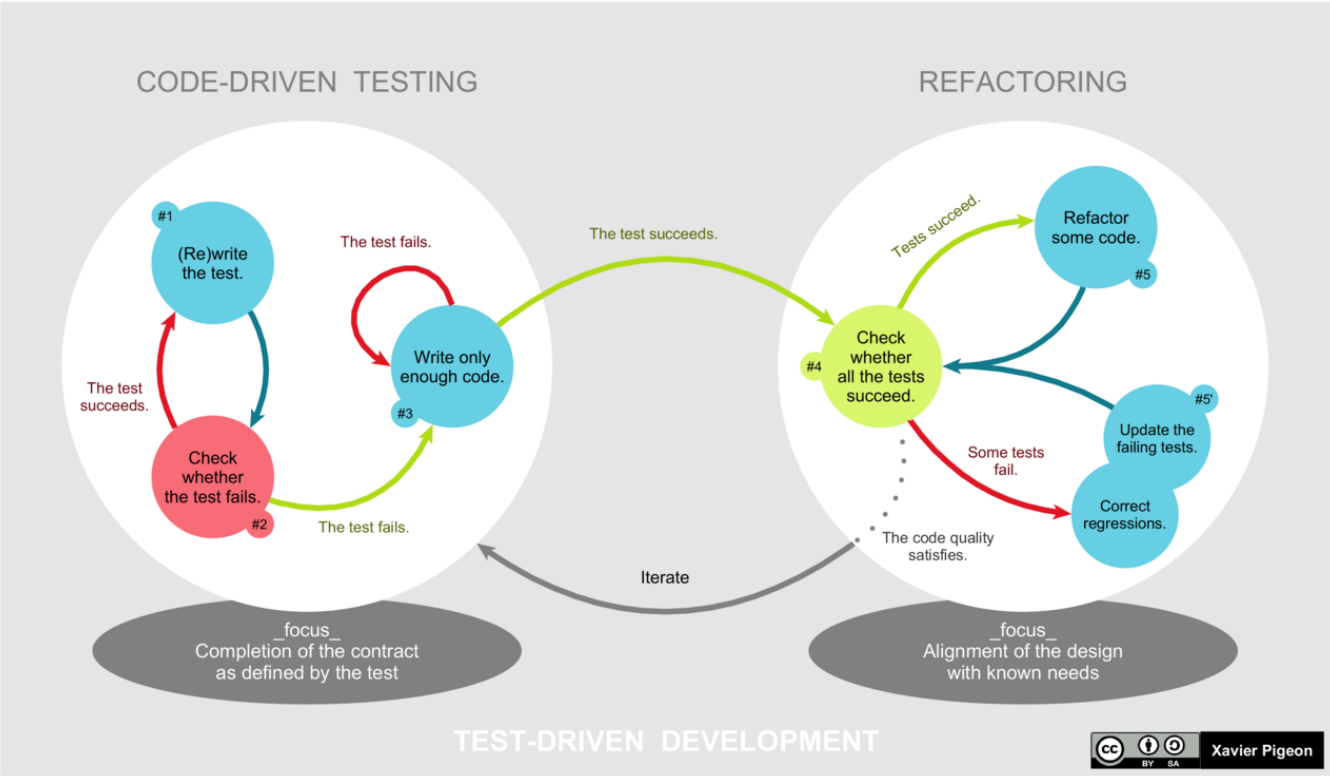
There are a number of published „Best practice“ guides for software development in different scientific fields. We have collected some general practices that help you to write FAIR software.

- Ten simple rules for documenting scientific software
- Oliver Melchert's best practices for small computational projects

Suresoft
SUSTAINABLE RESEARCH SOFTWARE

Best practice: Tests and Test-driven development (TDD)

- Include testing in the development process
- Each new piece of code is tested for functionality before it is added to the main branch
- Best practice: add incremental changes!
- TDD: First create a test for the desired functionality, then write the code that is able to fulfill the test requirements



Best practice: Refactoring

Code refactoring is the process of restructuring code without changing its original functionality.

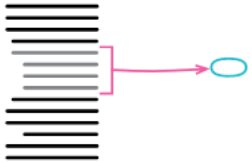
This helps to ensure that

- the code is more clearly structured and therefore easier to read and understand
- errors and weak points are easier to find and rectify
- the code is easier to extend and better to maintain

Martin Fowler, Refactoring: improving the design of existing code (German)

Robert C. Martin, Clean Code: Refactoring, Patterns, Testen und Techniken für sauberen Code

Extract Function



```
function printOwing(invoice) {
  printBanner();
  let outstanding  = calculateOutstanding();

  //print details
  console.log(`name: ${invoice.customer}`);
  console.log(`amount: ${outstanding}`);
}
```

```
function printOwing(invoice) {
  printBanner();
  let outstanding  = calculateOutstanding();
  printDetails(outstanding);

  function printDetails(outstanding) {
    console.log(`name: ${invoice.customer}`);
    console.log(`amount: ${outstanding}`);
  }
}
```

Martin Fowler, Refactoring catalog: https://refactoring.com/catalog/extractFunction.html

Best practice: Clean code

- There are different options how to write names, comments, functions and classes in your code
- Even though a “messy” written code might work, it is not re-usable
- Changing small habits can make a big difference!

In this example, it is better to define a function which contains the for-loop:

Do not

```
input_number = int(input("Enter a number"))

# check if input_number is a prime number
is_prime = True
for i in range(2, input_number):
    if input_number % i == 0:
        is_prime = False
        break

print(input_number, "is a prime:", is_prime)
```

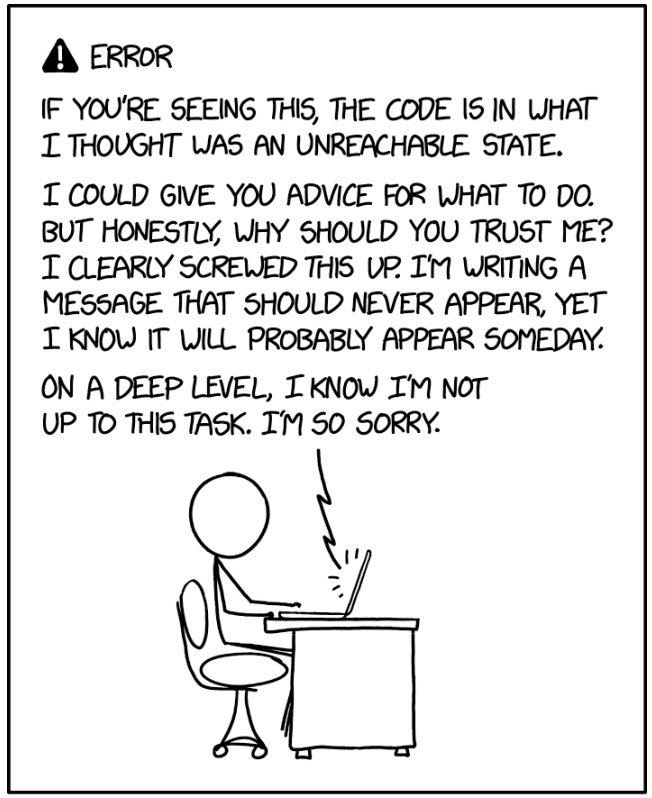
Do

```
def is_prime(number):
    prime_flag = True

    for i in range(2, number):
        if number % i == 0:
            prime_flag = False
            break

    return prime_flag


input_number = int(input("Enter a number"))
print(input_number, "is a prime:", is_prime(input_number))
```

https://suresoft.dev

Best Practice: Error messages

- Write error messages
- Provide solutions or where to find the information relevant to fixing the error.



NEVER WRITE ERROR MESSAGES TIRED.

https://xkcd.com/2200

Graphic: Unknown, via: https://community.spiceworks.com/topic/2105369-10-hilarious-error-messages-facepalm-worthy-computer-prompts-that-make-no-sense

Best practice: README Part I

- Give an overview of the project
- List the names and affiliation of people involved
- Environment and dependencies needed to run the code

Environment and dependencies

The provided code is written using Python (2.7.15+) and requires the functionality of

- numpy (>=1.8.0rc1)
- scipy (>=0.13.0b1)
- matplotlib (>=1.2.1)

All-optical Supercontinuum Switching (code and data)

Code repository for the article

"All-optical Supercontinuum Switching"

Oliver Melchert (1,2,3), Carsten Brée (4), Ayhan Tajalli (2), Alexander Pape (2,5), Rostislav Arkhipov (6), Stephanie Willms (1,2), Ihar Babushkin (1,2), Dmitry Skryabin (7), Günter Steinmeyer (8,9), Uwe Morgner (1,2,3), and Ayhan Demircan (1,2,3)

1. Cluster of Excellence PhoenixD, Welfengarten 1, 30167, Hannover, Germany
2. Institute of Quantum Optics, Leibniz University Hannover, Welfengarten 1 30167, Hannover, Germany
3. Hannover Centre for Optical Technologies, Nienburgerstr. 17, 30167, Hannover, Germany
4. Weierstraß Institute for Applied Analysis and Stochastics, Mohrenstraße 39, 10117 Berlin, Germany
5. VALO Innovations GmbH, Hollerithallee 17, 30419, Hannover, Germany
6. St. Petersburg State University, Universitetskaya nab. 7/9, St. Petersburg 199034, Russia
7. Department of Physics, University of Bath, Bath, BA2 7AY, UK
8. Max-Born-Institute (MBI), Max-Born-Str. 2a, 12489 Berlin
9. Institut für Physik, Humboldt-Universität zu Berlin, Newtonstraße 15, 12489 Berlin, Germany

This repository contains code and data analysis scripts for reproduction of simulated data and a draft versions of Figures 3 of the article.

The provided code implements the nonlinear propagation of optical pulses in a NLPM750 photonic crystal fiber in terms of the generalized nonlinear Schrödinger equation, including the effets of dispersion, self-phase modulation, self-steepening, Raman effect, and quantum noise.

Best practice: README Part II

- Details about included material
- License, Citation & Acknowledgements

Subfolder `/scripts` contains:

- `pyGNLSE.py` : driver script implementing the genaralized nonlinear Schrödinger equation.

License

This project is licensed under the MIT License - see the LICENSE file for details.

Acknowledgments

This work received funding from the Deutsche Forschungsgemeinschaft (DFG) under Germany's Excellence Strategy within the Cluster of Excellence PhoenixD (Photonics, Optics, and Engineering – Innovation Across Disciplines) (EXC 2122, projectID 390833453).

Included materials

The repository follows a modular structure:

```
numExp01_FIG03_propagationDynamics
├── data
├── FIG03_subfigures
│   ├── FIGS
│   │   ├── GNLSE_BlowWood_tMax8000.000000_Nt32768_zMax600000.000000_Nz15
│   │   ├── GNLSE_BlowWood_tMax8000.000000_Nt32768_zMax600000.000000_Nz15
│   │   └── GNLSE_BlowWood_tMax8000.000000_Nt32768_zMax600000.000000_Nz15
│   ├── getFigures.sh
│   ├── main_FIG03_subfigure.py
│   └── spectrogram.py
└── main_NLPM750_propagationDynamics_qNoise.py

provenance_data
├── dataProvenance.sh
├── get_info.py
└── provenance_numExp01.log

scripts
└── pyGNLSE.py

src
├── data_handler.py
├── raman_response.py
├── solver.py
└── utils.py

LICENSE
Readme.md
```

How to publish research software and code

- Why publish your data and software?
- Preparation of your software publication
  - Version control your documentation
  - Use automated documentation tools
  - Software citation
  - User guide and examples
- Publishing software
- Licences
- Linking journal articles with related data and software
- Example: Publish software via Zenodo

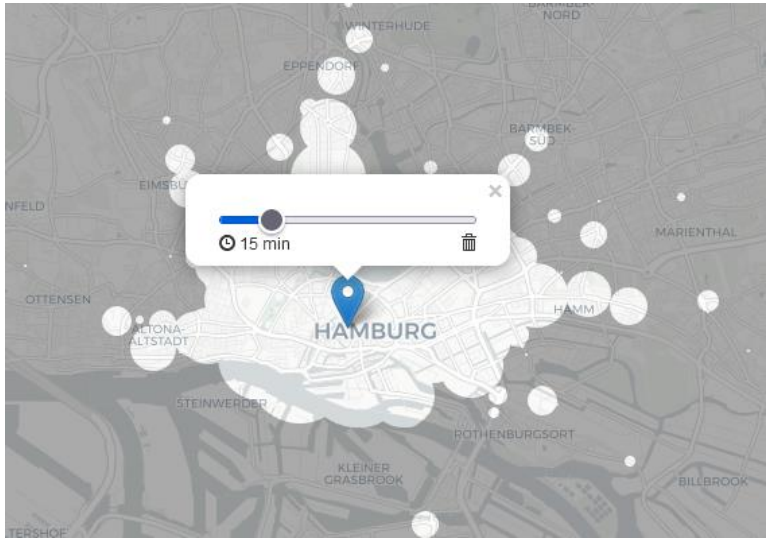
Why publish your data and software?

Open data are valuable and can be used to create new research output or tools of public interest:

- Participation: findtoilet.dk
- Empowerment of citizens: mapnificient
- Innovation: EHEC outbreak genome analysis

Reasons to publish your research software:

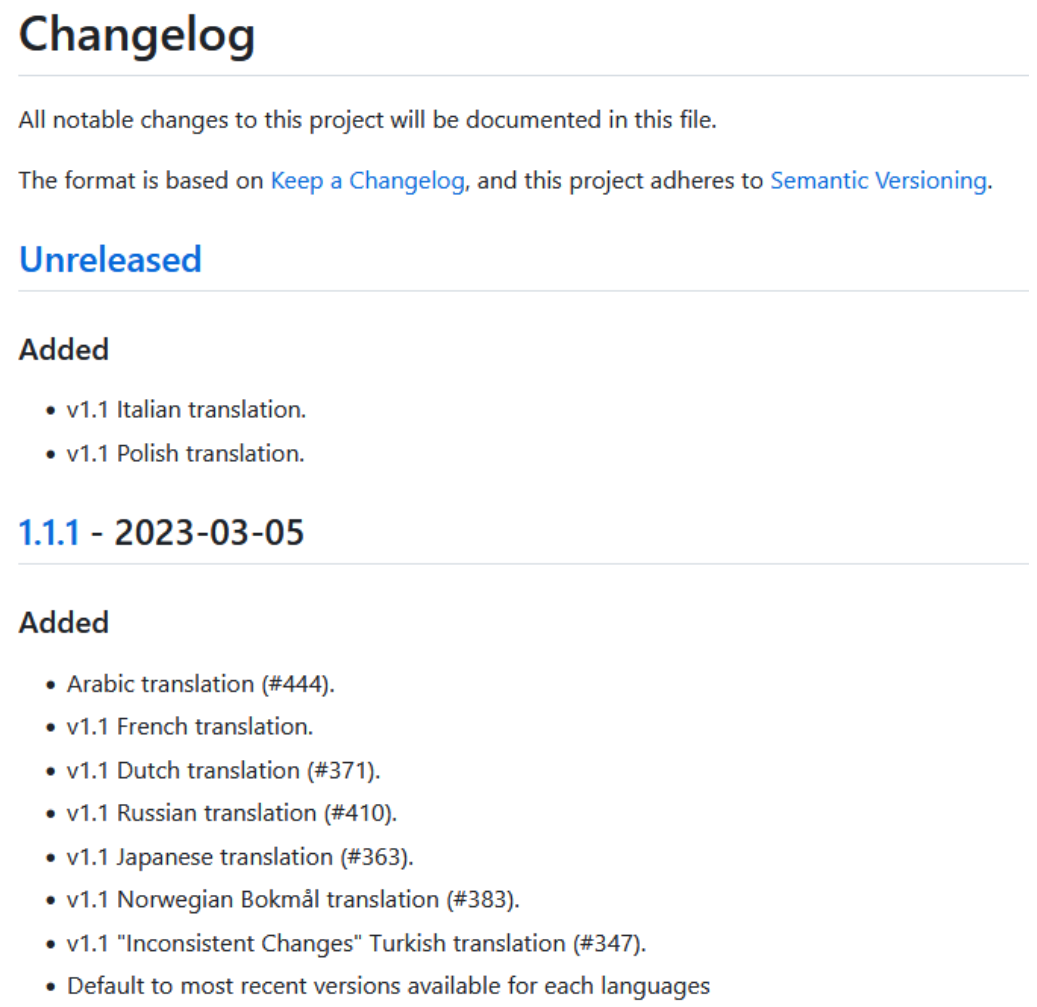
- To enable software citation
- To make the software FAIR
- To let software count towards evaluation



Mapnificent.net

Software publication: Version control your documentation

- Make it clear which documentation applies to which software version
- A changelog can make this task much easier
- There are useful services that can help you do this.



Changelog

All notable changes to this project will be documented in this file.

The format is based on Keep a Changelog, and this project adheres to Semantic Versioning.

Unreleased

Added

- v1.1 Italian translation.
- v1.1 Polish translation.

1.1.1 - 2023-03-05

Added

- Arabic translation (#444).
- v1.1 French translation.
- v1.1 Dutch translation (#371).
- v1.1 Russian translation (#410).
- v1.1 Japanese translation (#363).
- v1.1 Norwegian Bokmål translation (#383).
- v1.1 "Inconsistent Changes" Turkish translation (#347).
- Default to most recent versions available for each languages

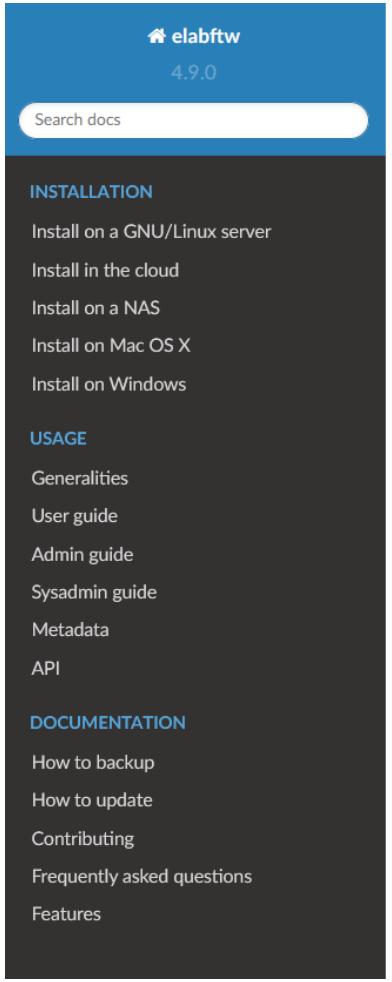
Screenshot: https://github.com/olivierlacan/keep-a-changelog/blob/main/CHANGELOG.md

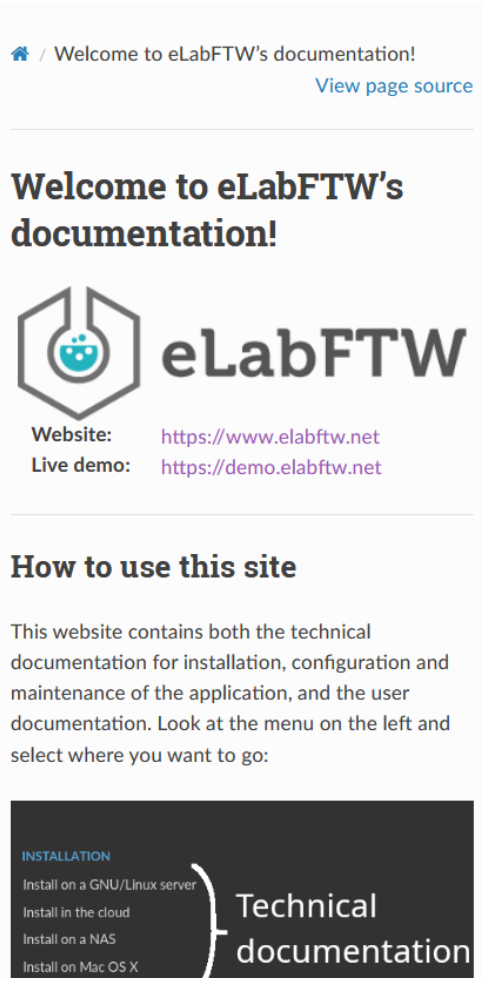
Best Practice: Use documentation tools

- Documentation of a project is the alpha and omega
- Complete and prompt documentation is essential
- Use tools to create a nice documentation site which helps others to use your software

Sphinx Python Documentation Generator:

```
docs
├── build
├── make.bat
├── Makefile
└── source
    ├── conf.py
    ├── index.rst
    ├── _static
    └── _templates
```





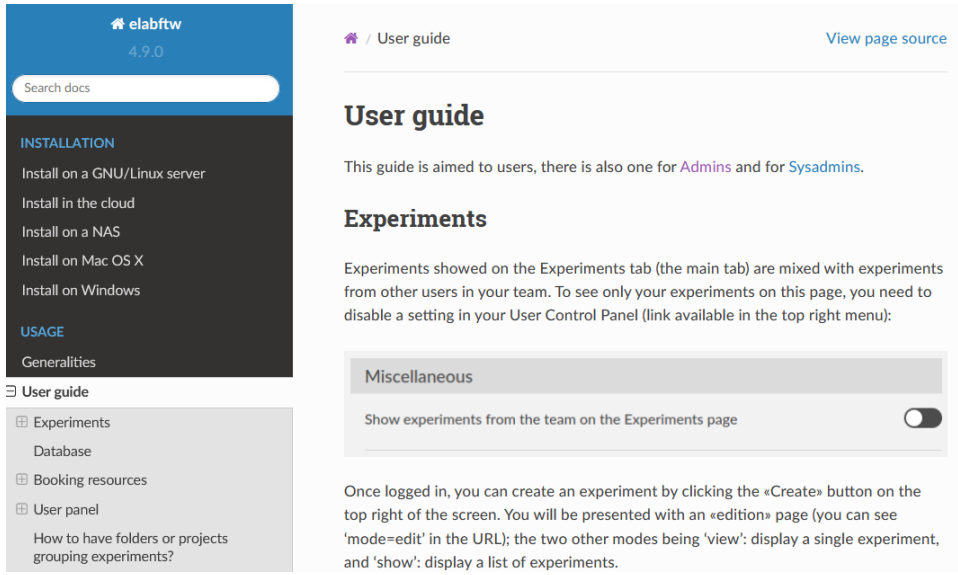
Software publication: Software Citation

- Provide information on how to cite your code
- Be sure to always properly cite other people's code that you reuse as well

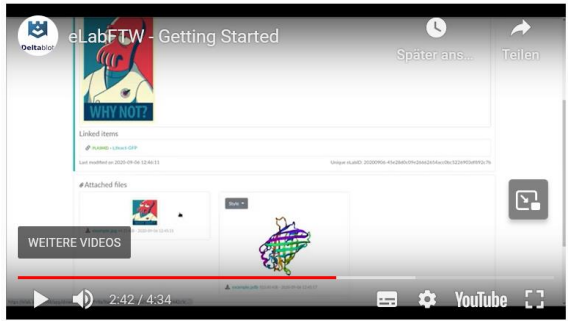
```
# This CITATION.cff file was generated with cffinit.
# Visit https://bit.ly/cffinit to generate yours today!

cff-version: 1.2.0
title: Cheese_TAX_Alert
message: >-
  If you use this software, please cite it using the
  metadata from this file.
type: software
authors:
  - given-names: Sheryl
    family-names: Mc Sniff
    email: SMS@gmail.com
    affiliation: University of Dogford
repository-code: 'https://git.eu/McSniff/cheesetaxalert'
repository: 'https://doi.org/10.123456789/mcsniff'
abstract: >-
  the software can be installed in a refrigerator so that as
  soon as the refrigerator door is opened, the Puppy
  receives a warning signal that the Cheese Tax must be
  collected.
keywords:
  - puppy
  - cheese
  - tax
license: MIT
version: '1.0'
date-released: '2023-09-01'
```

Software publication: User guide and examples

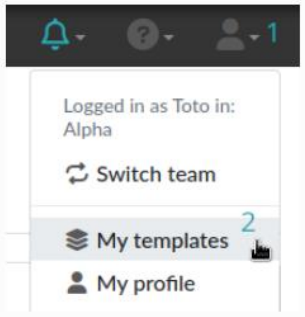
- People might not use your software if it takes too much time to get started
- Add examples, a tutorial, videos – anything that helps to show the functionalities of your software
- If you have numerous examples, use a special section or directory
- Try your user guide on someone who does not know your software yet



Video tutorials



Screenshots



Publishing software

- Publish software in a publication repository (like Zenodo or your institutional data repository)
  - This gives you:
    - An unique and persistent identifier (e.g. DOI)
    - An identifier that points to the specific version of your software
- Provide citation metadata for your software (via CFF)
- License your code
- Possibility of additional publication in a software journal

Repository publication → software journal → papers

Important: The source code repository (e.g. GitHub, GitLab) is not a publication repository!

Licenses

Common software licenses:

- MIT
- MPL 2.0
- GPL 3.0 – only

Choose an open source license

Licenses for text and data:

Creative Commons licenses

- CC0 – no name attribution, no restrictions
- CC-BY – author attribution when using the data
- CC-BY-SA – author attribution and share under the same conditions

Choose a CC license

Example: Overview of the MIT-License

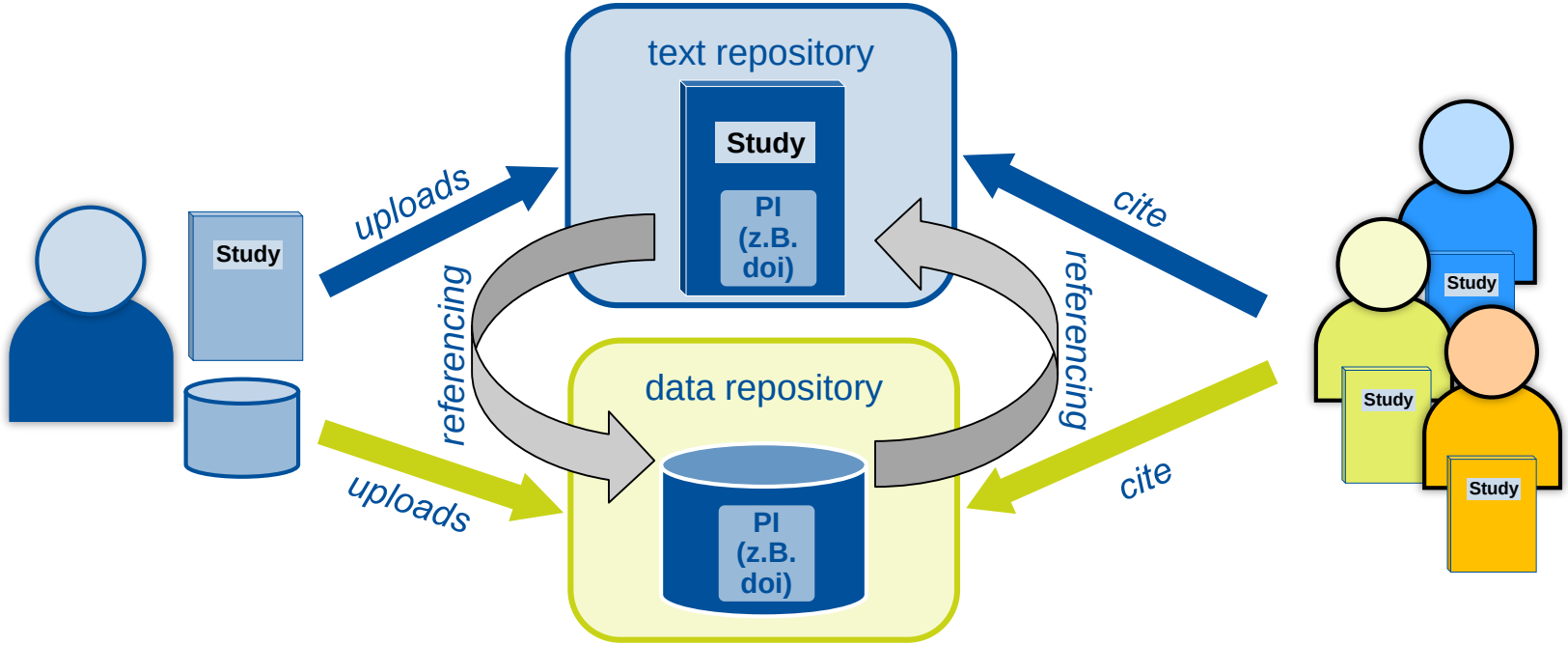
MIT License

A short and simple permissive license with conditions only requiring preservation of copyright and license notices. Licensed works, modifications, and larger works may be distributed under different terms and without source code.

Permissions	Conditions	Limitations
Commercial use	License and copyright notice	Liability
Distribution		Warranty
Modification		
Private use		

https://choosealicense.com/licenses/mit/

Linking journal articles with related data and software



further reading

Diana Kwon (2019): The Push to Replace Journal Supplements with Repositories. Online article, 19 August 2019, on the website of „The Scientist“.

go to article

LUH also provides its own institutional text repository for open access publications.

go to text repository

Summary

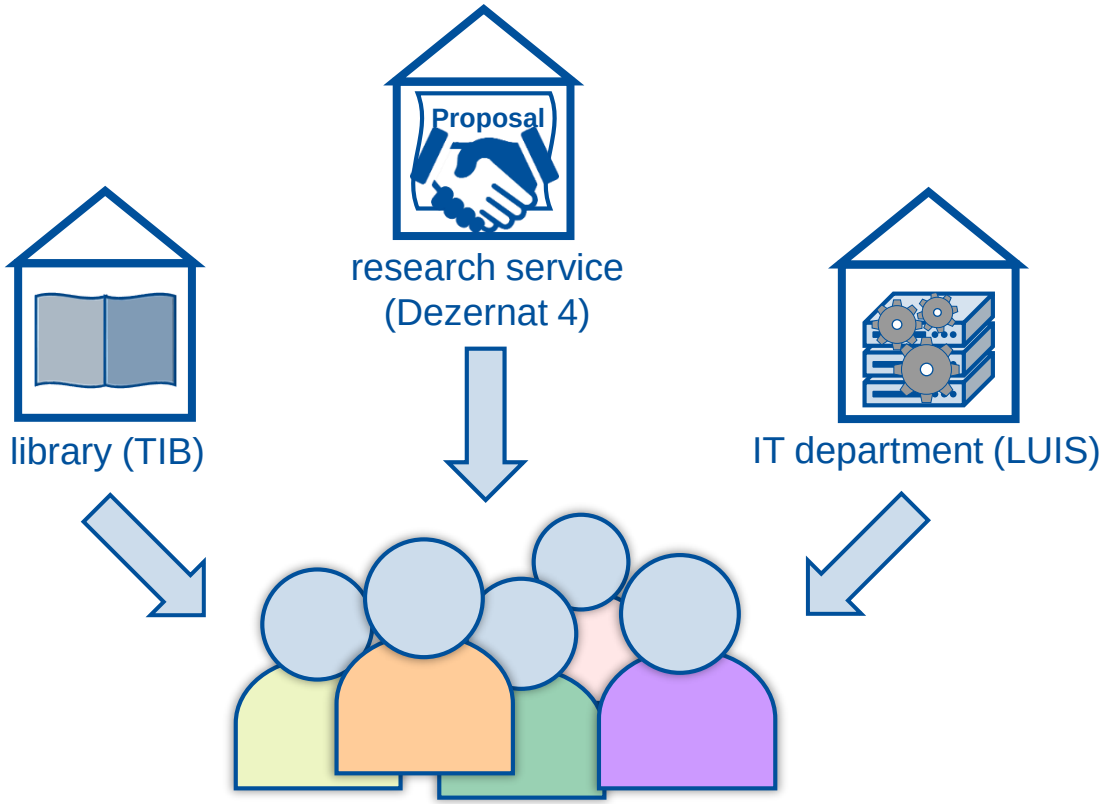
- Software management happens before you even start coding:
  - Clarify responsibilities
  - Agree on standards and methods and write them down (SMP)
  - Recognize that data and software management are work tasks that will consume some of your time
- Develop a culture that values data- and software management
  - Include the best practices in your everyday work
  - Think of your future self and anyone who might want to re-use your code
  - Engage in projects of others: Create and solve issues, reuse instead of setting up new

https://xkcd.com/1421/

Supporting services and initiatives

- The Research Data Support Team of LUH
- External information and support
- RSE working groups and initiatives

The Research Data Support Team of LUH



Sign up for our monthly newsletter on RDM!

i

We train and counsel LUH members on the following topics, among others:

- documentation and publication of data
- DMP and RDM policies
- RDM statements in funding proposals
- LUH services and infrastructures for data management
- legal issues (in cooperation with the legal department and the data protection office)
- practical implementation of data management in research processes

Please note as well the additional information, guides and training courses on our website.

go to website of the Research Data Support Team

External information and support

Courses, talks and schools:

Suresoft Project: Workshop schedule with courses on best practices in research software engineering

Hessian Research Data Infrastructures: Data and Code Schools, Data Talks

Helmholtz Information & Data Science Academy:
Courses, schools, workshops & talks

Self-training courses:

Suresoft Knowledge Hub: Workshops on Git foundations, Clean Code, Software Testing, CI and more

Software Carpentry: You can work through the lessons on the Unix Shell, Git, Programming with Python or R by yourself

RSE working groups and initiatives

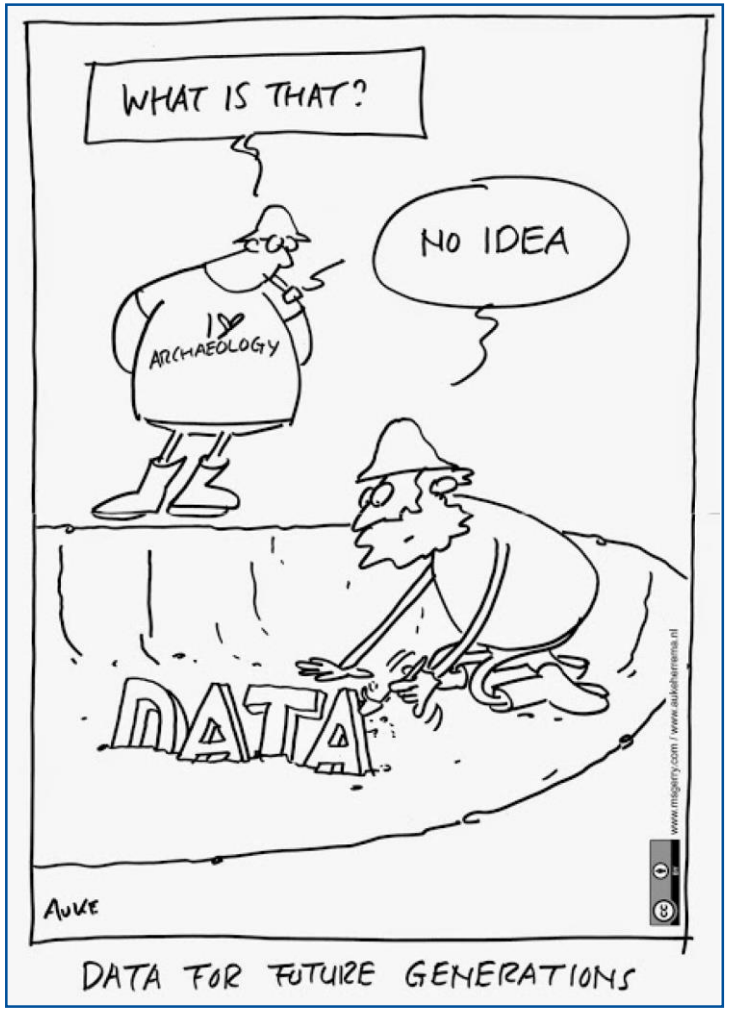
Research Software Engineers (RSEs)
- German association (de-RSE e.V.)
- monthly call, Chat, Blog
- International conferences for and by Research Software Engineers

Research Data Alliance (RDA):
International network of RDM specialists with a special focus on technical aspects.

Software Sustainability Institute (UK)
- Motto: “Better software, better research”
- Research Software Healthcheck: Evaluation tool to check your software
- online Research Software Camps

NFDI: The federal government and the state governments jointly fund the development of a national research data infrastructure (NFDI). X consortia are developing disciplinary standards, establish services and offer trainings.

Thank you for taking this course!



by Auke Herrema