ScaDS.AI DRESDEN LEIPZIG

CENTER FOR SCALABLE DATA ANALYTICS AND ARTIFICIAL INTELLIGENCE

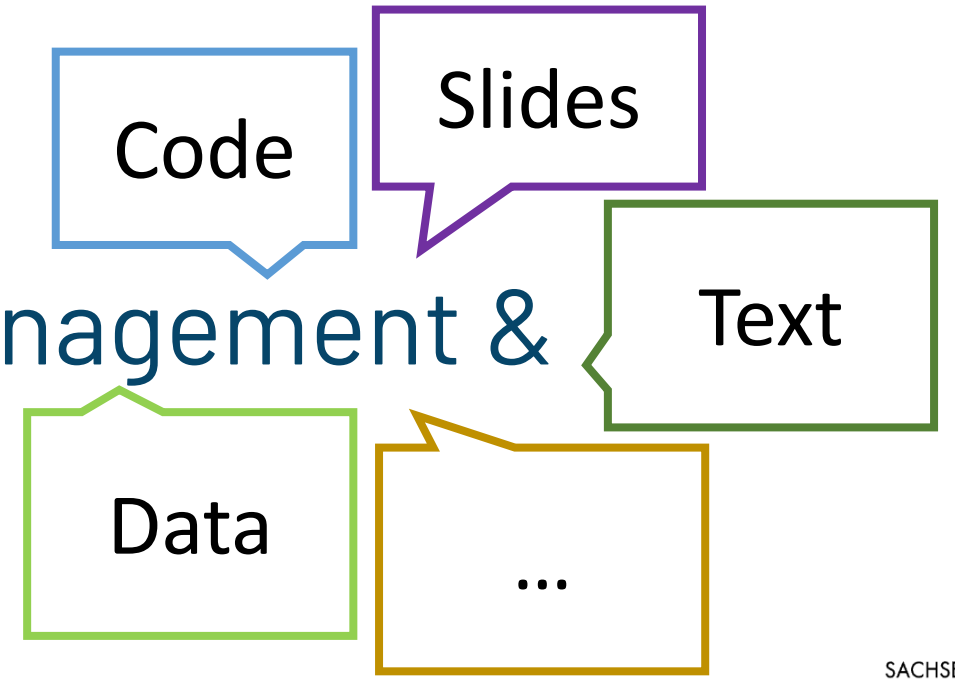
NFDI 4 BIOIMAGE

NATIONAL RESEARCH DATA MANAGEMENT INFRASTRUCTURE FOR MICROSCOPY AND BIOIMAGE ANALYSIS

GloBIAS Global BioImage Analysts' Society

GLOBAL BIOIMAGE ANALYST'S SOCIETY

Research Data Management & Open Science



Robert Haase

GEFÖRDERT VOM

Bundesministerium für Bildung und Forschung

SACHSEN

Diese Maßnahme wird gefördert durch die Bundesregierung aufgrund eines Beschlusses des Deutschen Bundestages. Diese Maßnahme wird mitfinanziert durch Steuermittel auf der Grundlage des von den Abgeordneten des Sächsischen Landtags beschlossenen Haushaltes.

Quiz

- When you shared materials over the internet, which *platform* did you use?

Onedrive/Google cloud/Dropbox/etc.	Zenodo/Figshare/ arxiv/F1000	Email	Other
			

Closed science

Why are some science-related materials/data/code not shared?

- Risk of being scooped
- Fear of blaming oneself (imposter syndrome)
- Lack of awareness (who is allowed to publish *my work*?)
- Assumption: it’s not worth the effort.

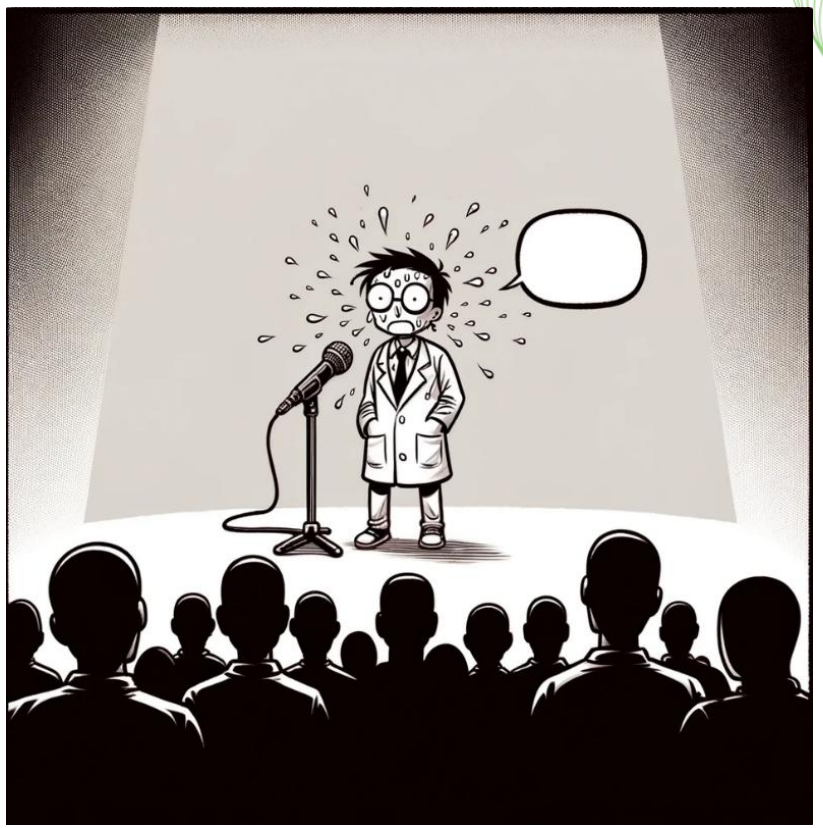


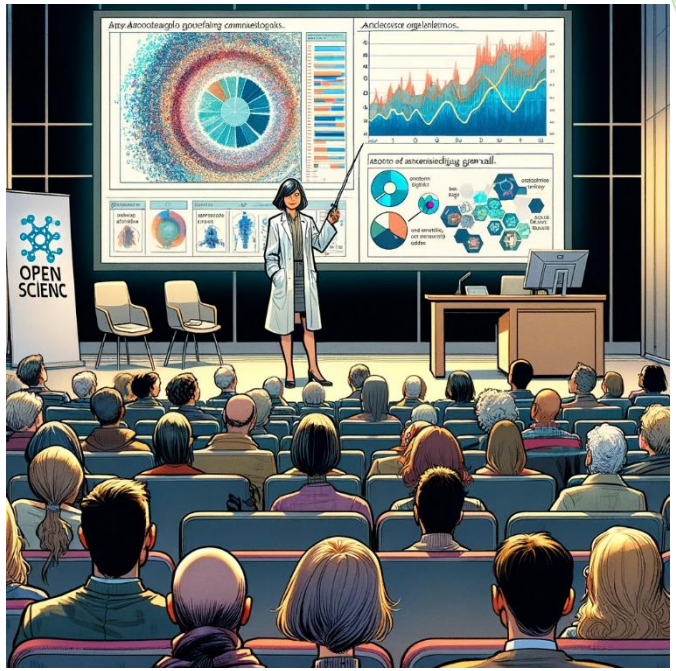
Image was created using Generative AI (Dall-E)

Open Science

- Research related (hot topics)
- Often tailored towards general audience (science communication)
- Earliest at the time a manuscript is published (e.g. as preprint)

Open Training

- Routine tasks (colder topics)
- Transfer of domain-specific knowledge



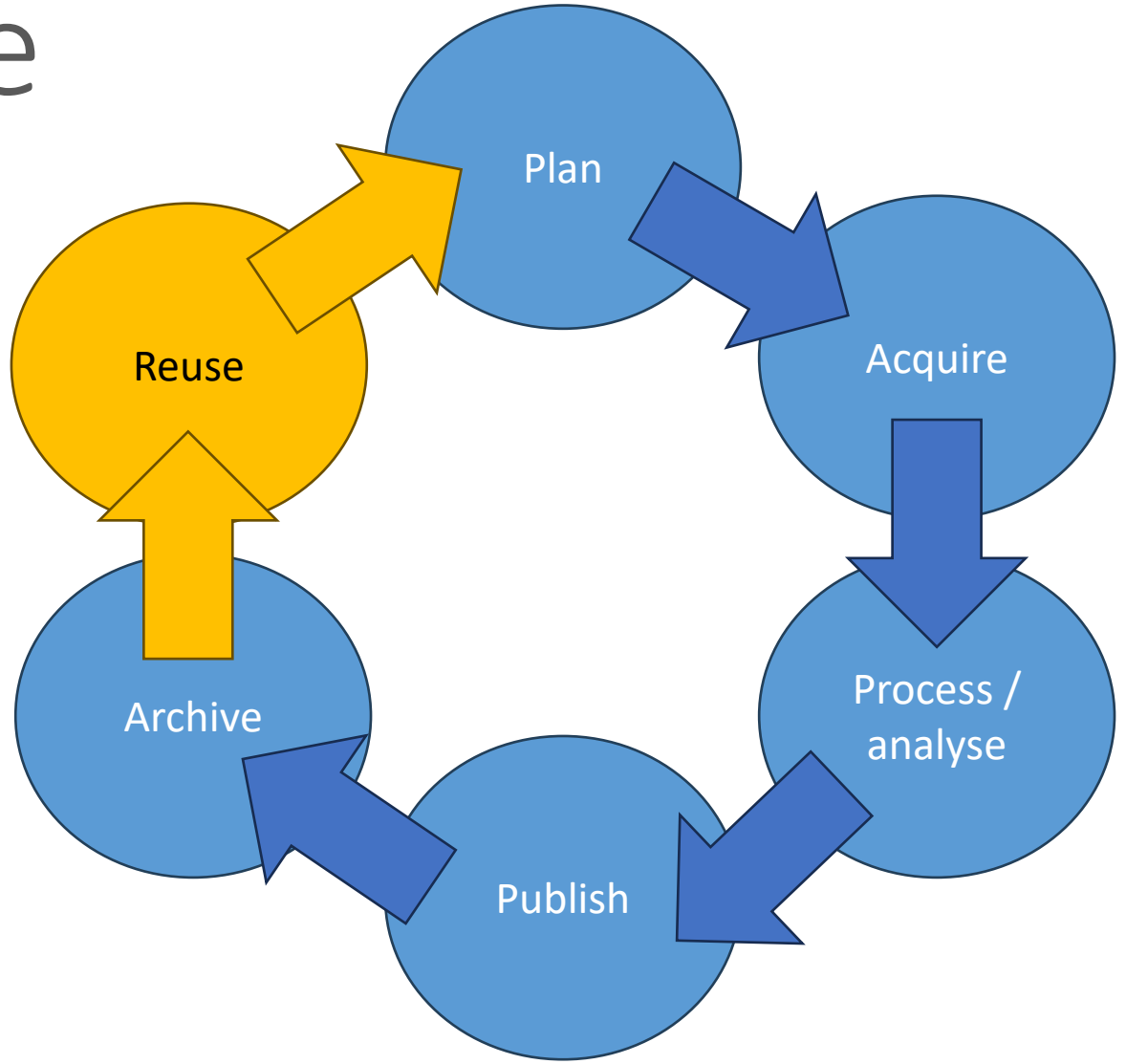
Research Data Management (RDM)

- All activities, processes, terms, persons which have relationships with data
  - Processing
  - Storage
  - Organization
  - Publication
  - …
- In routine: working with data

Image was created using Generative AI (Dall-E)

RDM Life Cycle

- Processes are ideally cyclic
- Closing the loop is a major the challenge

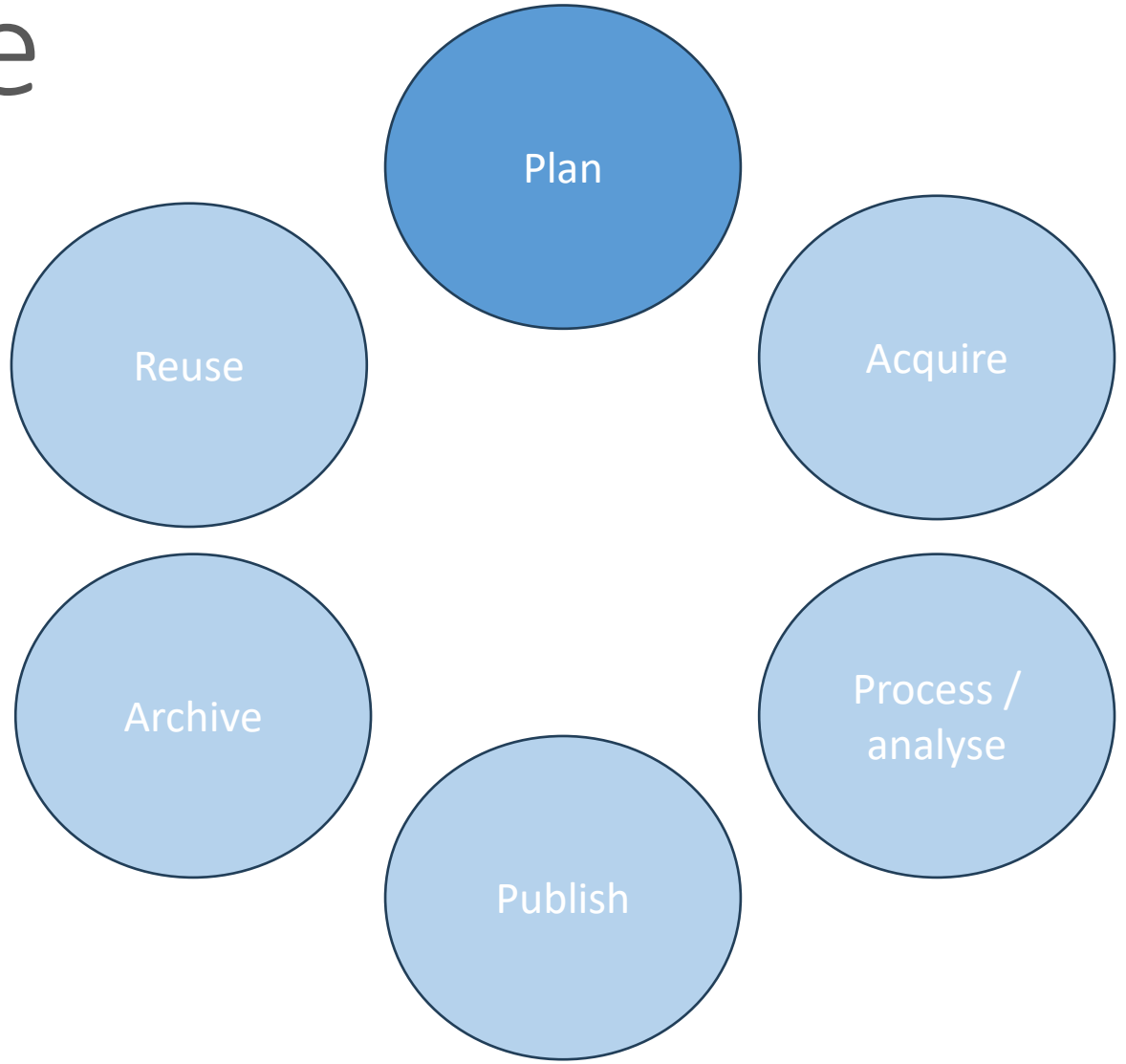


Adaptiert von:
https://forschungsdaten.info/themen/informieren-und-planen/datenlebenszyklus/

RDM Life Cycle

Plan

- Cost
- Benefit
- Quality
- Strategic decisions



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Data Management Plans (DMPs)

- Define responsibilities and procedures early!

"Data / materials we produce will be published under CC-BY 4.0"

"Robert will do this by end of 2025!"

DMP

- Only if procedures are defined early, everyone can follow them.
- Licenses are important when assembling materials (-> Copyright)
- Meta-data might have *higher quality* if the person responsible for publishing the data is aware of their duties.

Are we going to publish data / materials / code?

What license can we use?

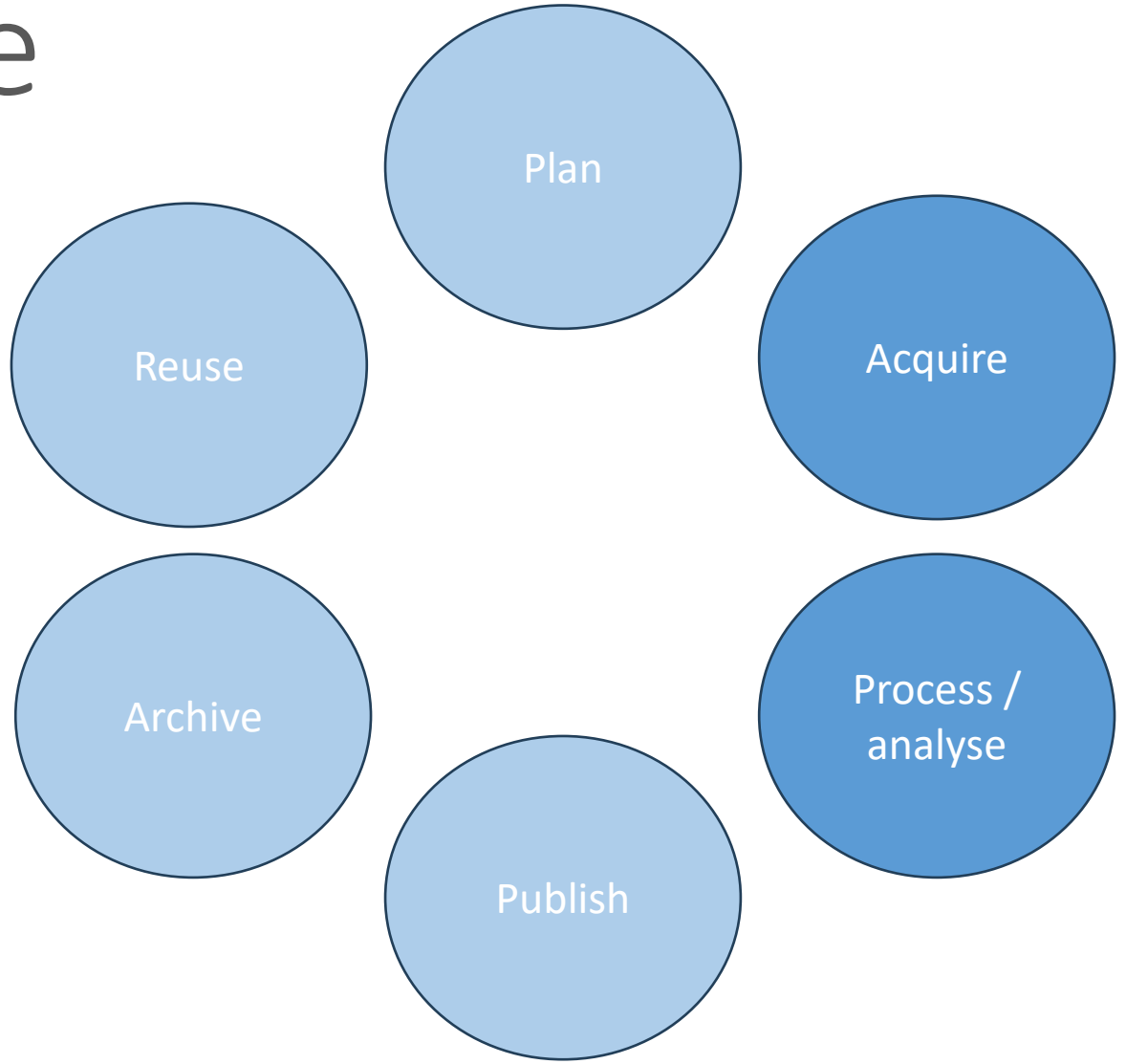
Deciding by the end of the project is too late!

RDM Life Cycle

Acquisition + Processing

- Types of data
- Terms and conditions
  - Usage rights
  - Copyright

- IT infrastructure
  - HPC
  - USB-Drives
- Backup



Adaptiert von:
https://forschungsdaten.info/themen/informieren-und-planen/datenlebenszyklus/

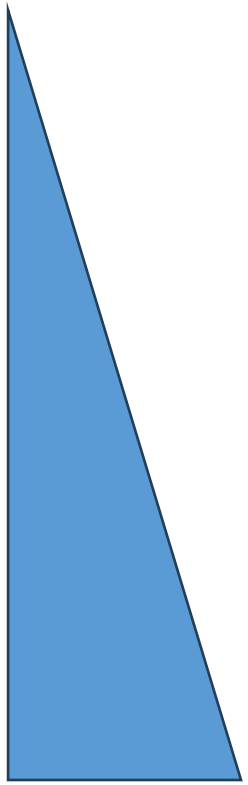
Types of data

- Structured data
  - Tables, databases
- Unstructured data
  - Texte, emails, videos, pictures
- Semi-structured data
  - Surveys
  - Scientific images

Image was created using Generative AI (Dall-E)

Types of data

- Openly accessible data
  - „open data“
  - „open source“ software
- Business data
- Research data
  - Hot / cold
- Personal data
- Secret data



In need of protection (schutzbedürftig)

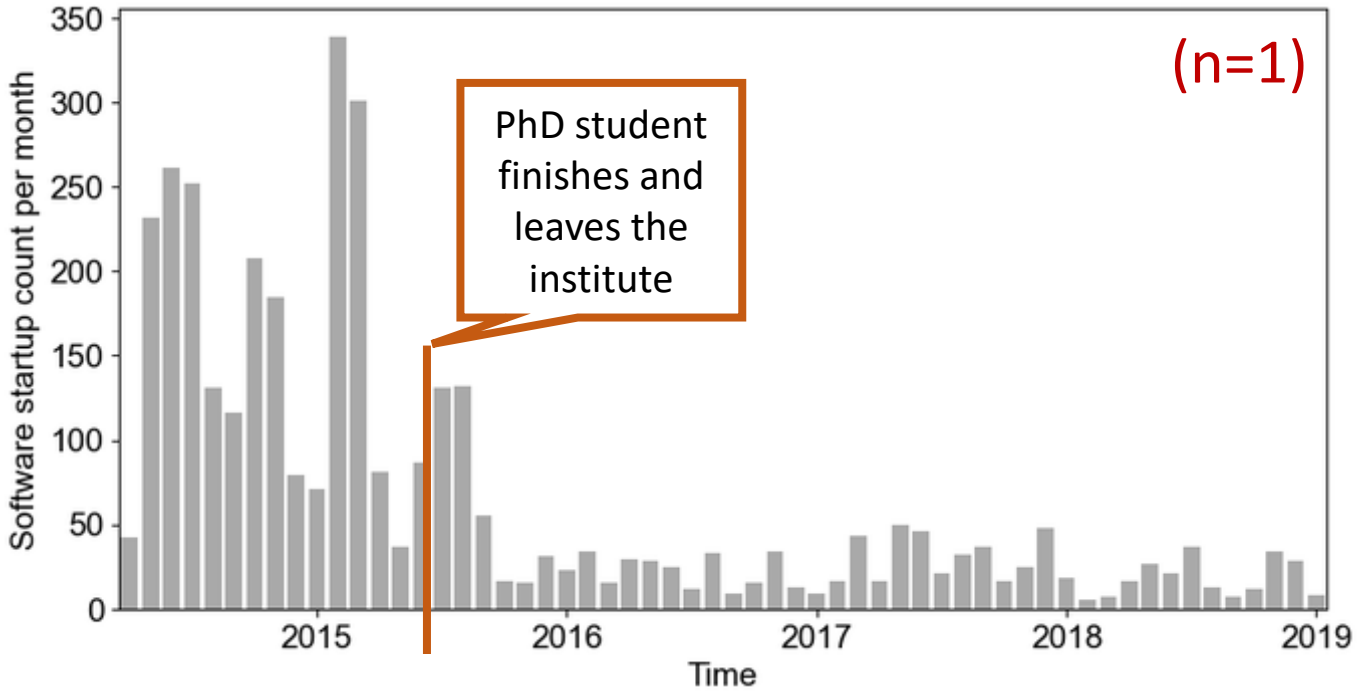
Image was created using Generative AI (Dall-E)

Version control [for code]

- Me, during my Phd:

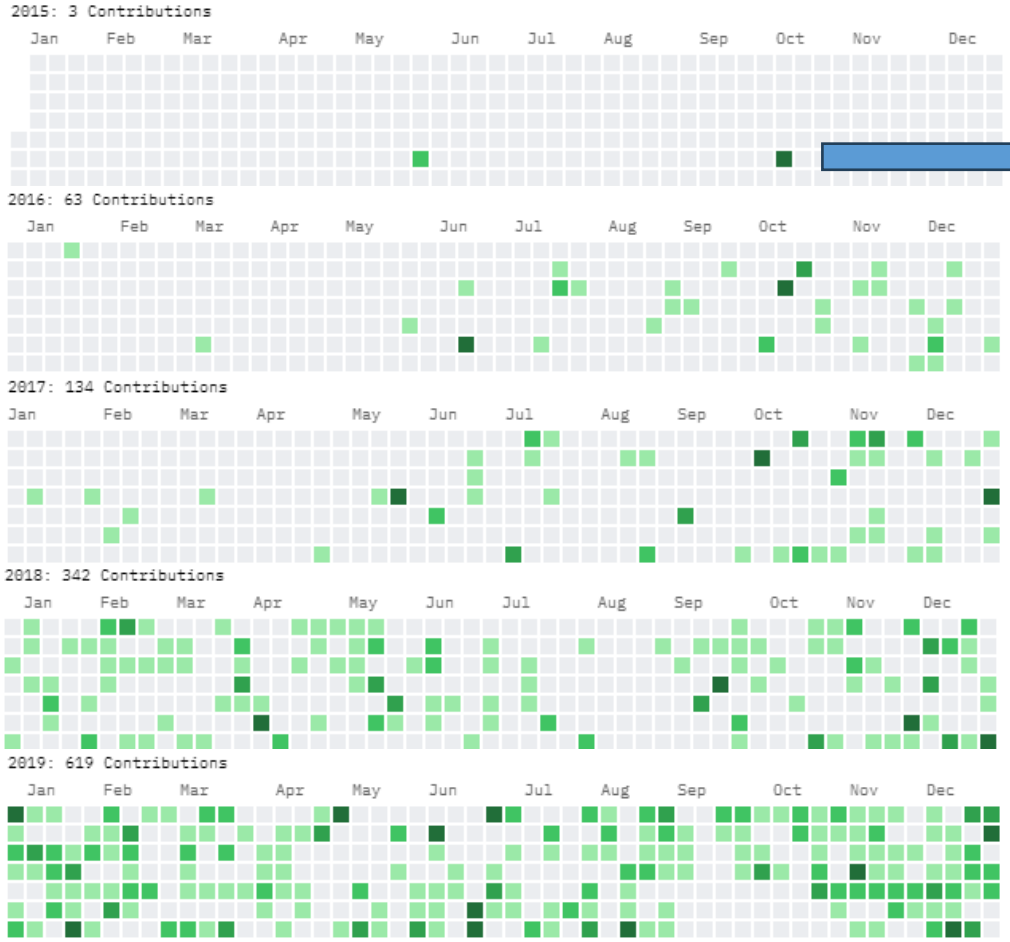
geisterr - Kopie (2).exe	2/27/2013 4:43 PM
geisterr - Kopie.exe	3/26/2012 9:53 PM
geisterr.exe	2/18/2015 3:09 PM
geisterr_alpha.exe	2/20/2014 8:44 AM
geisterr_alpha2.exe	1/7/2014 1:41 PM
geisterr_alpha3.exe	1/8/2014 11:26 AM
geisterr_alpha4.exe	1/15/2014 2:09 PM
geisterr2013.exe	12/17/2013 9:55 AM
geisterrbilder.exe	3/22/2013 4:38 PM
histogeisterr.exe	4/29/2013 2:19 PM

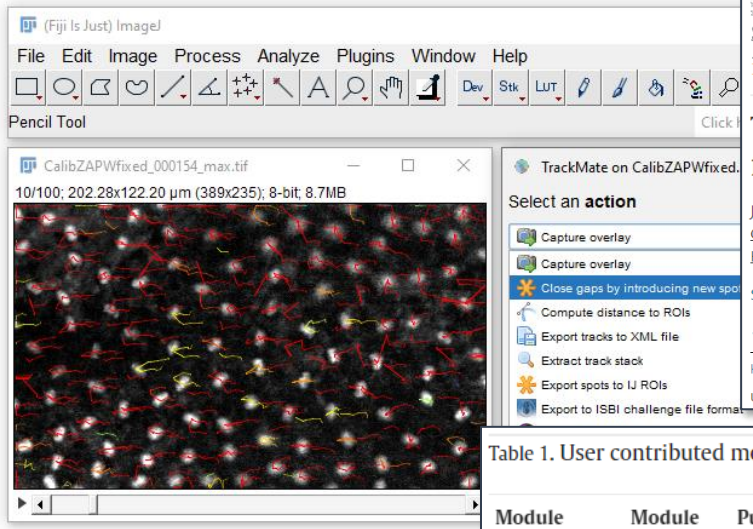
„Geisterr“ usage statistics



Version control [for code]: git

Github contributions





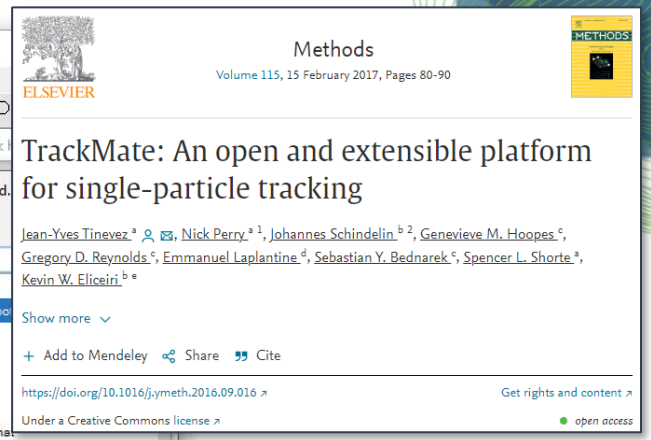


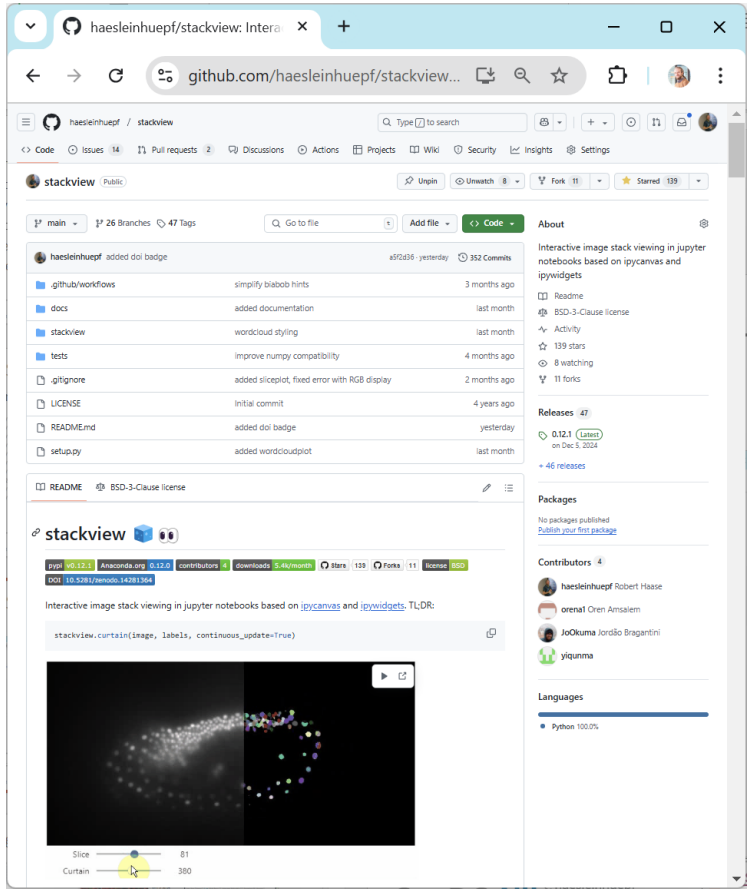
Table 1. User contributed modules of TrackMate v3.4.0.

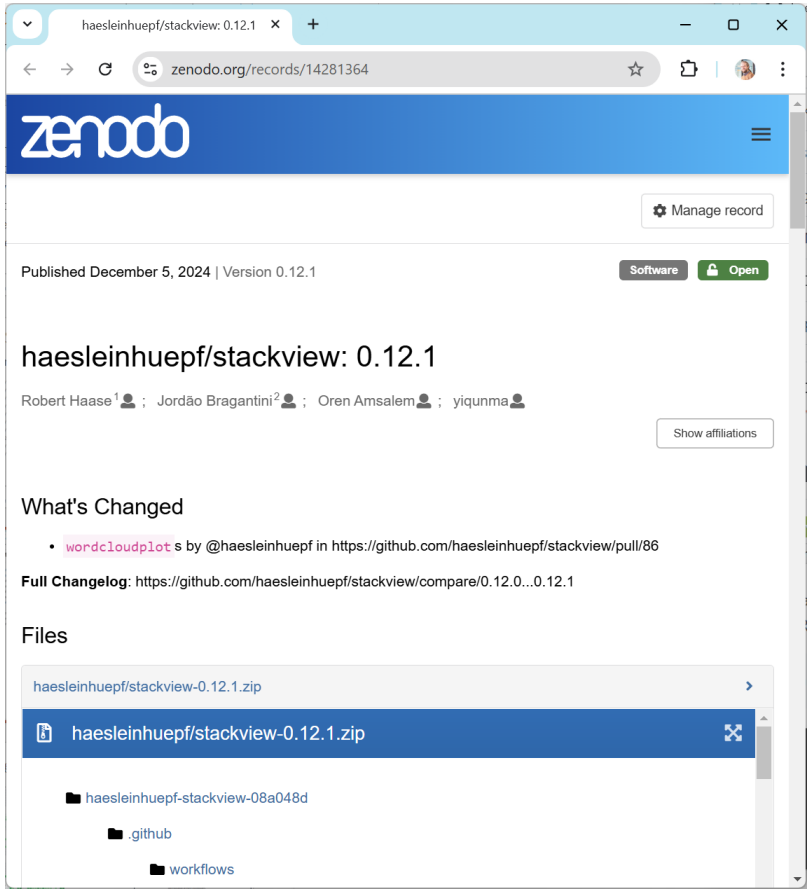
Module name	Module type	Purpose	Author	Location
Linear tracker	Particle-linking	Linking transported particles by extrapolating their velocity	Ronny Sczech	https://github.com/chicoronny/RonnyTrackMate↗
Batch mode	Plugin	Runs TrackMate in batch, reading		
Close gaps	Generic action	Close gaps in tracks by creating spots in missing frame by linear interpolation of their coordinates	Robert Haase	Integrated into TrackMate v3.4.0

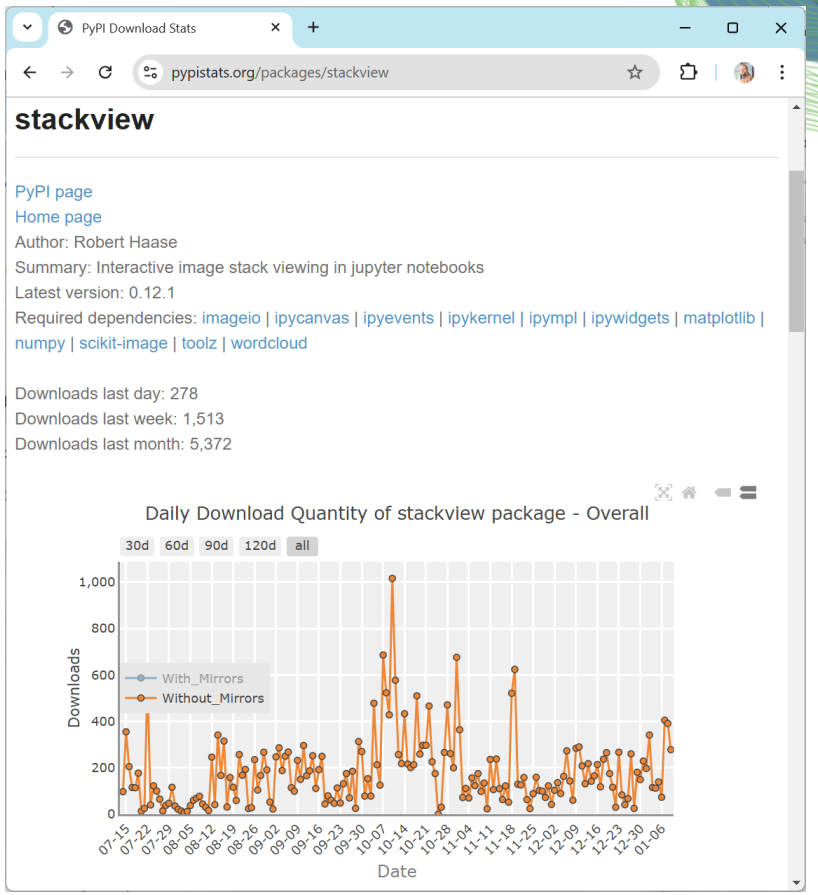
Note: The colour-code is not consistent between the years

Version control [for code]: git

- Me, today:

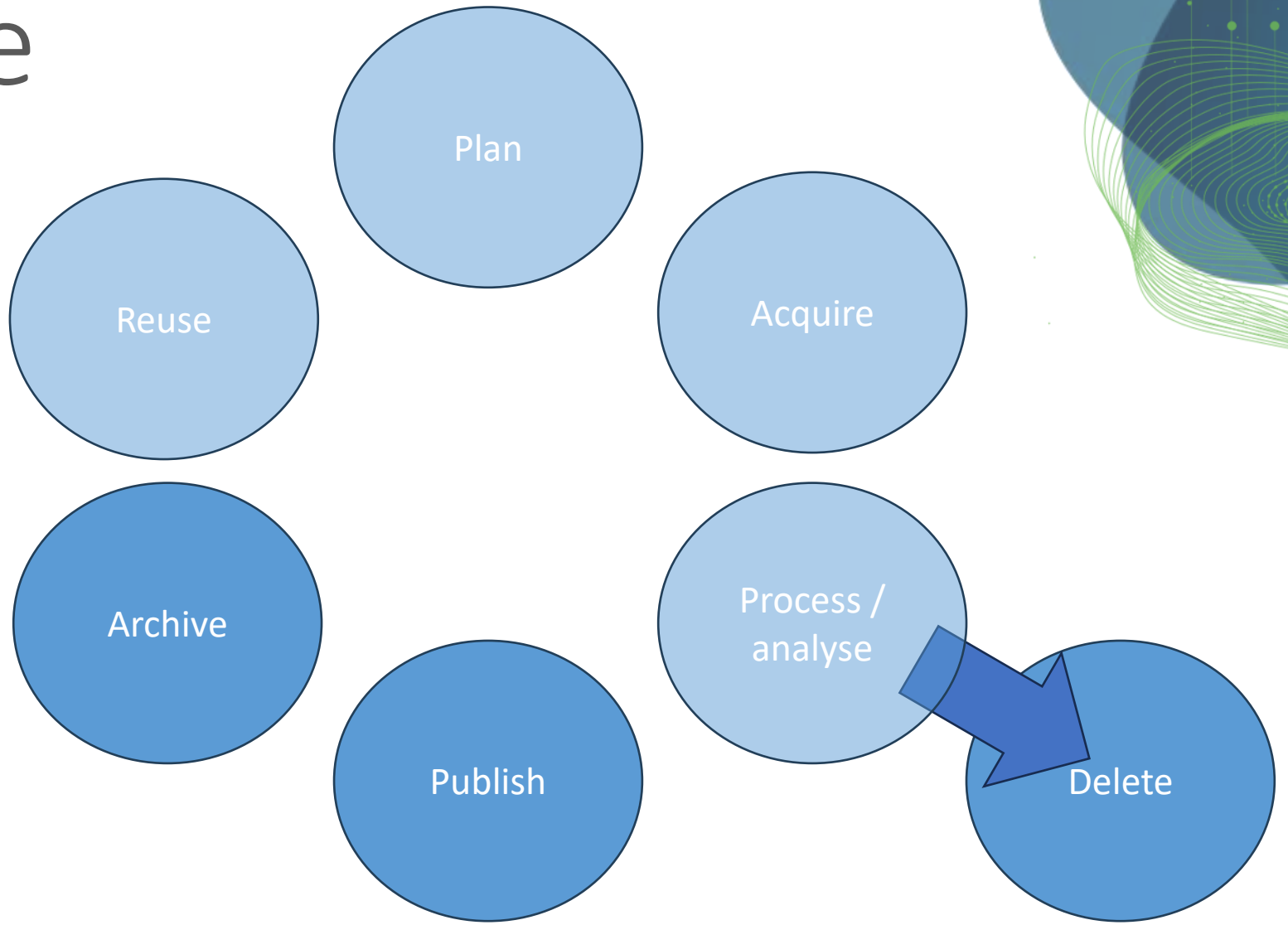






RDM Life Cycle

- Right to publish
- Regulatory aspects
  - Research data: archive 15 years
- Authorship
- Registration (-> Findable)



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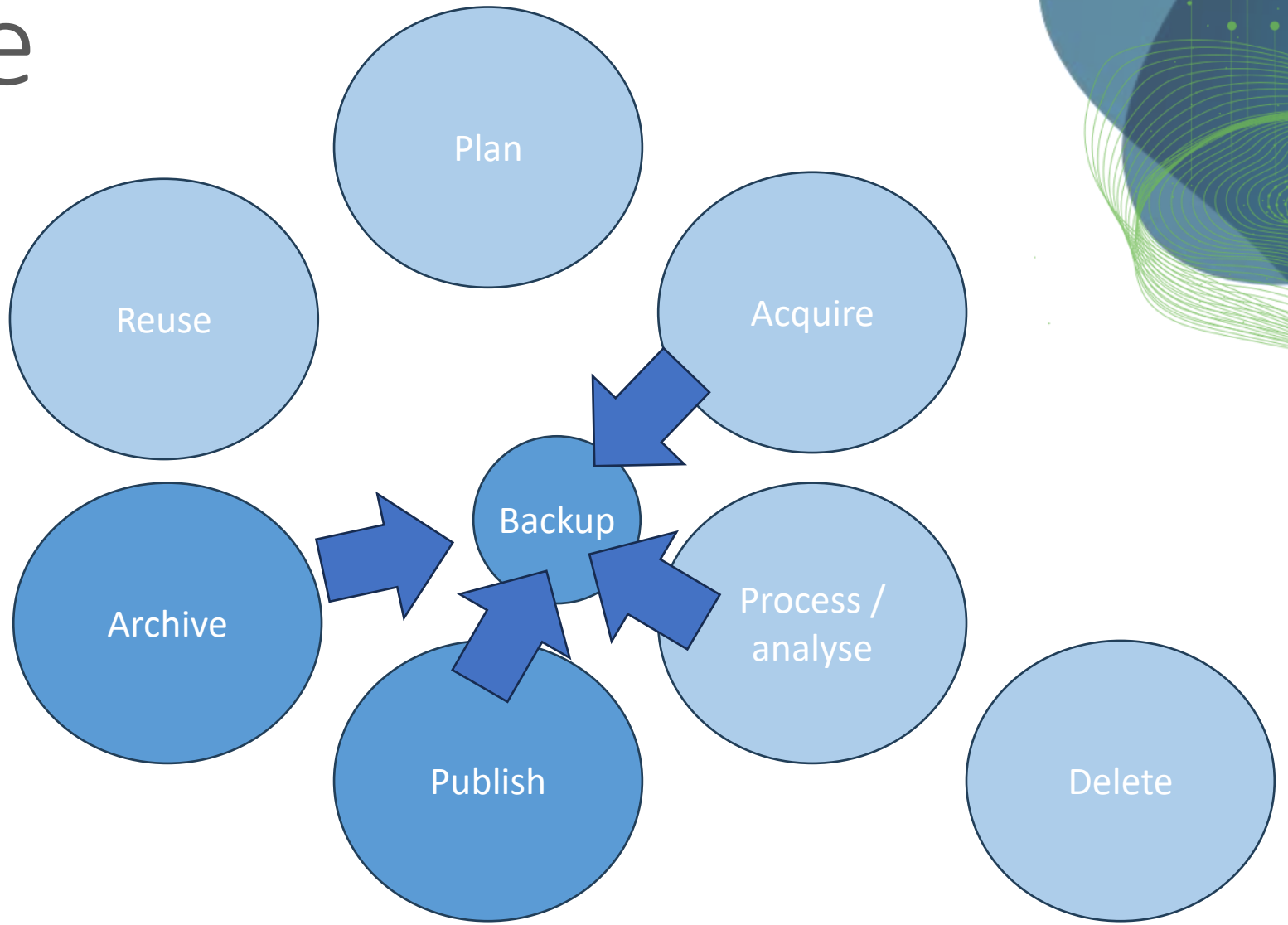
RDM Life Cycle

- Backup: Regular copy of (all) files
  - Conflict: Some personal data needs to be deleted, should not go into backup
- Publication: Selection of curated files for external use
- Archive: Selection of curated files for later use (not necessarily public)



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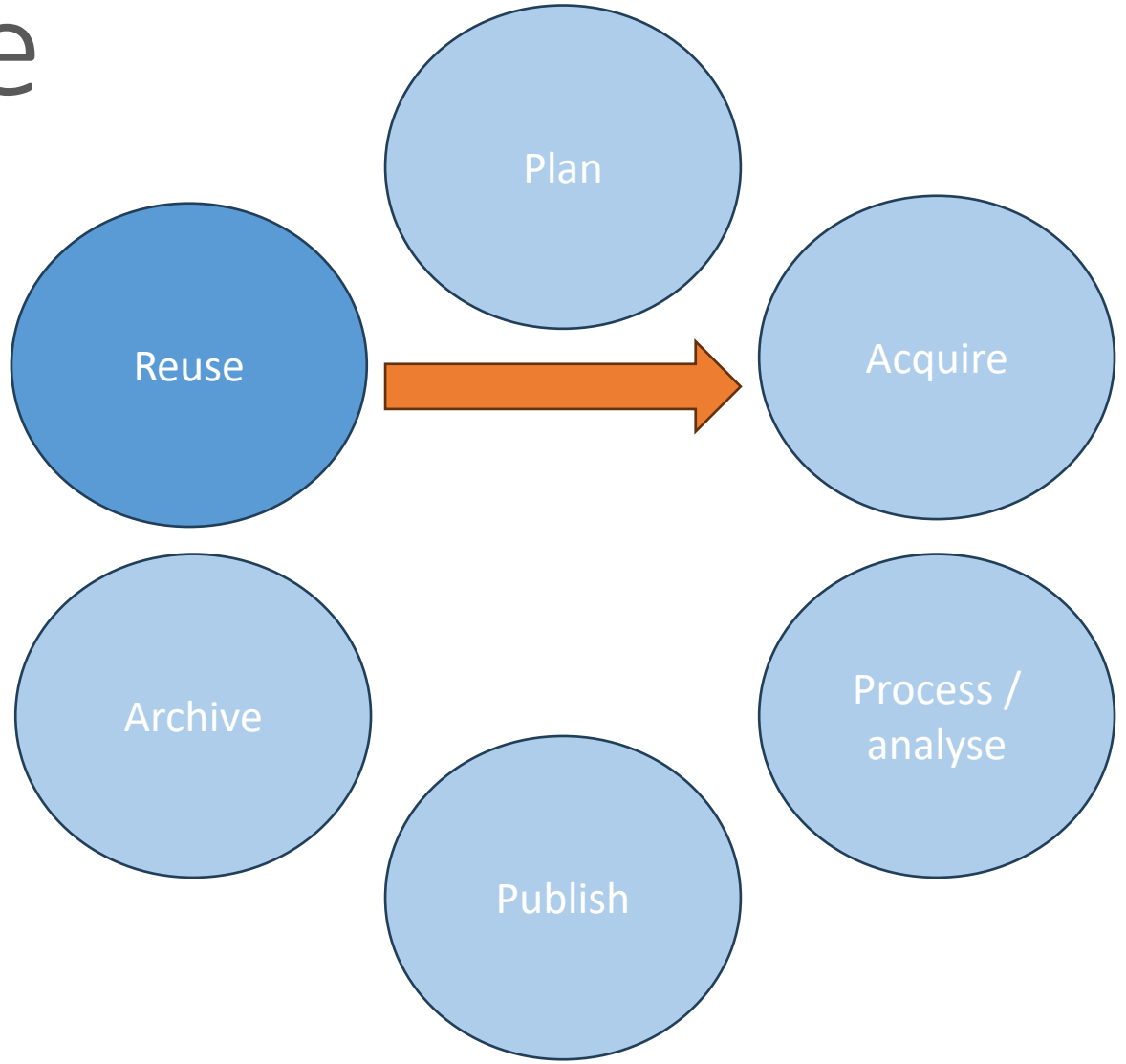
RDM Life Cycle

- Potential future benefit
- Sustainability
- Important: Licensing
  - Has impact on next cycle / acquisition



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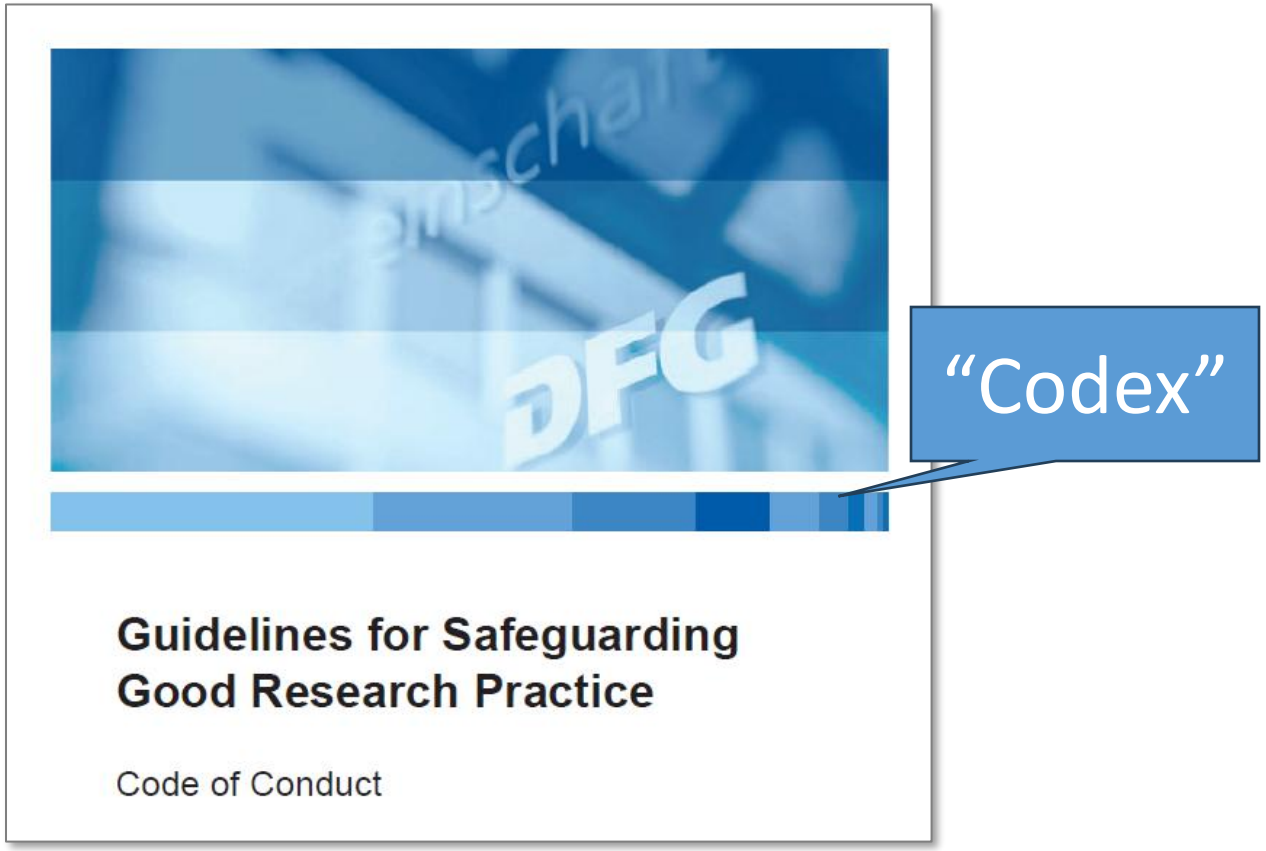
Scientific culture

Public access to research results -> Reusability



"Codex"

Guideline 13: Providing public access to research results

- As a rule, researchers make all results available as part of scientific/academic discourse. In specific cases, however, there may be reasons not to make results publicly available (in the narrower sense of publication, but also in a broader sense through other communication channels); this decision must not depend on third parties. Researchers decide autonomously – with due regard for the conventions of the relevant subject area – whether, how and where to disseminate their 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. Software programmed by researchers themselves is made publicly available along with the source code. Researchers provide full and correct information about their own preliminary work and that of others.

Explanations:

In the interest of transparency and to enable research to be referred to and reused by others, whenever possible researchers make the research data and principal materials on which a publication is based available in recognised archives and repositories in accordance with the FAIR principles (**F**indable, **A**ccessible, **I**nteroperable, **R**eusable). Restrictions may apply to public availability in the case of patent applications. If self-developed

Scientific culture

DFG Deutsche Forschungsgemeinschaft

About Us | Funding | Basics and Topics | Funded Projects | News

DFG > News > News and Current Topics > Information for Researchers > Package of Measures to Support a Shift in the Culture of Research Assessment

Information for Researchers, No. 61 | September 1, 2022

Package of Measures to Support a Shift in the Culture of Research Assessment

DFG changes proposal forms and introduces mandatory CV template / The aim is to support a shift in the culture of research assessment / Improvement of equal opportunity practices

DFG changes proposal forms and introduces mandatory CV template / The aim is to support a shift in the culture of research assessment / Improvement of equal opportunity practices

Successful science and research require suitable framework conditions. The Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) ensures these conditions by regularly conducting analyses, providing the relevant information and adapting its procedures accordingly. The DFG set out the challenges and fields of action in a position paper on academic publishing published in May of this year: it sees both the academic community as a whole and itself as a funding organisation as being responsible for initiating a cultural shift towards research assessment that is geared more towards equal opportunity and attaches even greater importance to the substance of research. In the interests of bringing about such a shift, it is up to research funding organisations to broaden the spectrum of accepted publication formats, to attach greater value to content-based evidence of achievement and to strengthen the recipient side of publishing. The DFG has launched a comprehensive and far-reaching package of measures in order to fulfil this mandate.

Binding CV template across all funding programmes

For this reason, the assessment of a researcher's accomplishments must be holistic and based on substantive qualitative criteria. In order to strengthen qualitative evaluation criteria over quantitative indicators, the DFG will be introducing a curriculum vitae template that will be mandatory across all programmes from 1 March 2023 (the template will be adapted shortly for proposals under the Collaborative Research Centre and Research Training Group programmes; information will be provided separately in this regard). The template adopted by the DFG Senate allows applicants to provide both narrative and tabular information, thereby facilitating a holistic view of the applicant's academic career in the review and evaluation process.

In addition to the mandatory information required in order to assess eligibility, applicants may also provide details of special circumstances or additional services to scholarship such as committee activities or the establishment of research infrastructures. As such, the template provides the basis for a qualitatively sound assessment of academic performance that takes greater account of the respective stage of the individual's life and career. Accordingly, reviewers are now instructed to consider applicants' academic performance in the context of their individual curriculum vitae and career stage.

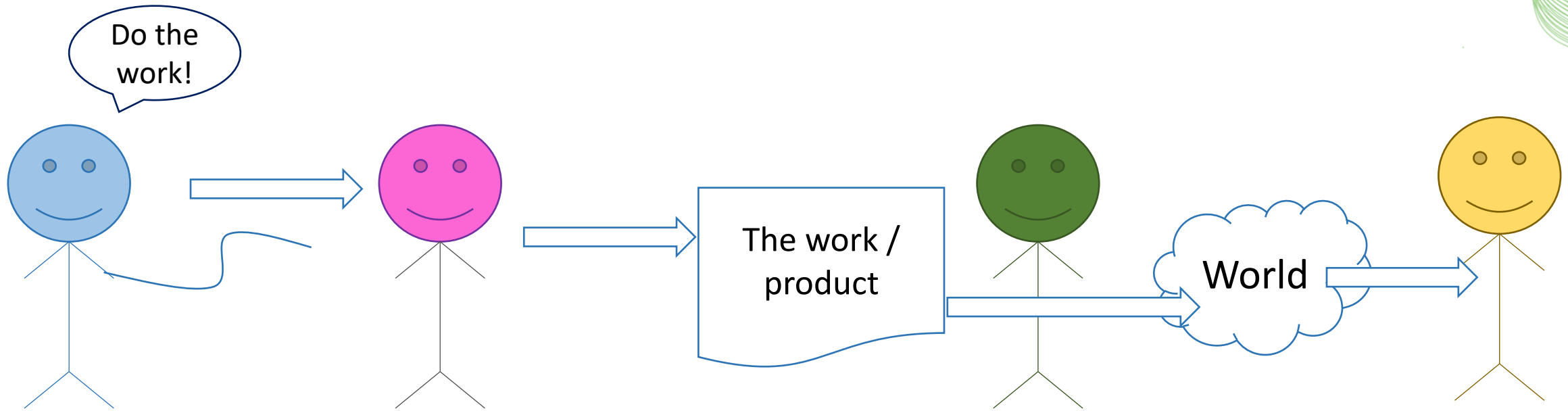
Publication details in proposals and CVs

Performance assessment based on content-related qualitative criteria also explicitly includes ensuring that the entire spectrum of academic publication types are equally displayed and acknowledged in funding proposals and CVs. In addition to a maximum of ten publications in the more common publication formats, the CV can therefore now list up to ten further sets of research outcomes and findings that have been publicised in a variety of other ways, including articles on preprint servers, data sets or software packages, for example. In DFG proposals, the project-specific list of publications will be included in the general bibliography. The intention here is to shift the focus of the review and the evaluation of a proposal away from the list of publications and towards the substance of the applicant's accomplishments. In order to document their own published preliminary work, applicants can typographically highlight (e.g. in bold) a maximum of ten of their own publications in the bibliography that are important for the project. No information on quantitative metrics such as impact factors and h-indices is required in the CV or the proposal, and such information is not to be considered in the review. The relevant details are included in DFG forms and review instructions.

These modifications and innovations reflect the fact that the DFG is continuing to promote the cultural shift in research assessment that was advocated in May with the publication of the position paper on academic publishing. The DFG hopes that this refocus – away from quantitative indicators and towards the substance of scholarship – will lead to improved equality of opportunity and a higher-quality basis for review overall.

Am I allowed to publish my stuff?

- … it depends… on who is responsible



Copyright holder,
e.g. employer / PI of the author

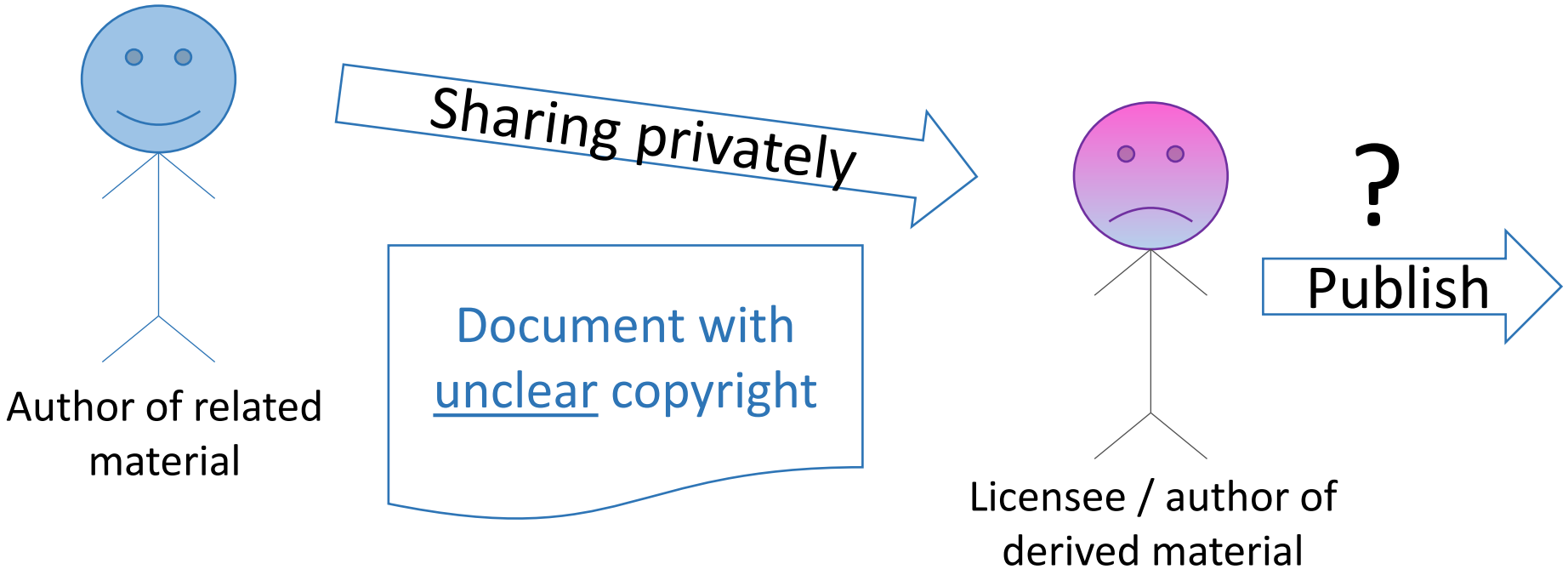
Author
Creator of the work

Publisher
The person who made the work available

Licensee
The person who uses / reuses the material

Am I allowed to publish my stuff?

- … it depends… on what materials served as basis



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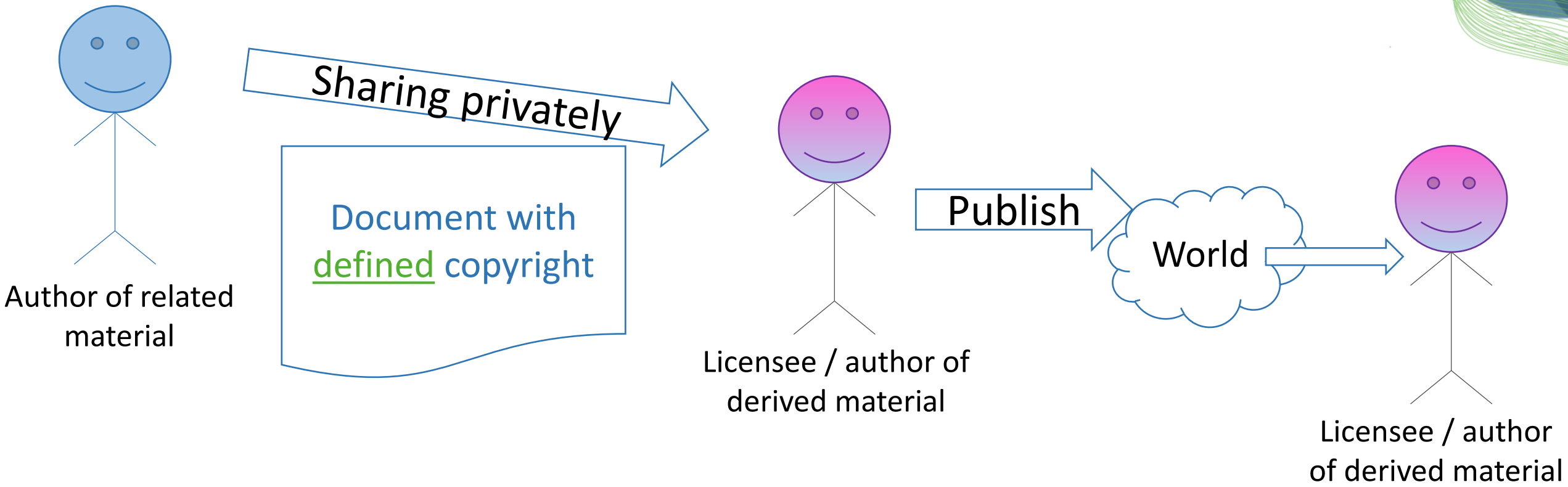
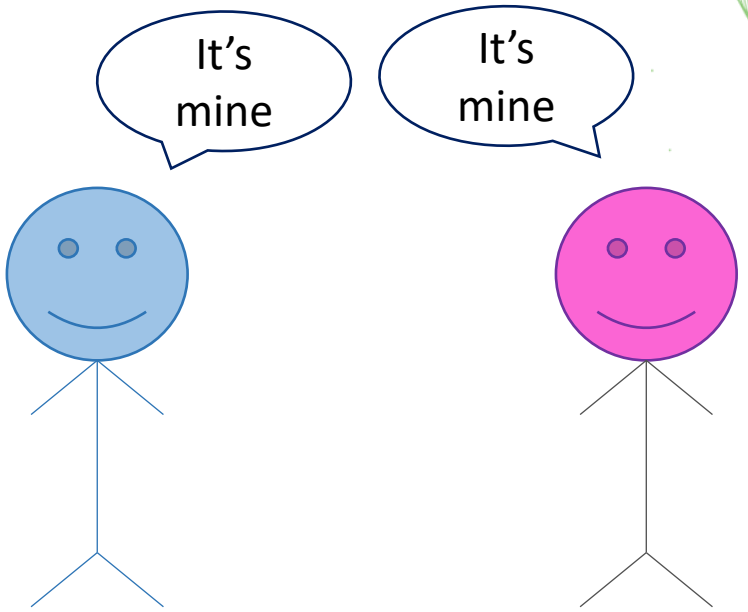


Public versus institutional repositories

Conflict of interest between employers and scientists

- Universities seek to keep things secret and potentially exploit them commercially (licenses, startups, …)
- Scientists need to publish to advance their career.
- Hints:
  - Decide early during the project what will be published and by who (-> DMP)
  - Check your job description! (Is “Programming” or “model training” part of it?)

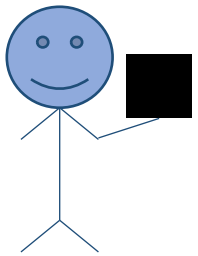


Copyright holder, e.g. employer / PI of the author

Author
Creator of the work

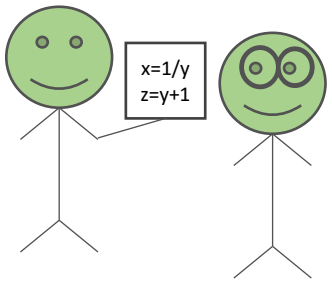
Openness of software / projects

Closed source



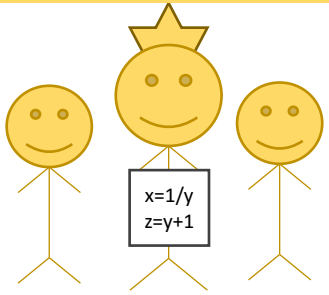
- Open to collaborations
- “Black box”
- Compiled code (e.g. C/C++)
- Good for protecting intellectual properties ($$$)

Open source



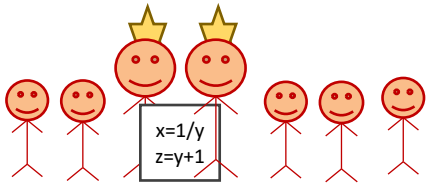
- Code available to read
- Not necessarily executable code
- No maintenance / support efforts

Benevolent dictatorship



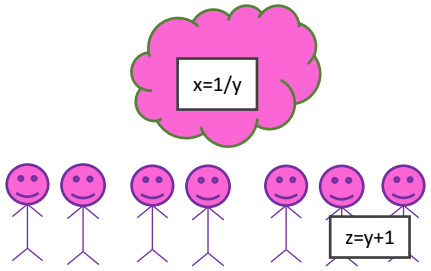
- Open to contributions
- Single maintainer, often overwhelmed
- Efficient decision making
- Bus factor ≈1

Community driven



- Open to contributions
- Partially democratic
- Board of maintainers (core developers)
- Long-winded decision making

Openly extensible



- Openly extensible; without maintainers involved
- Partially community driven

Hardware device drivers

Custom data analysis scripts

scikit-image, scipy, OpenCL

Python, numpy

Read more: https://coiled.io/blog/stages-of-openness/

Standard for sharing: The FAIR-principles

- Findable
- Accessible
- Interoperable
- Reusable

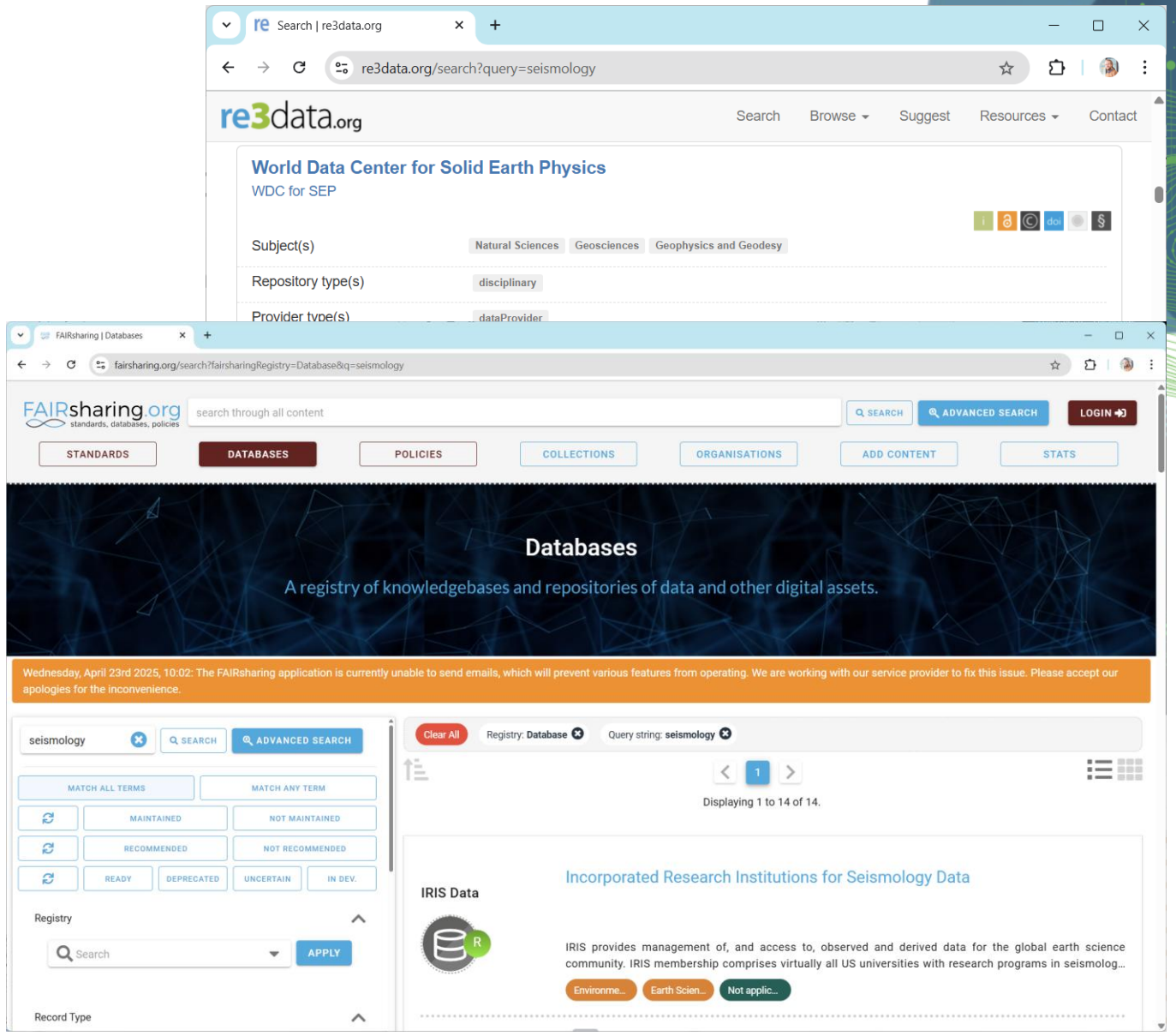
Findability

Domain-specific

- Search repository registries for your field!

Guidelines

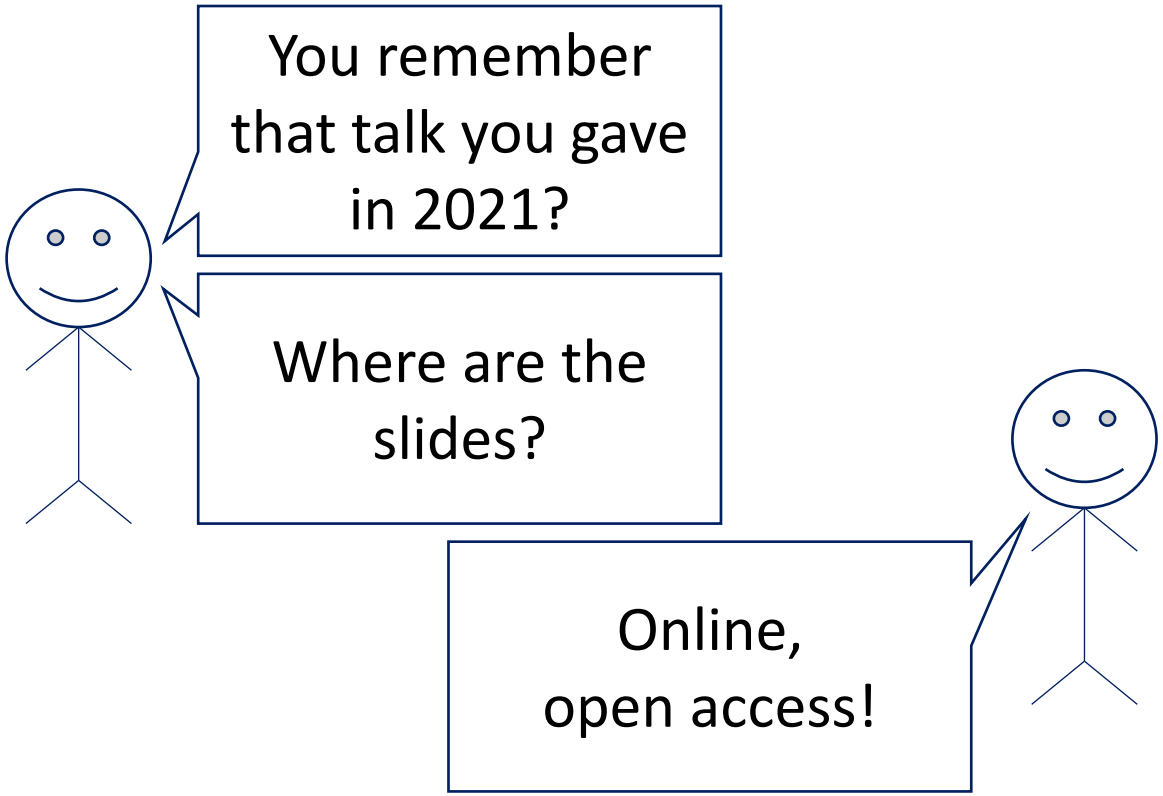
- Publish where your community publishes
- Publish where everyone publishes (beyond your community)
- Publish in your local institute's infrastructure

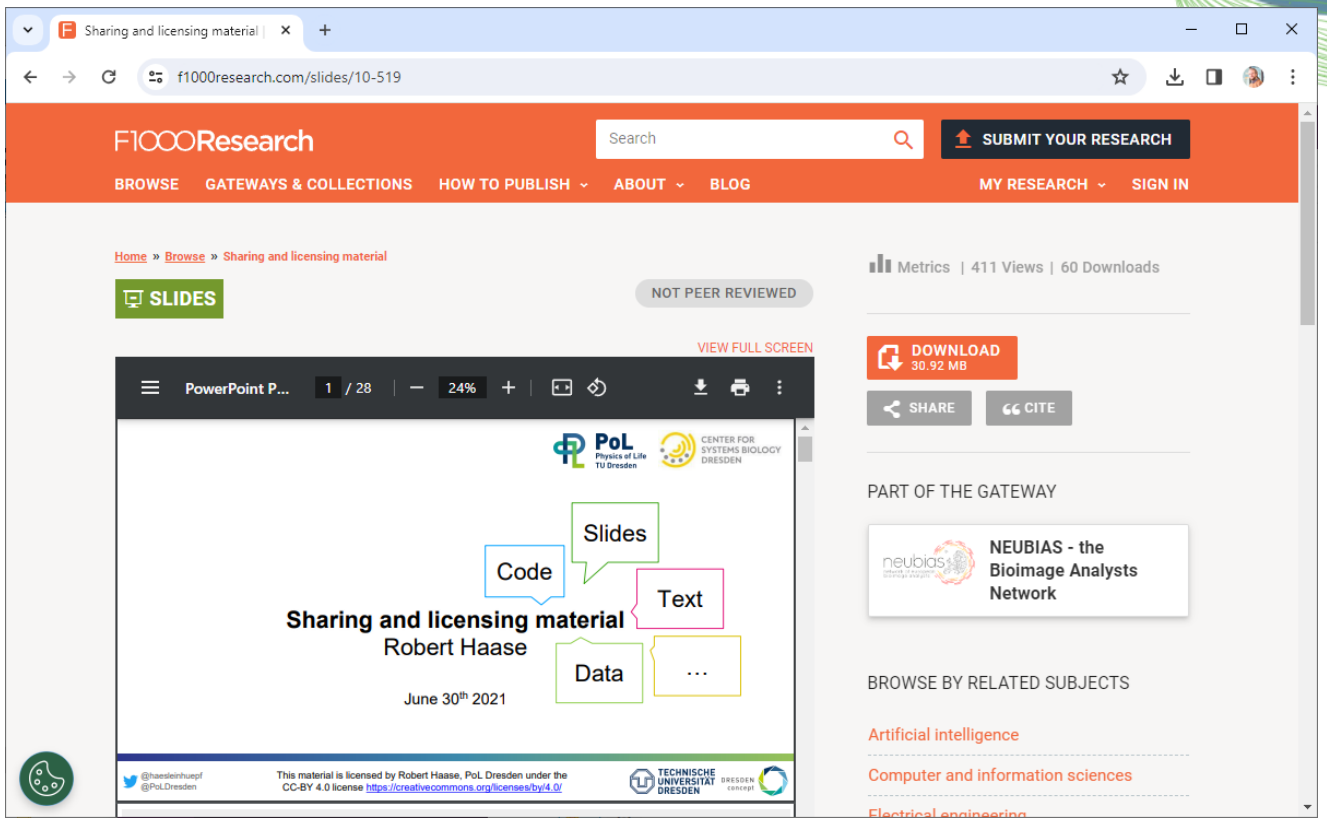


https://www.re3data.org/search?query=seismology
https://fairsharing.org/search?fairsharingRegistry=Database&q=seismology

Incentives: Findability

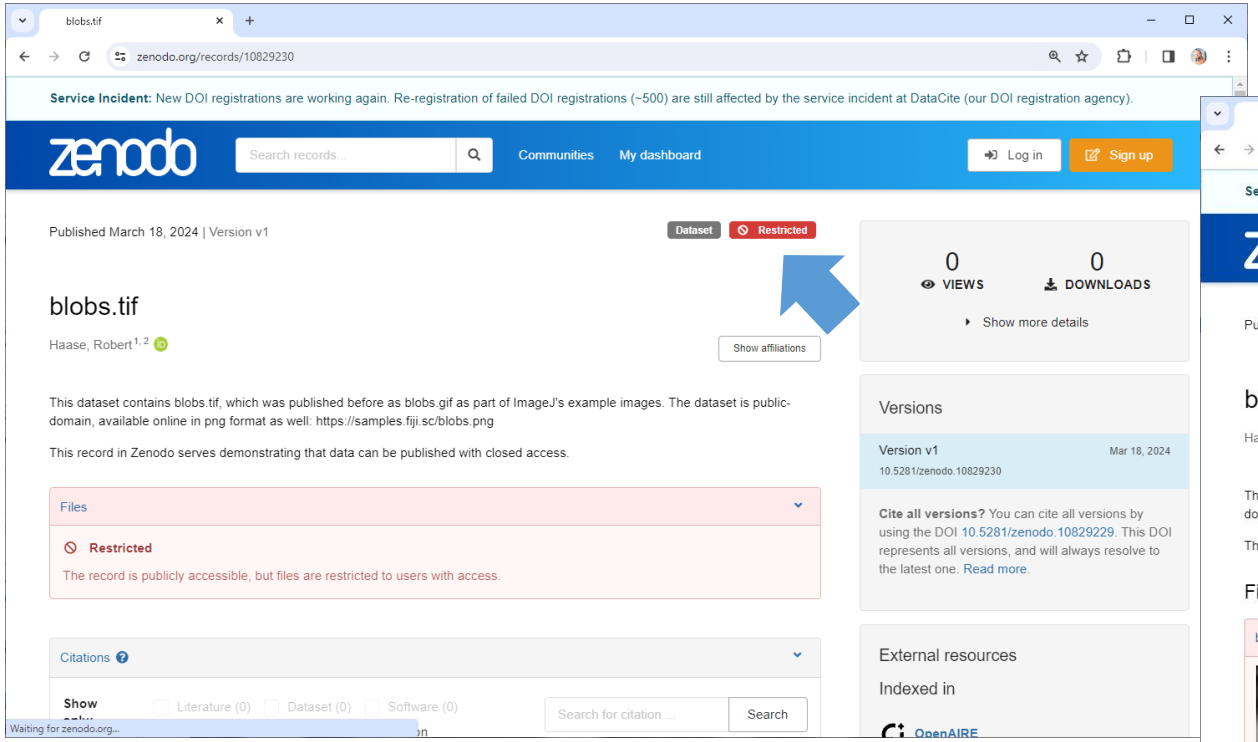
- Your *future-self* will thank you, because they will find your work

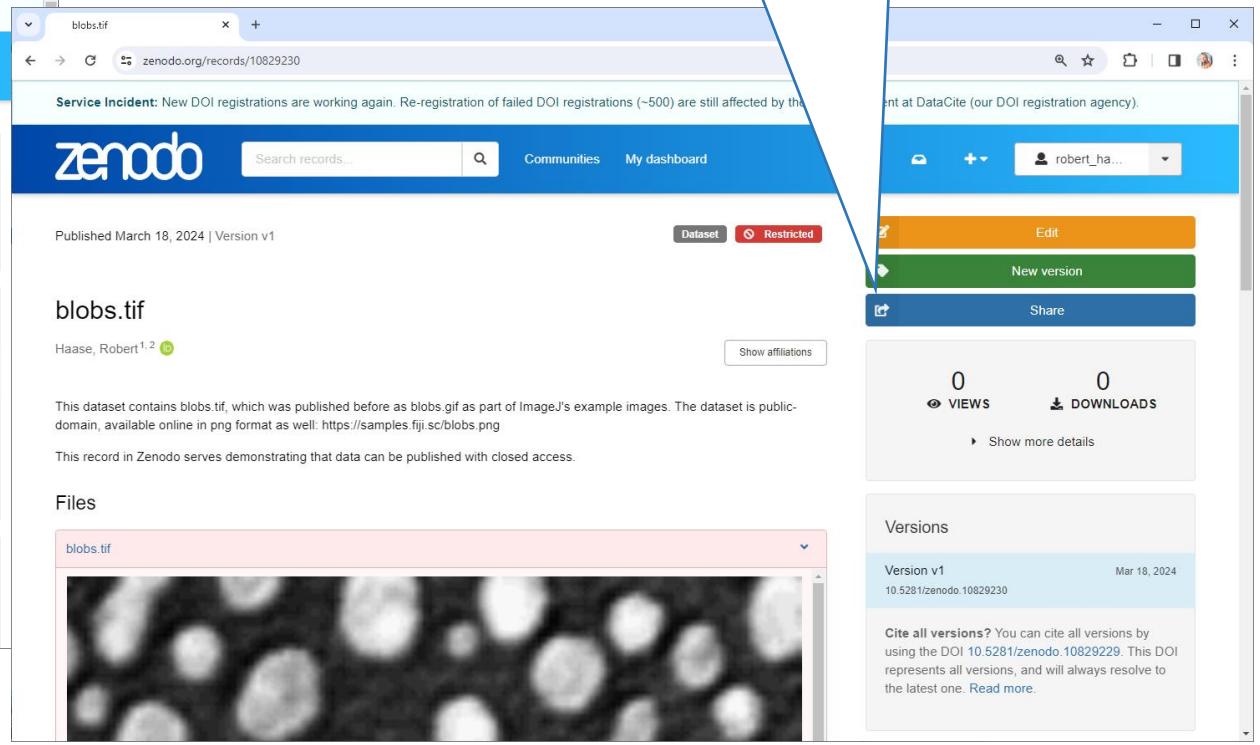


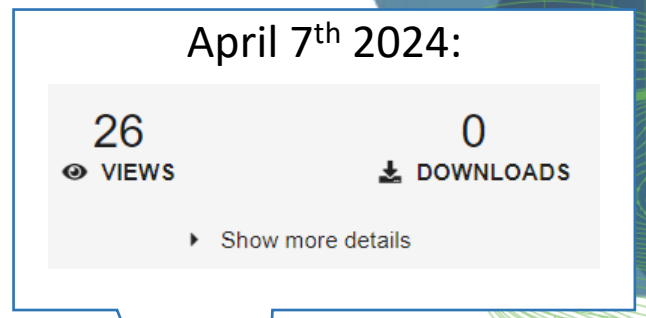


Accessibility

- The A in FAIR does not necessarily stand for Open Access







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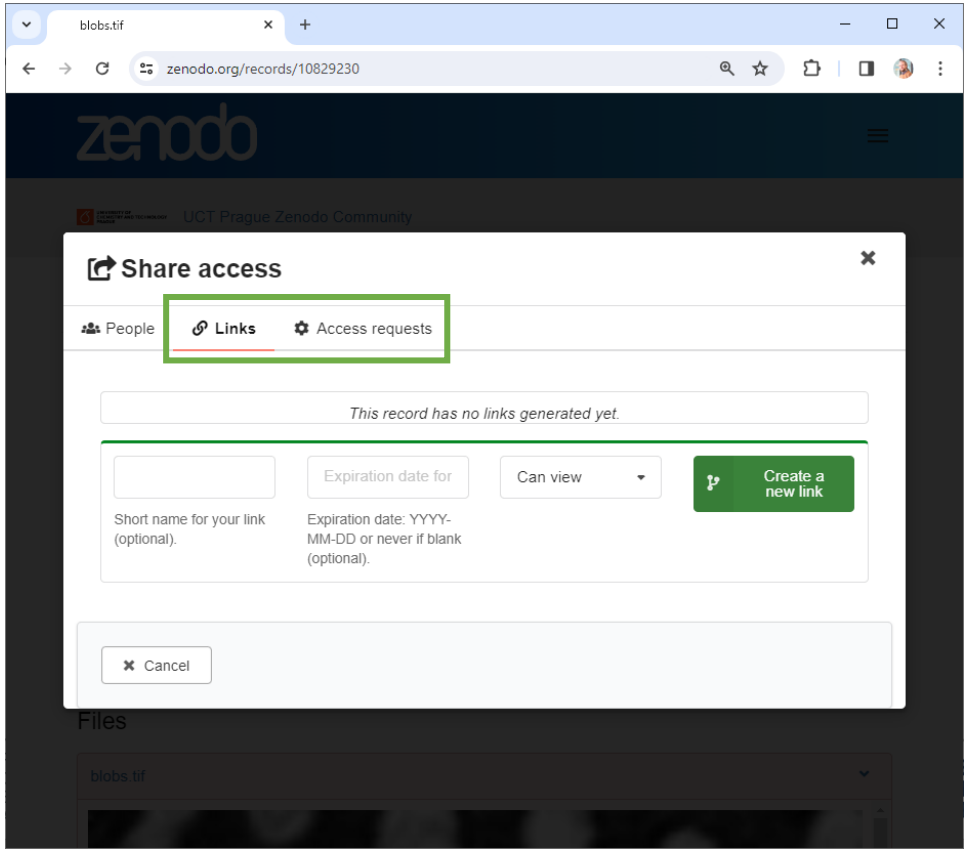

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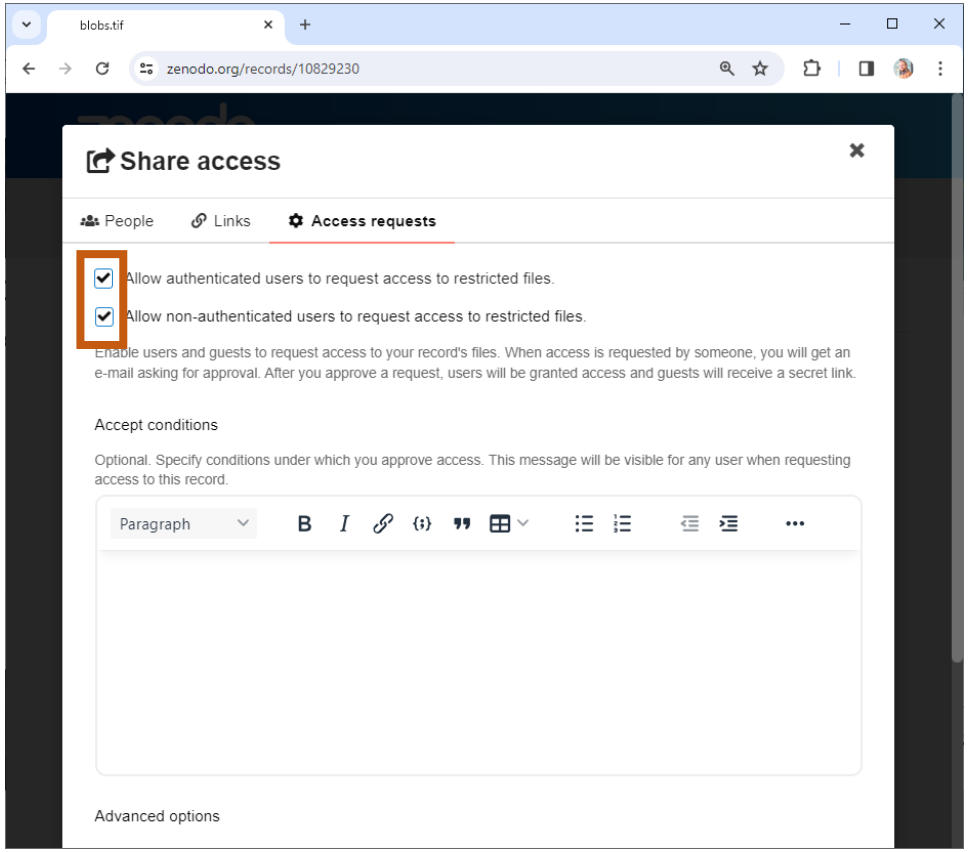
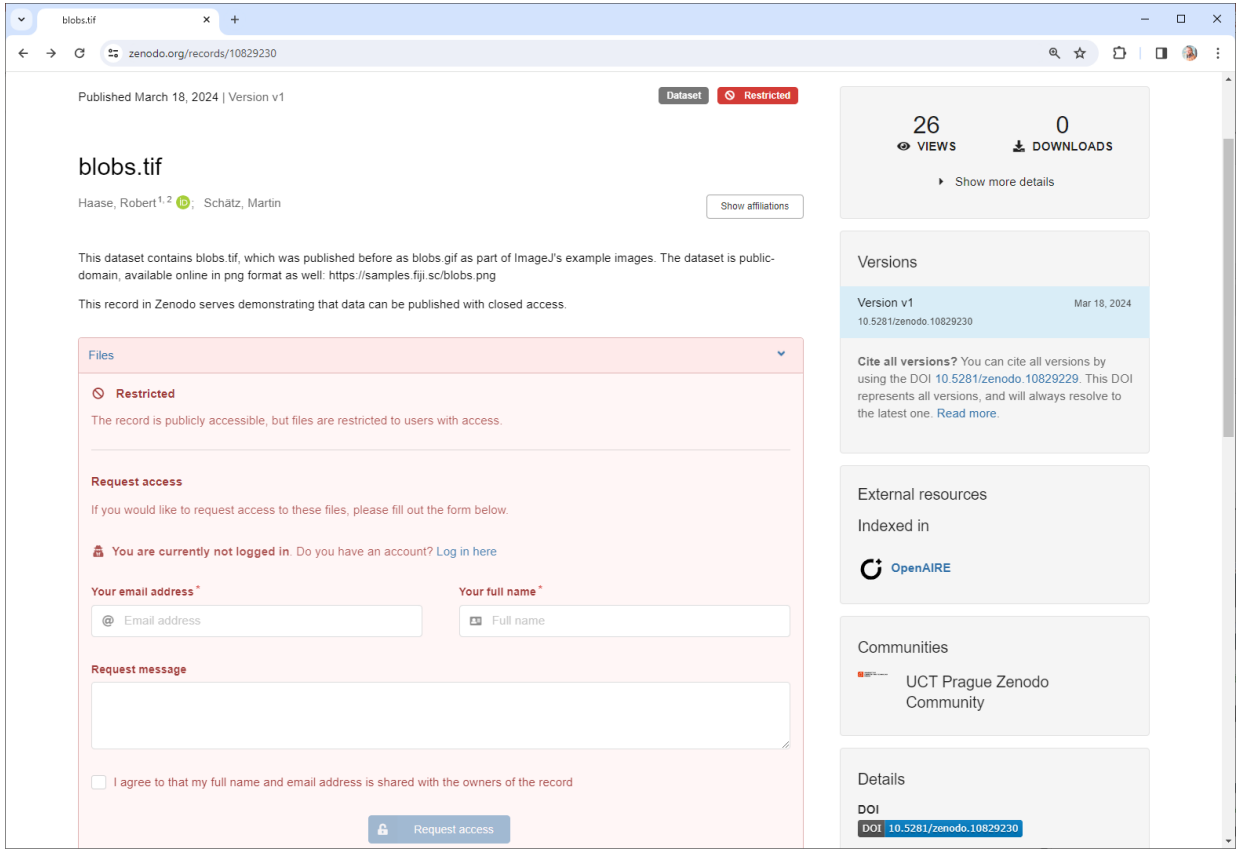




Interoperability

- 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

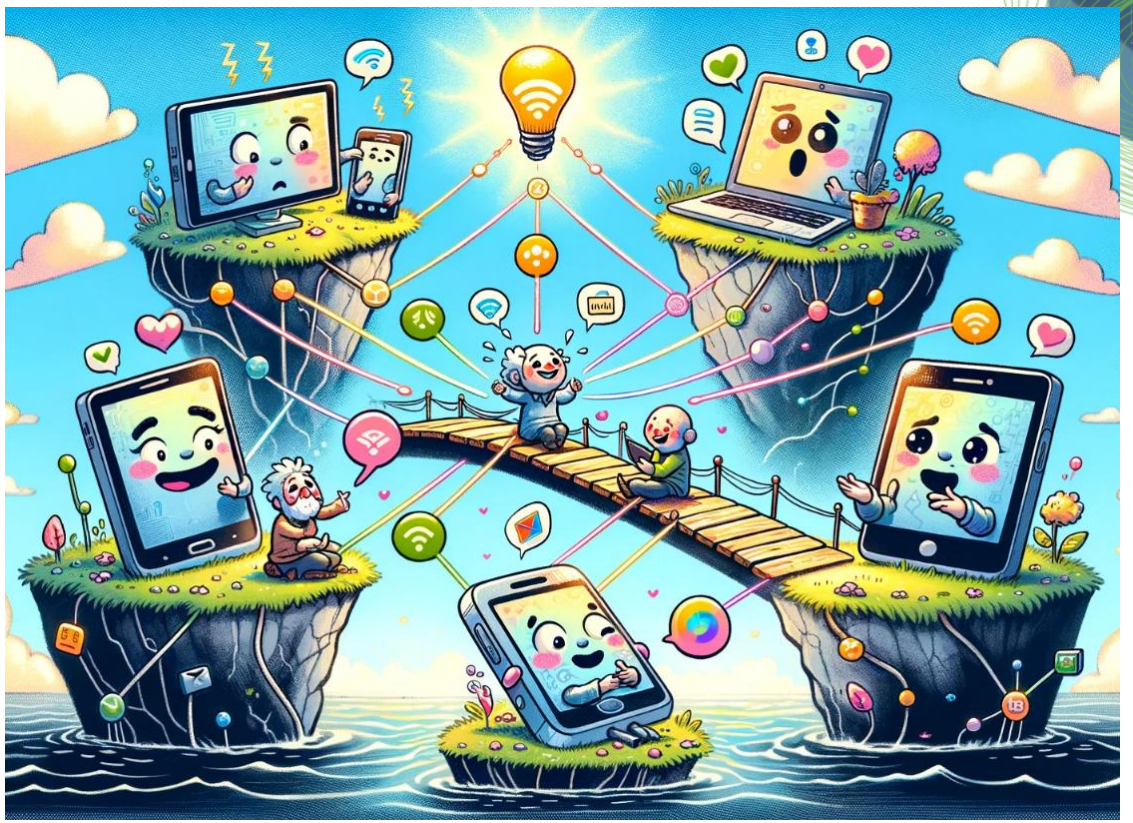
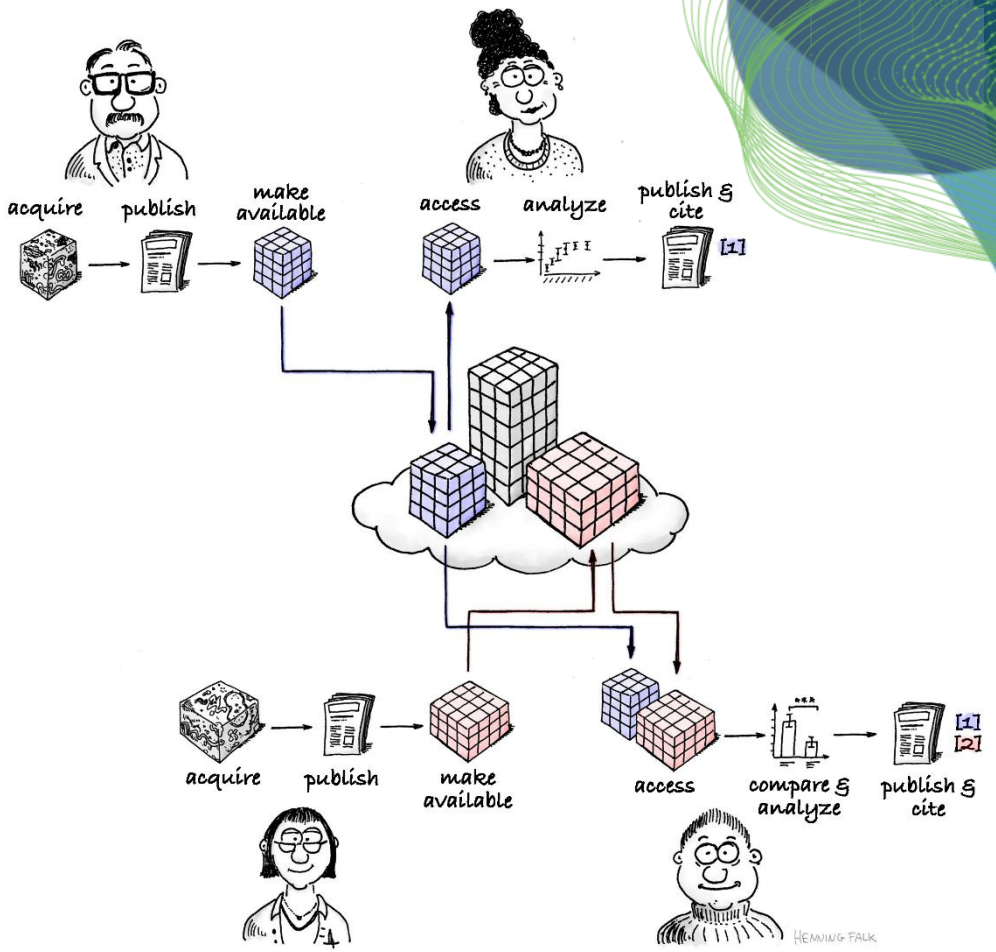


Image was created using Generative AI (Dall-E)
https://www.go-fair.org/fair-principles

Reusability

- 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

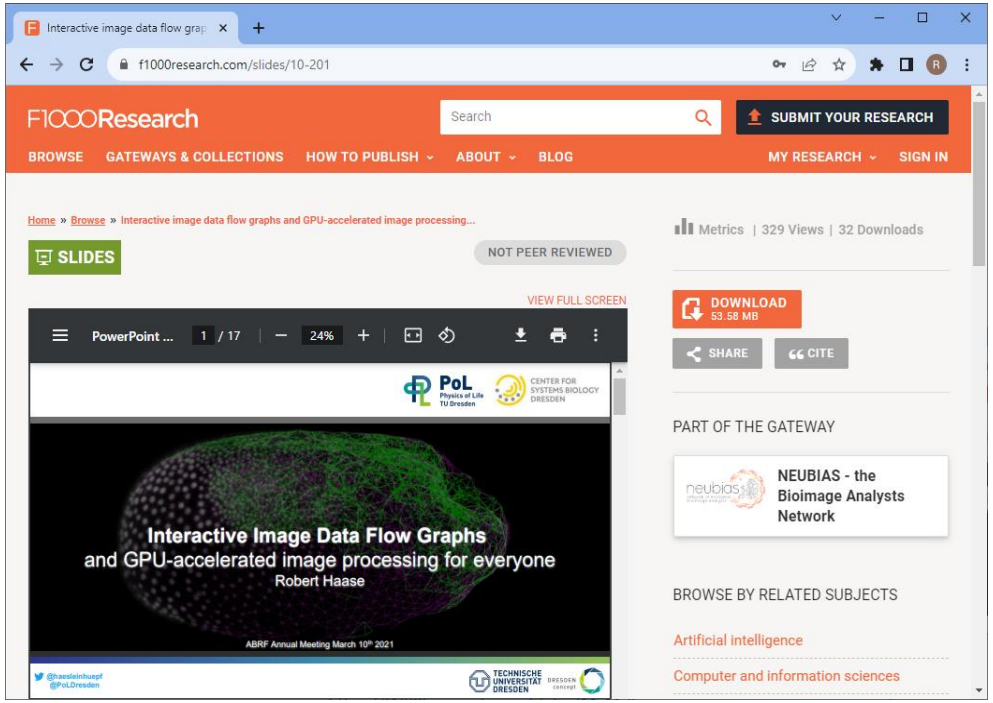


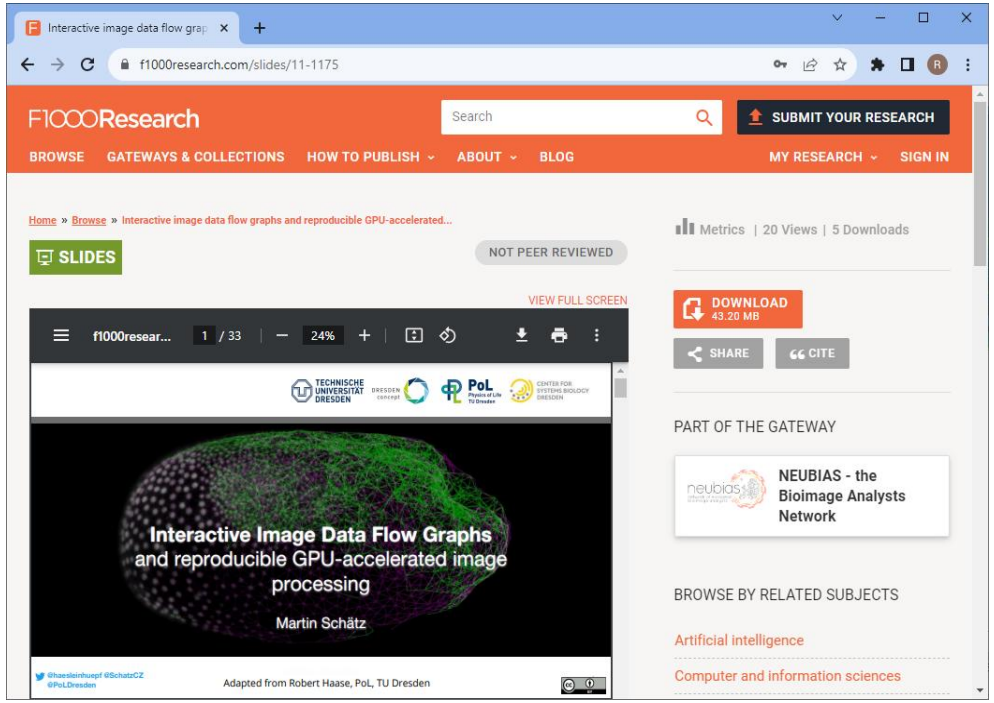
https://www.go-fair.org/fair-principles/

Drawing made by Henning Falk, ©2022 NumFOCUS, reused under a CC BY 4.0 license

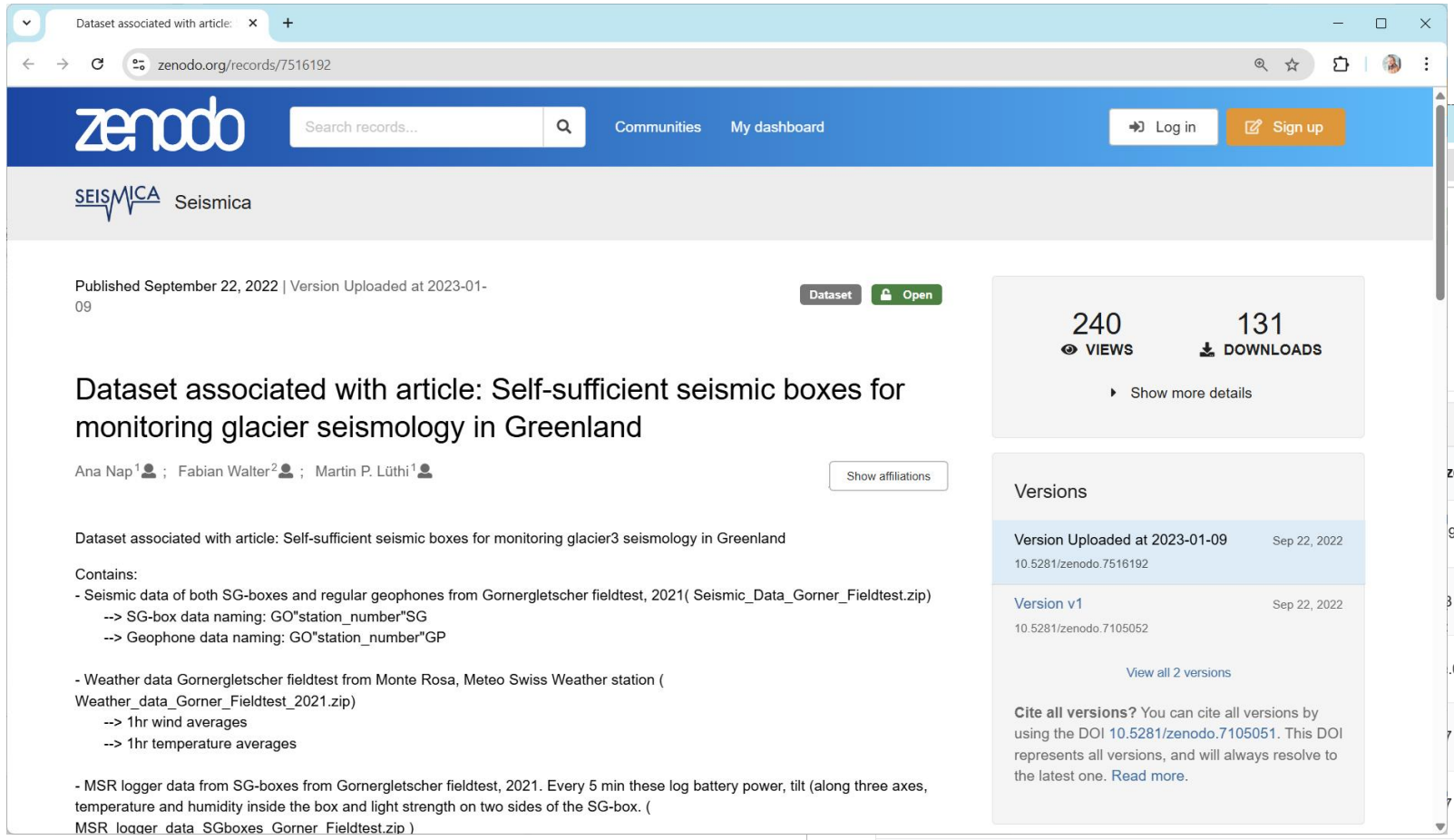
Incentives: Reusability

- Open Educational Resources
  -> Others teach how to use your *tools & methods*





Incentives: Citability



Where to share what?

Manuscripts

- https://eartharxiv.org/
- https://arxiv.org/

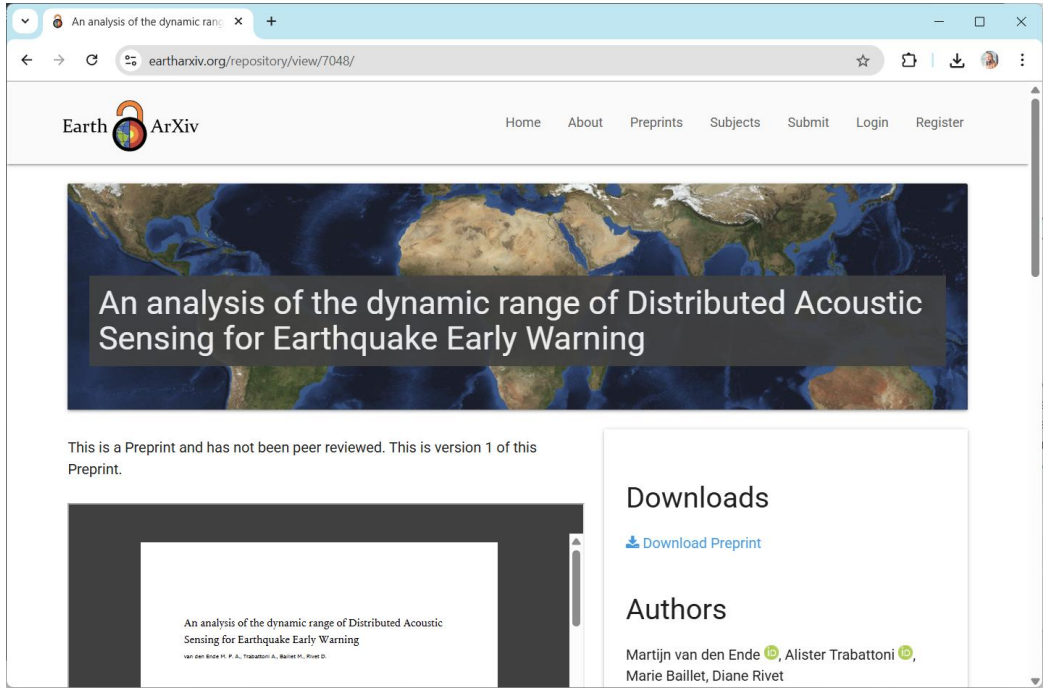
Code, Models & Data

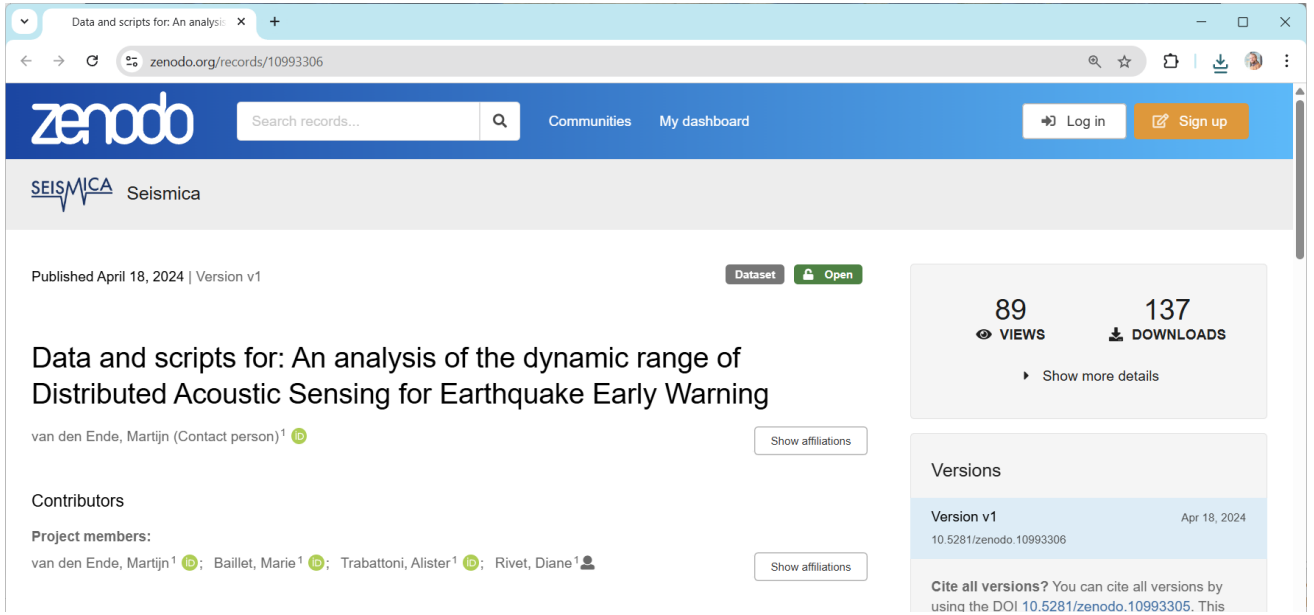
- https://github.com
- https://huggingface.co

Ongoing work on code and models

- https://zenodo.org

Publicly funded archive



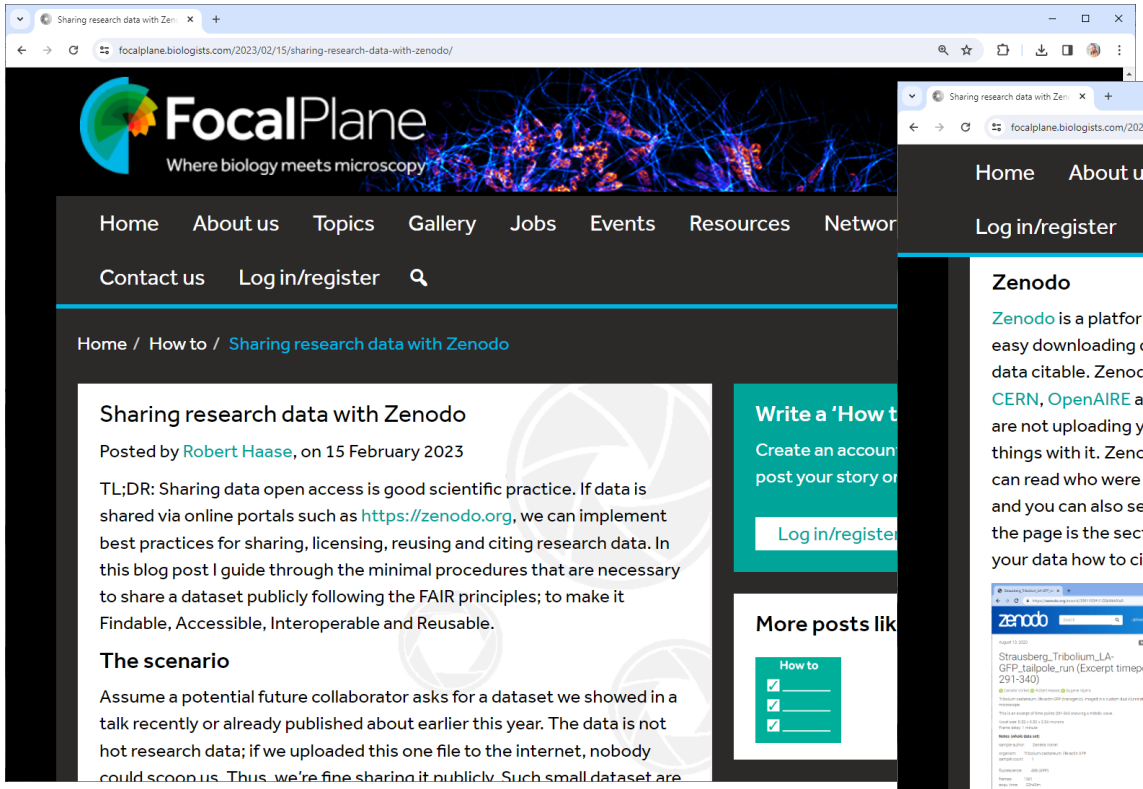


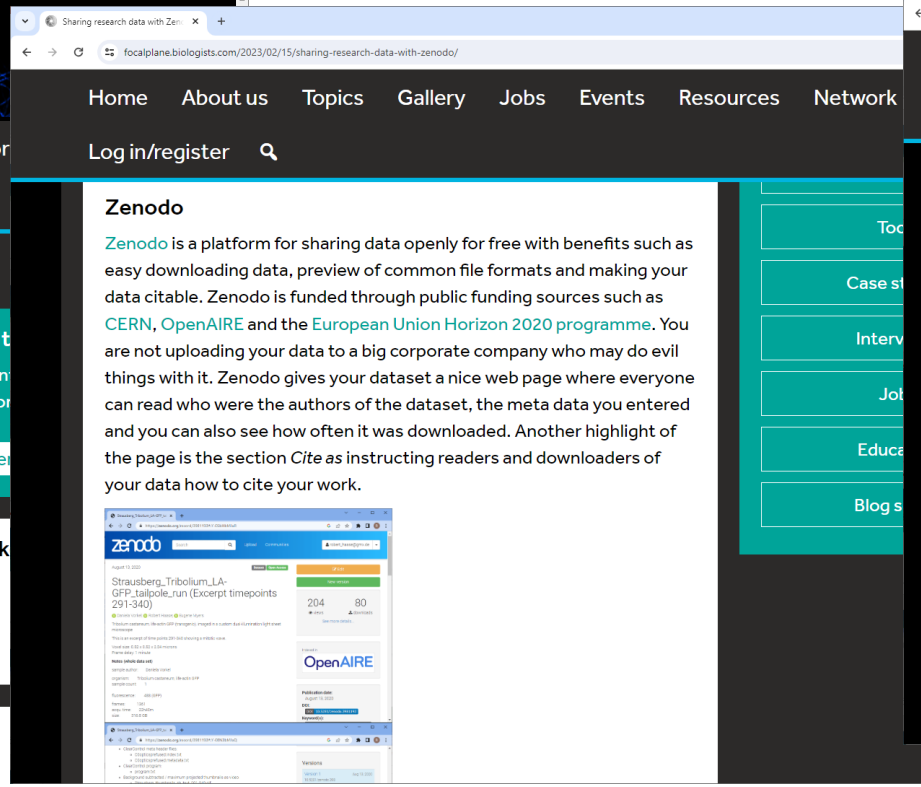
https://doi.org/10.31223/X5KH5R

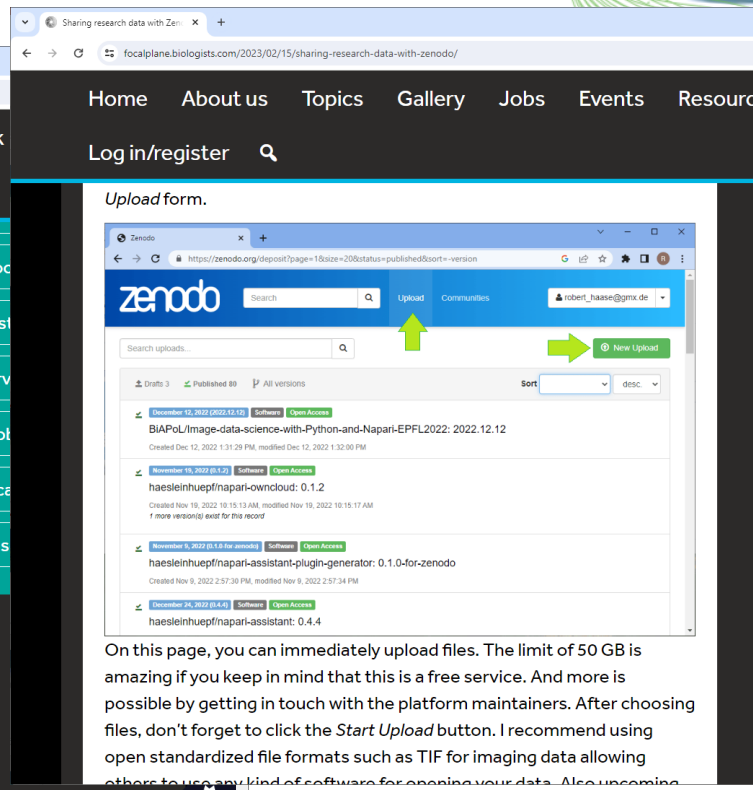
https://doi.org/10.5281/zenodo.10993305

Sharing files on Zenodo

- … is easier than you think







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CENTER FOR SCALABLE DATA ANALYTICS
AND ARTIFICIAL INTELLIGENCE

Research Software Management

Robert Haase

GEFÖRDERT VOM
Bundesministerium
für Bildung
und Forschung

SACHSEN
Diese Maßnahme wird gefördert durch die Bundesregierung aufgrund eines Beschlusses des Deutschen Bundestages.
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Quiz

- How do you typically install Python packages on your computer?

pip install …

conda install …

uv add …

<other>

Conda environments

- What is the difference between

`pip install …`

and

`conda install …`

?

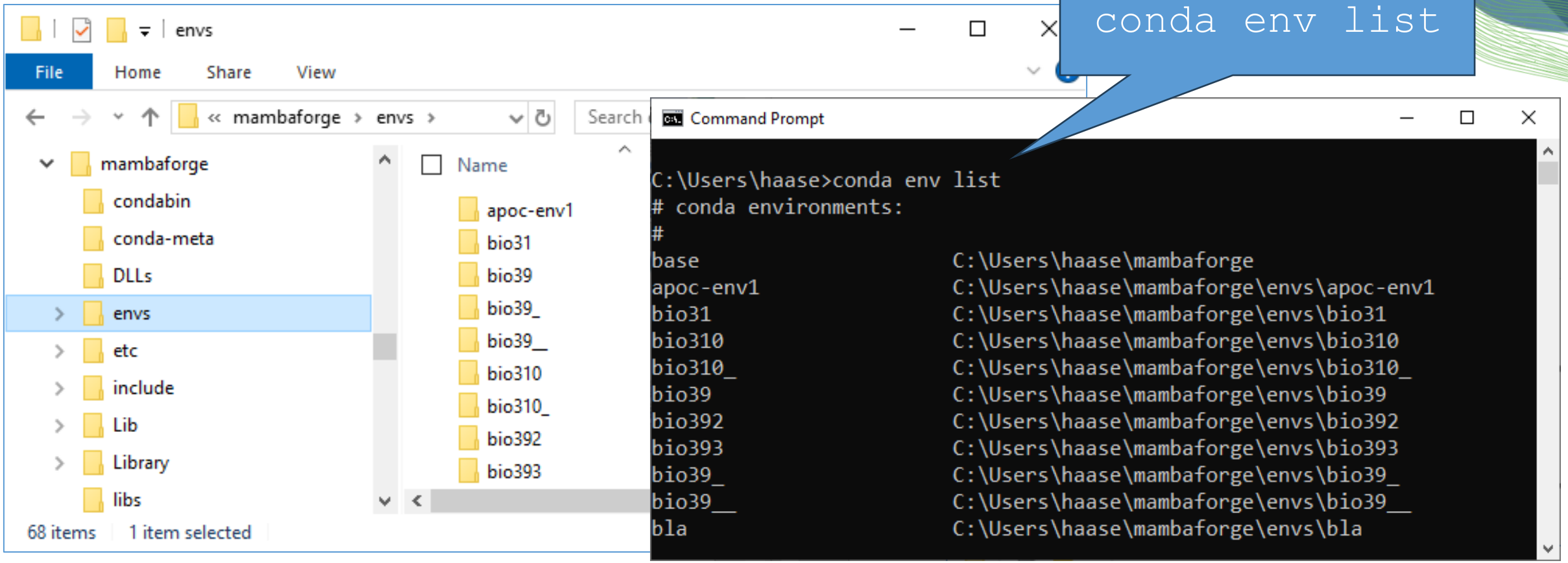
Conda environments

- Conda is a package manager
  - Allows to install Python packages
  - Allows to install other stuff (git, JDK)

- Conda is an environment manager
  - Virtual environments
  - Import/export/distribute environments

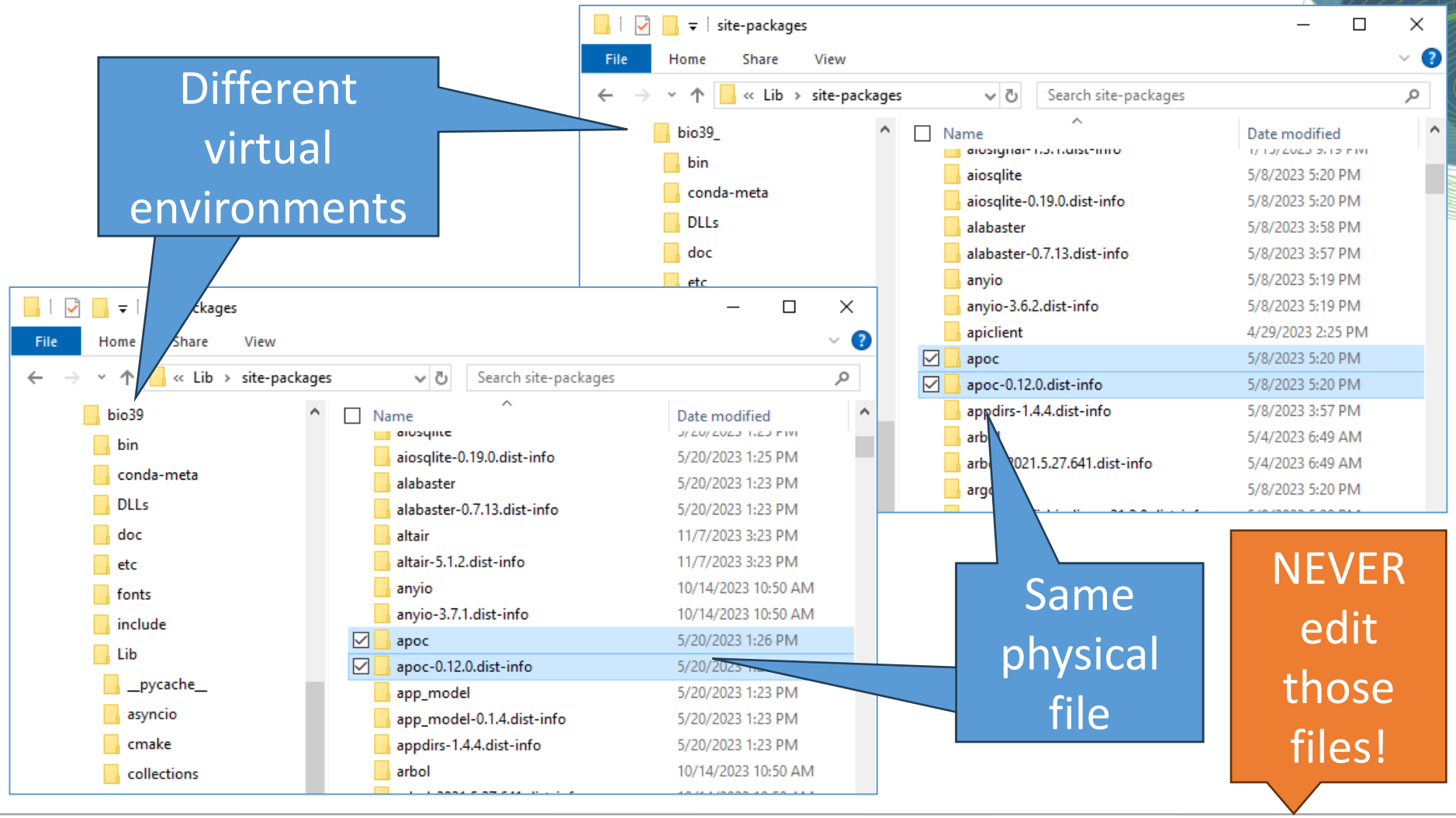
Conda environments

- A conda environment is *just a folder*



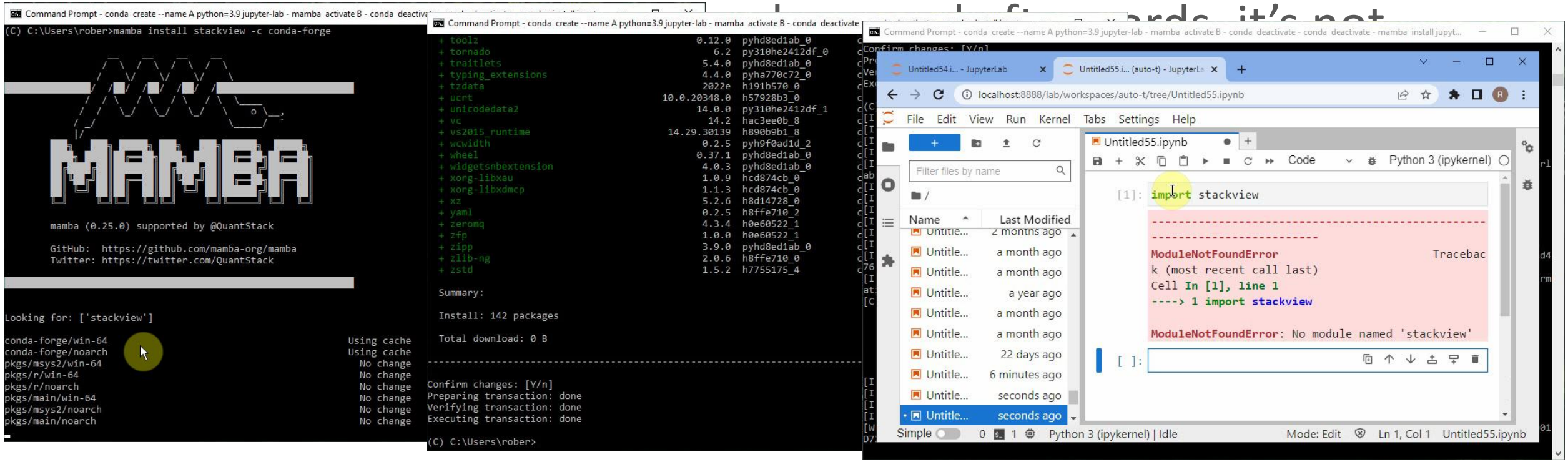
Conda environments

- Packages within the folders are just linked
- If you change a file in env1, the same file in env2 is changed.



Broken [conda] environments

- Common case of confusion in the Python ecosystem
- Happens to everyone – it's just a matter of time.



Background

- The base-environment is special.
- You install packages into the base environment, if you do not run `conda activate my_env`
- You can run base-software from within other environments

Base

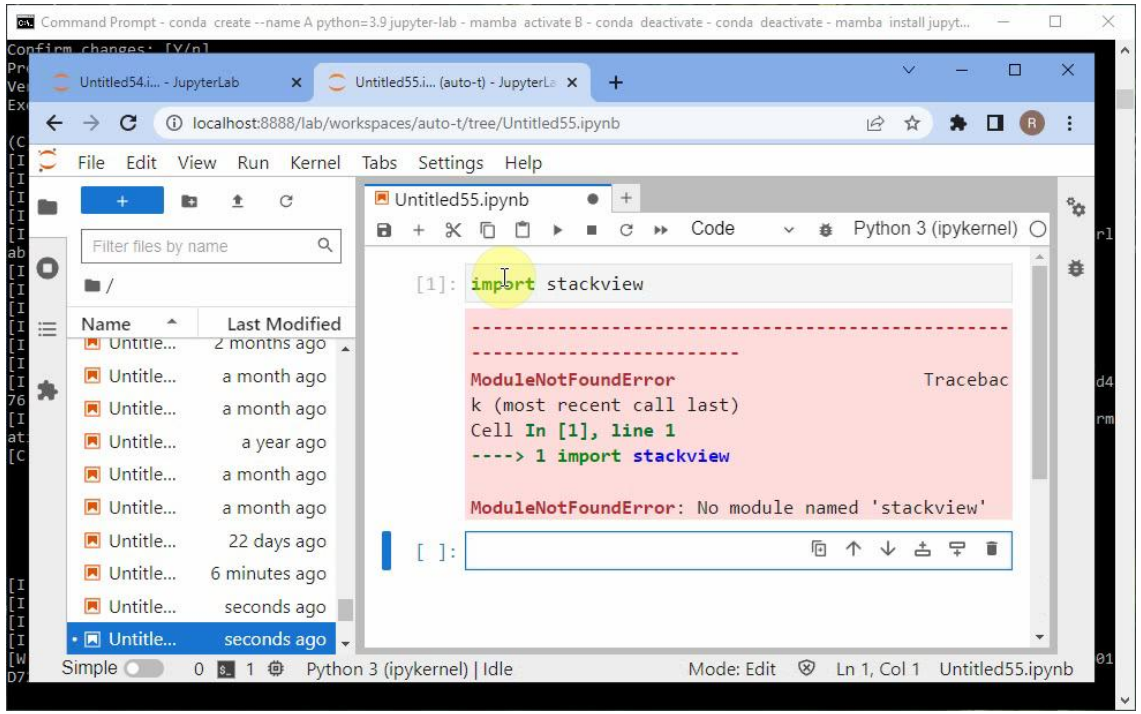
Installed packages:

`Jupyter lab`

my_env

Installed packages:

`stackview`



Broken [conda] environments

- The only cure: Uninstall and reinstall [Ana]conda.

- Alternatively:
  - Create a new environment for every project.
  - `conda activate my_env`
  - Do not install project-specific stuff in the base-environment.

Broken [conda] environments

Do not install anything in the base environment

Always call conda activate … before doing anything

Documenting dependencies

- Recommendation: Maintain a document with the dependencies (and versions) you need in your project
  - The conda way

environment.yml - Notepad

File Edit Format View Help

```
name: cellpose-test
channels:
  - conda-forge
  - pytorch
dependencies:
  - python=3.8
  - pytorch=1.12
  - devbio-napari
  - cellpose-napari
```

Ln 3, C 100% Windows (CRLF) UTF-8

In case your environment is screwed up, you can rebuild it any time.

```
conda env create -f environment.yml
```

  - The pip way

requirements.txt - Notepad

File Edit Format View Help

```
numpy>=1.21
andas~=1.4.0
napari~=0.4.11
matplotlib~=3.5.0
scikit-image~=0.19
umap-learn~=0.5.1
hdbscan~=0.8.27
scikit-learn~=1.0
numba~=0.55.1
```

Ln 2, 100% Windows (CRLF) UTF-8

```
pip install -r requirements.txt
```

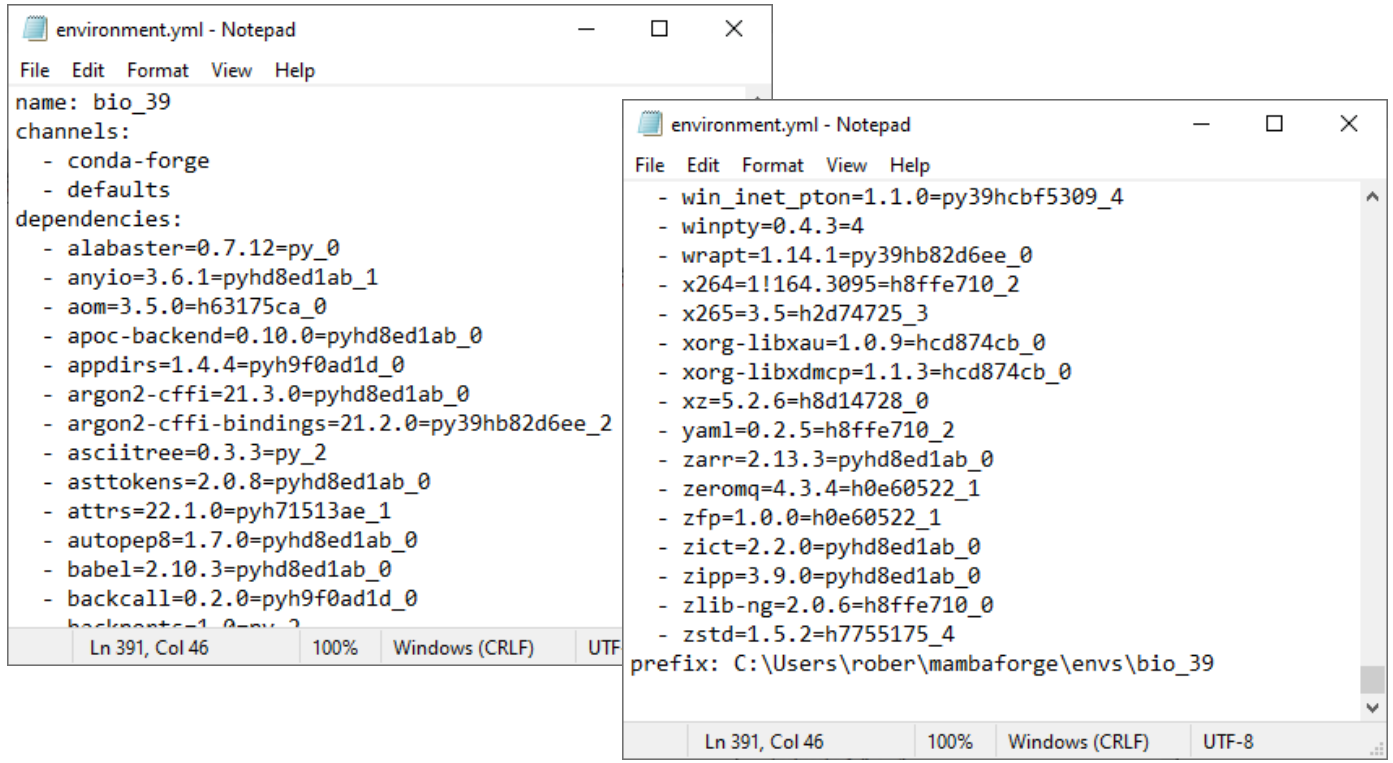
Your future self will thank you

https://conda.io/projects/conda/en/latest/user-guide/tasks/manage-environments.html#creating-an-environment-from-an-environment-yml-file
https://pip.pypa.io/en/stable/cli/pip_install/#examples

Documenting dependencies

- Exporting all installed libraries + versions

```
conda env export > environment.yml
```



Excellent way to document which dependencies were *actually* used…

It is *questionable* if re-creating an environment from this yml file works.

Installing dependencies

- A difference between pip and conda:

```
pip install package_a
```

```
conda install package_a
```

Depends on:
numpy<1.22.0

Dependency conflict

```
pip install package_b
```

```
conda install package_b
```

Depends on:
numpy>=1.22.0

passes

fails

Because the environment cannot be solved

Installing dependencies

- A difference between pip and conda:

```
pip install git
```

fails

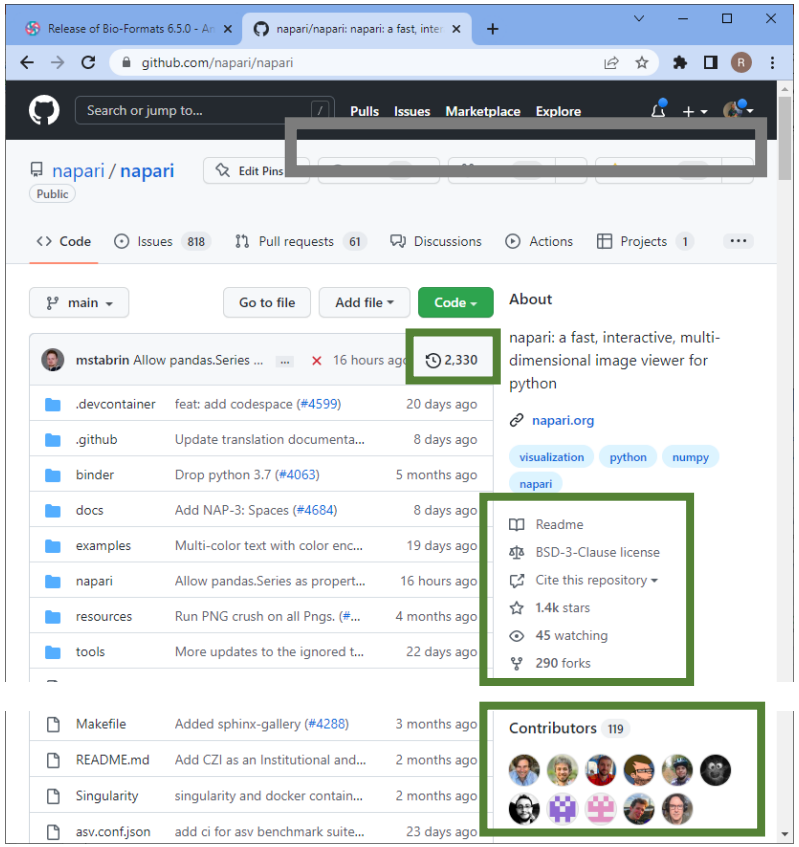
Because git is not a python package

```
conda install git
```

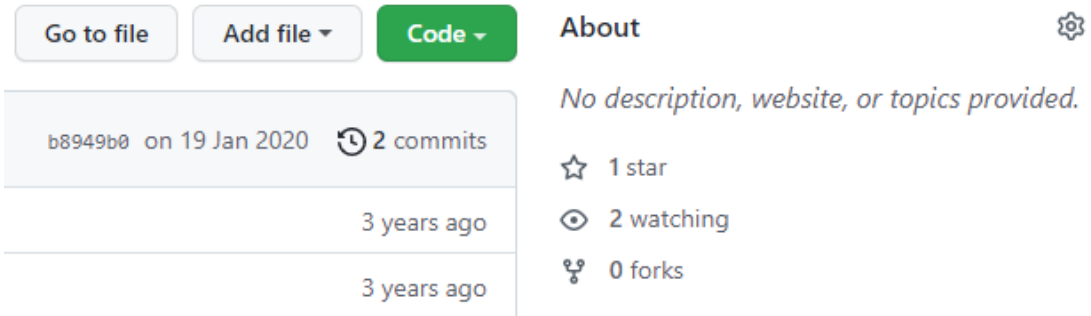
passes

Software quality indicators

- Visit the project's github or gitlab page and review indicators.



- **Stars**: People like software, similarly to posts on Bluesky
- **Watching**: People receive updates for new releases
- **Forks**: People made a copy of the code, e.g. to contribute to the project
- **Contributors**: People who contributed to the code
- **Commits**: Changes to the code



Software quality indicators

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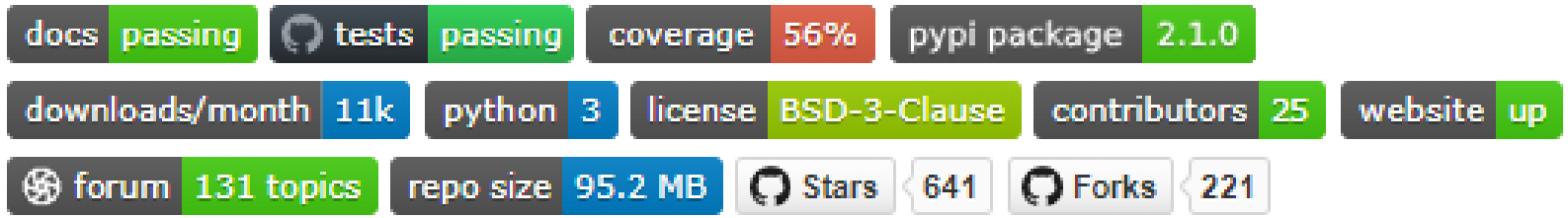
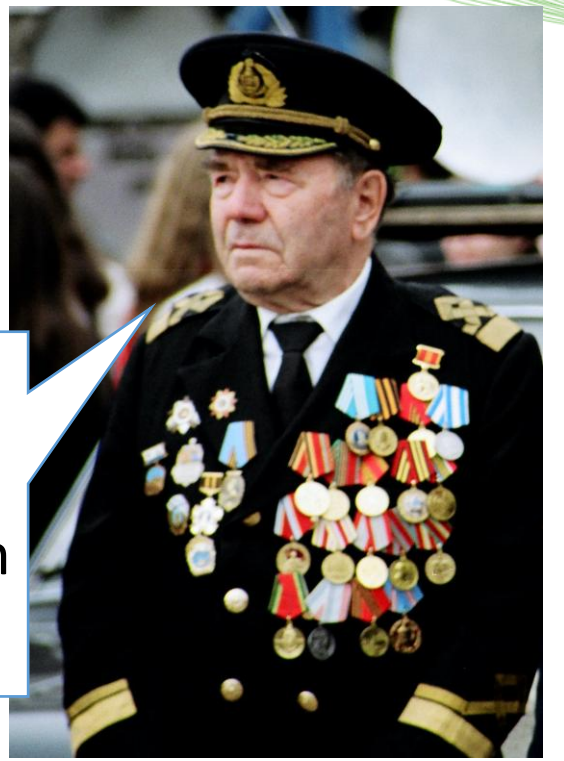


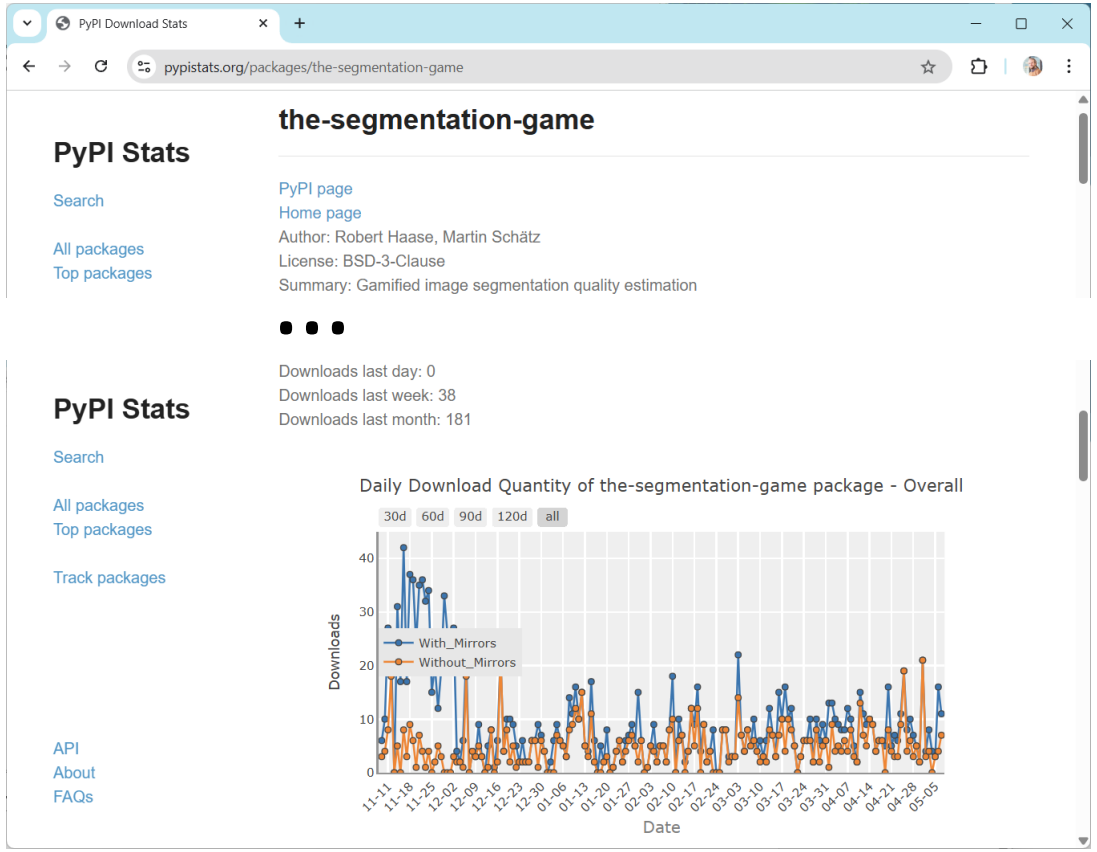


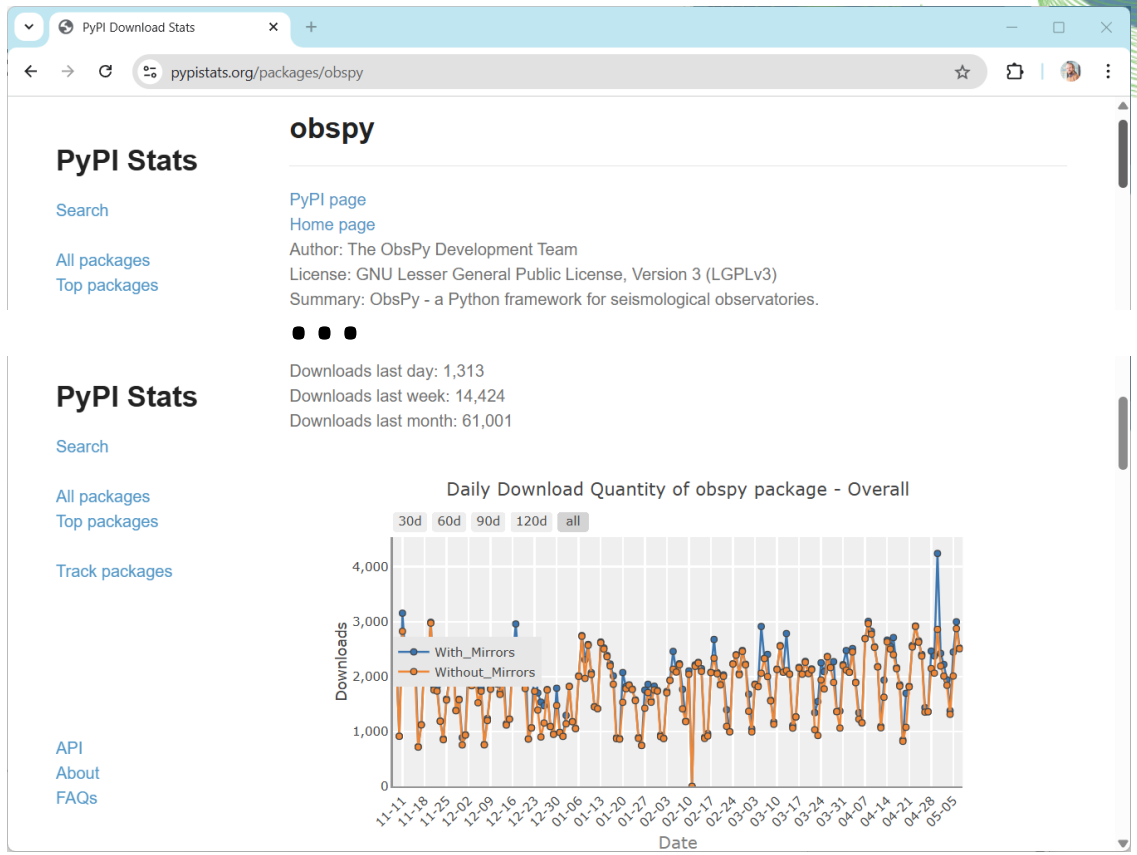
Note, github badges cannot be *deserved*. Developers put them there

Image source: Adapted from https://www.pexels.com/photo/shallow-focus-photo-of-two-persons-wearing-military-uniform-2859046/

Software quality indicators

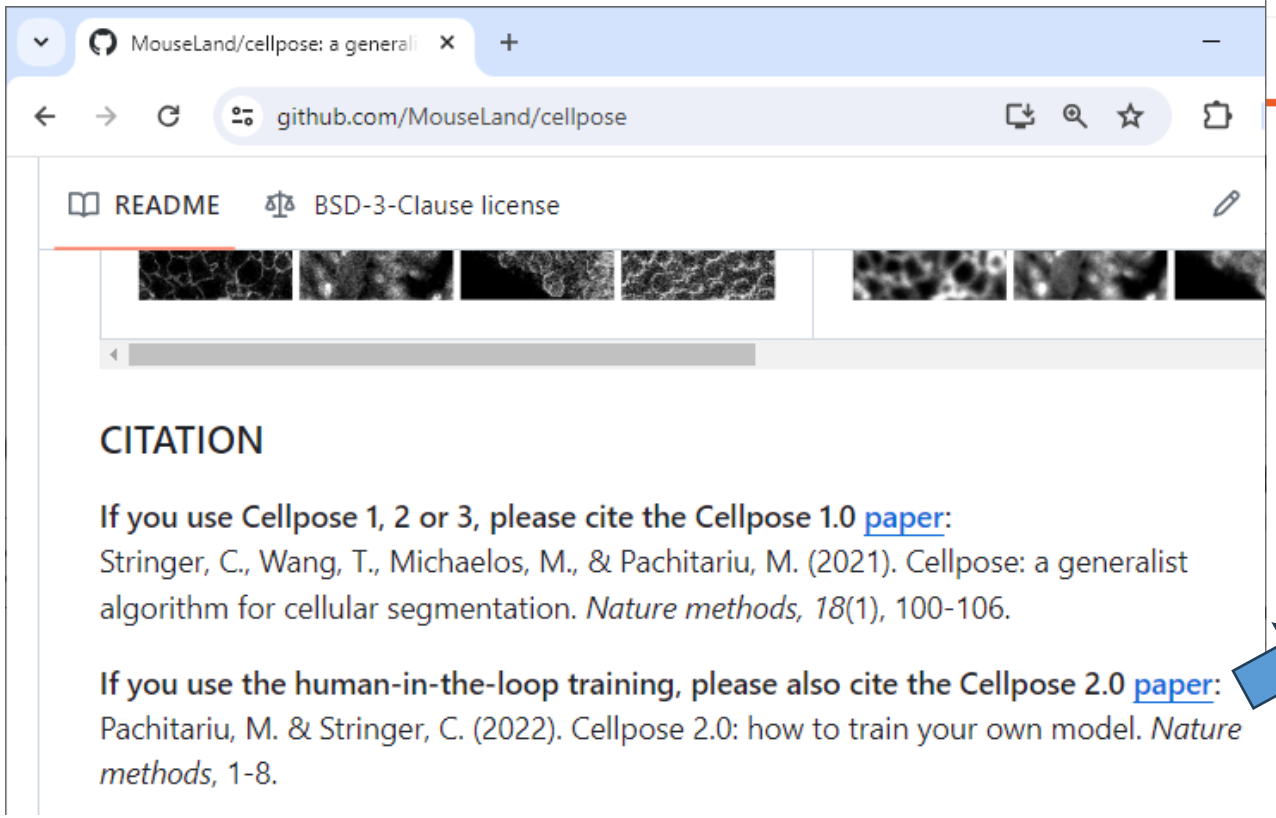
- Download statistics: pypi

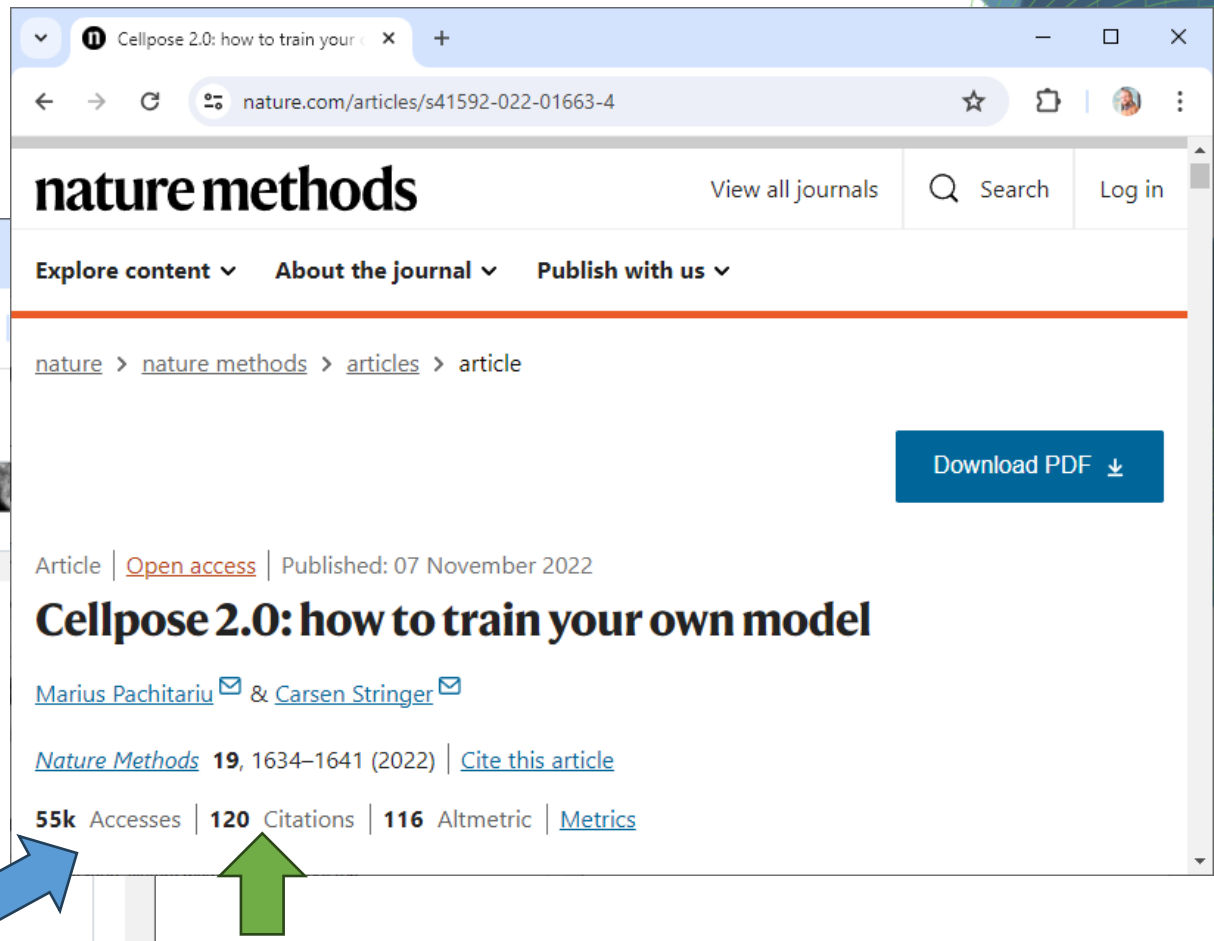


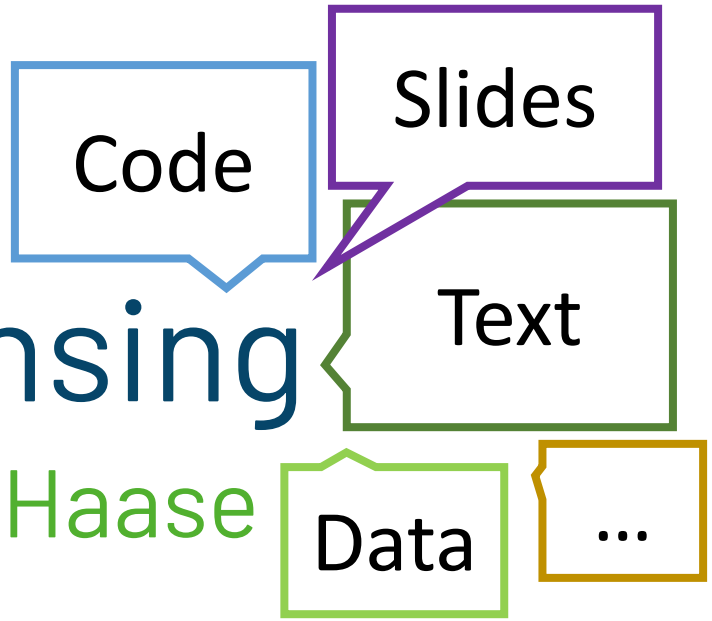


Software quality indicators

- Scientific publications







Licensing

Robert Haase

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What are the consequences of this sentence?

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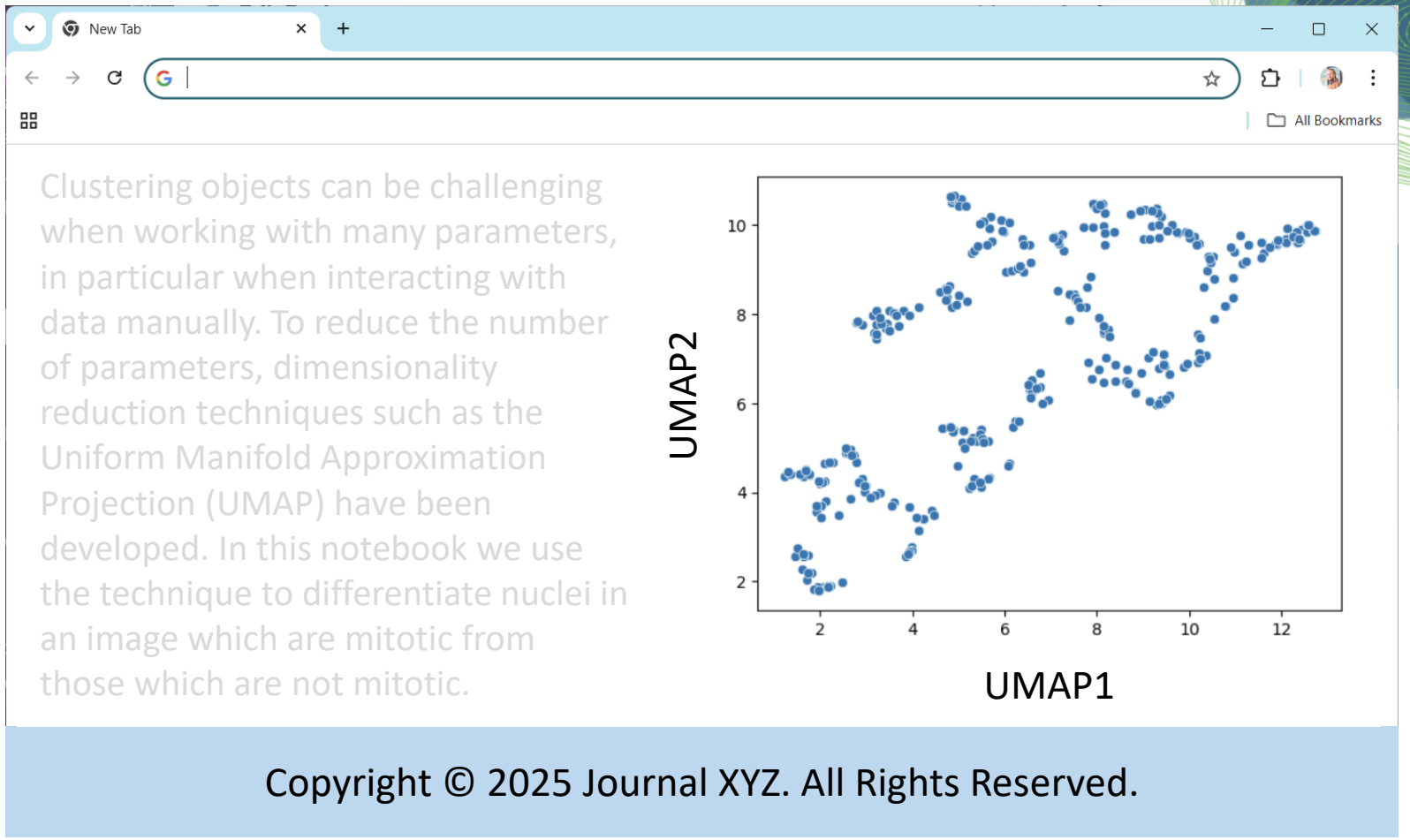
Quiz

- When you shared materials publicly on the internet, which *license* did you use?

None	Public Domain	Creative Commons	BSD/GPL/ MIT/…
			

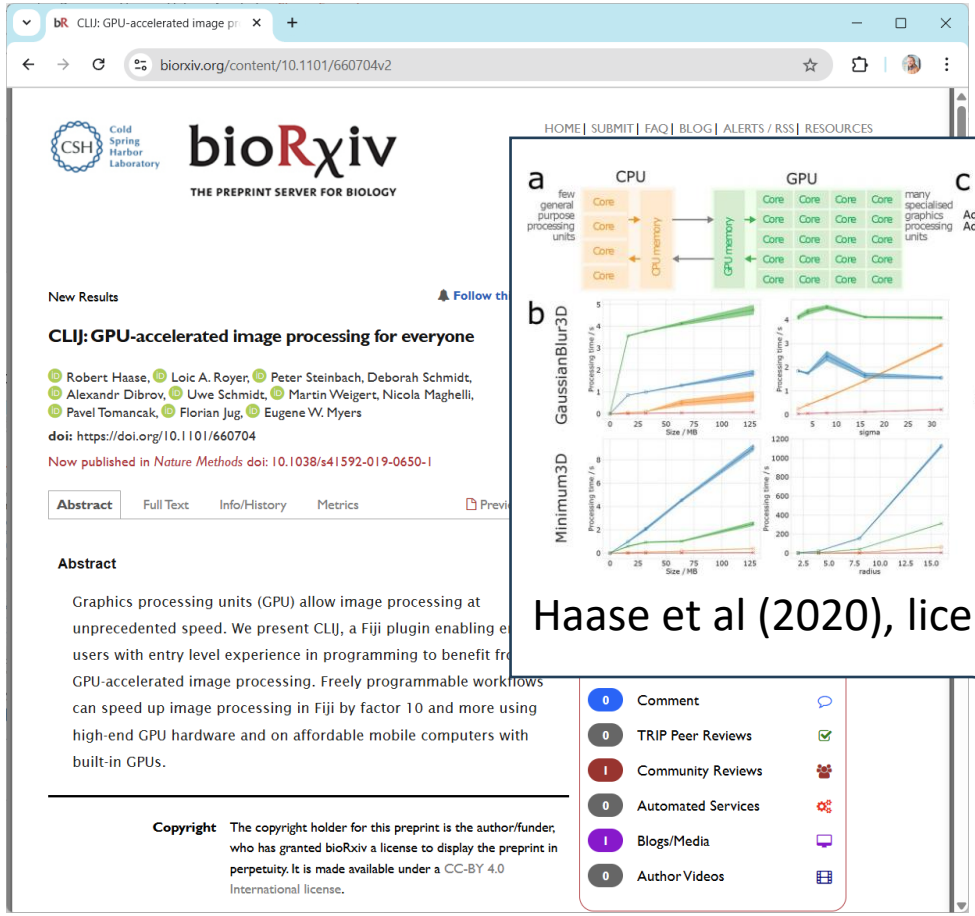
Quiz

How can you reuse this plot?
What is allowed?



Hint: Search for pre-prints

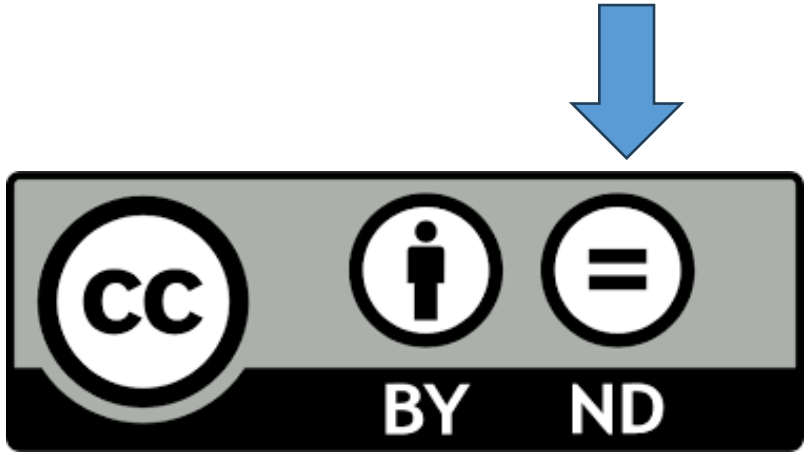
In case a journal doesn't allow reusing figures from a paper, search for the corresponding preprint!



Haase et al (2020), licensed CC-BY 4.0

Licensing: Permissive versus restrictive

- Who knows what the ND stands for?



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"permissive"

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"restrictive"

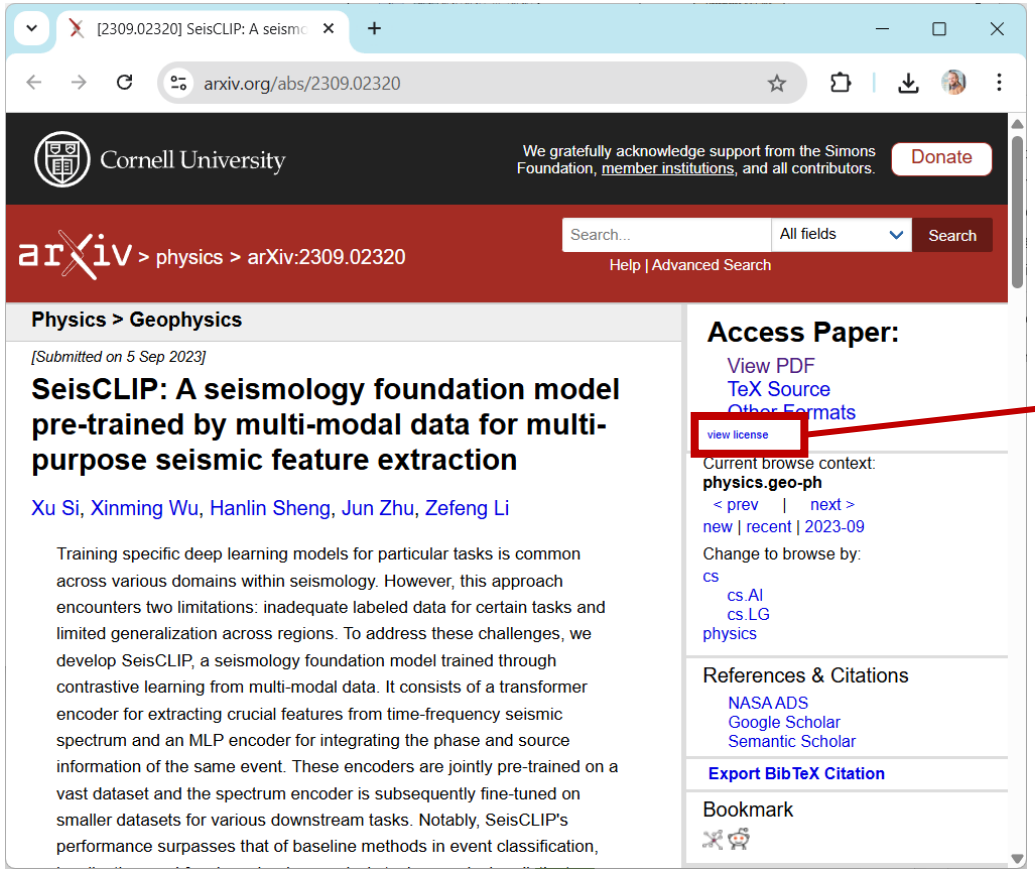
Licensing: Permissive versus restrictive

I hope nobody feels hurt
by the following slides.

I just would like to make a point.

Licensing: Permissive versus restrictive

Example



I would love to show you a Figure from this paper!

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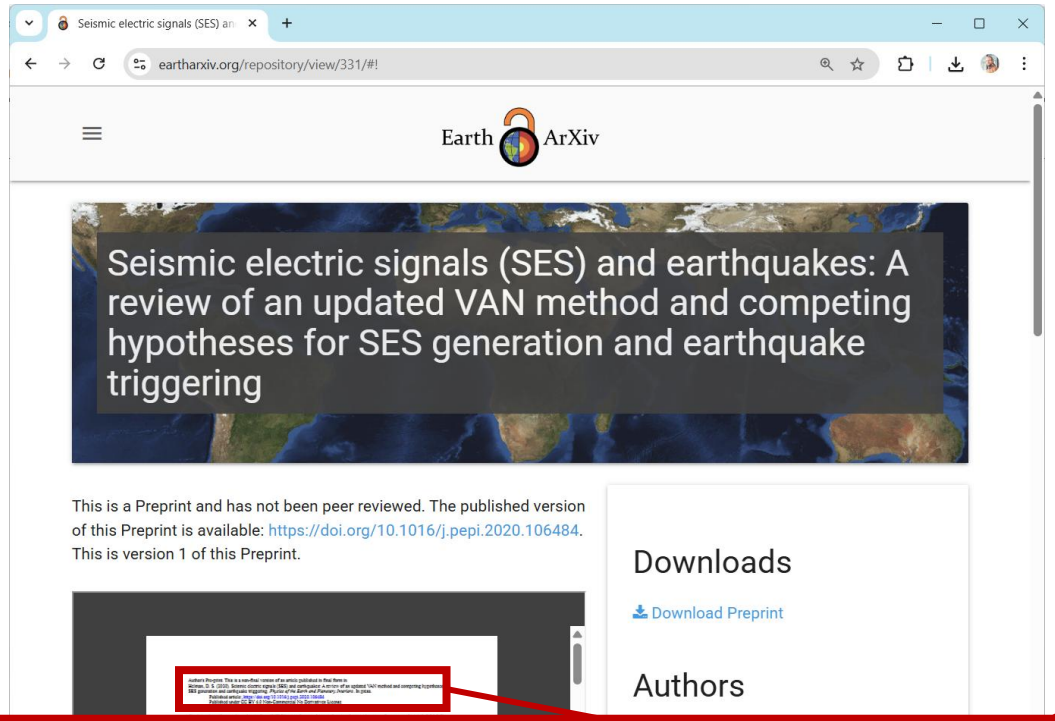
But I'm not allowed!

Licensing: Permissive versus restrictive

Example



I would love to show you a Figure from this paper!

But I'm not allowed!

Author's Pre-print. This is a non-final version of an article published in final form in
Helman, D. S. (2020). Seismic electric signals (SES) and earthquakes: A review of an updated VAN method and competing hypotheses for SES generation and earthquake triggering. *Physics of the Earth and Planetary Interiors*. In press.
Published article: https://doi.org/10.1016/j.pepi.2020.106484
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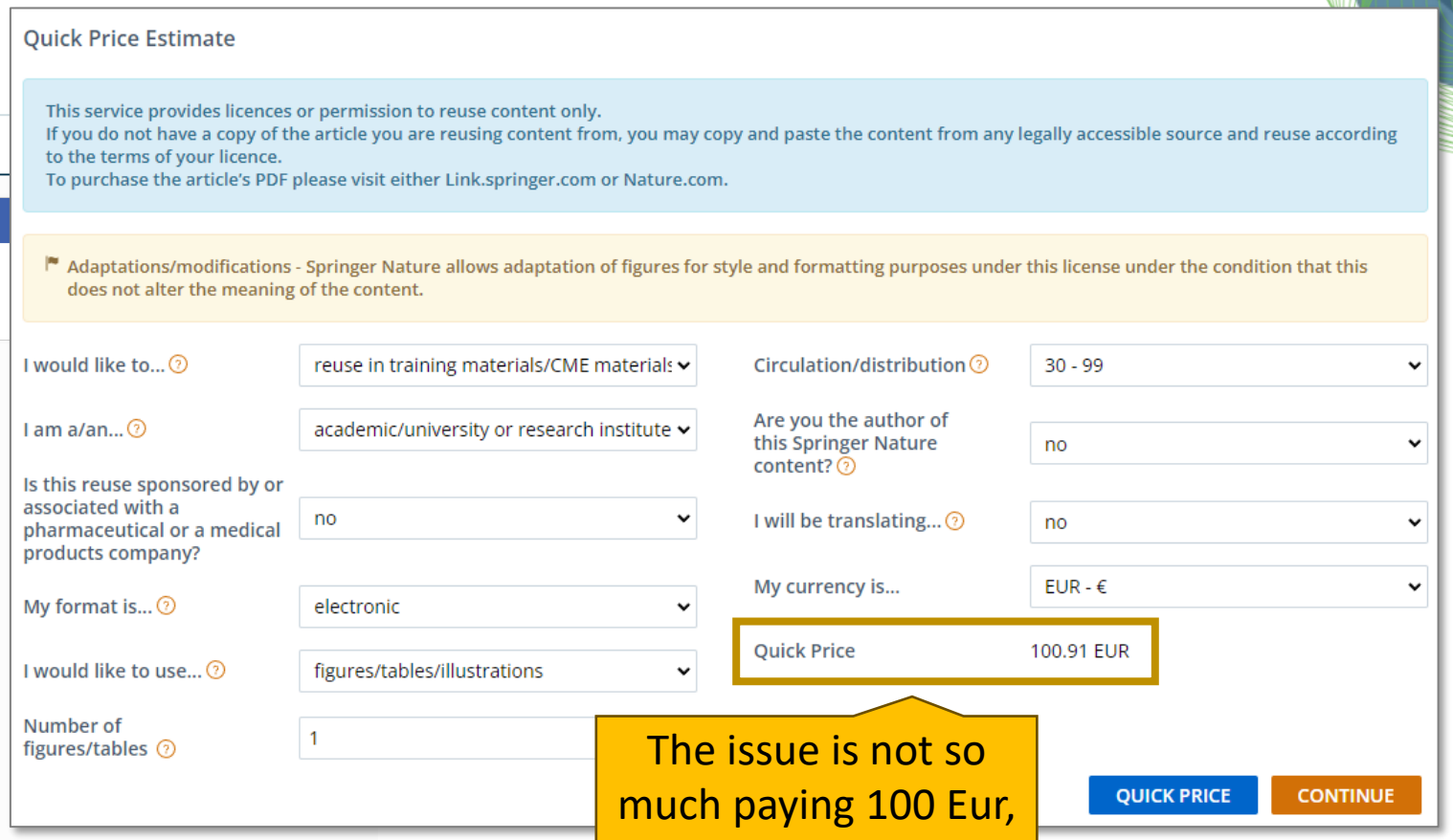
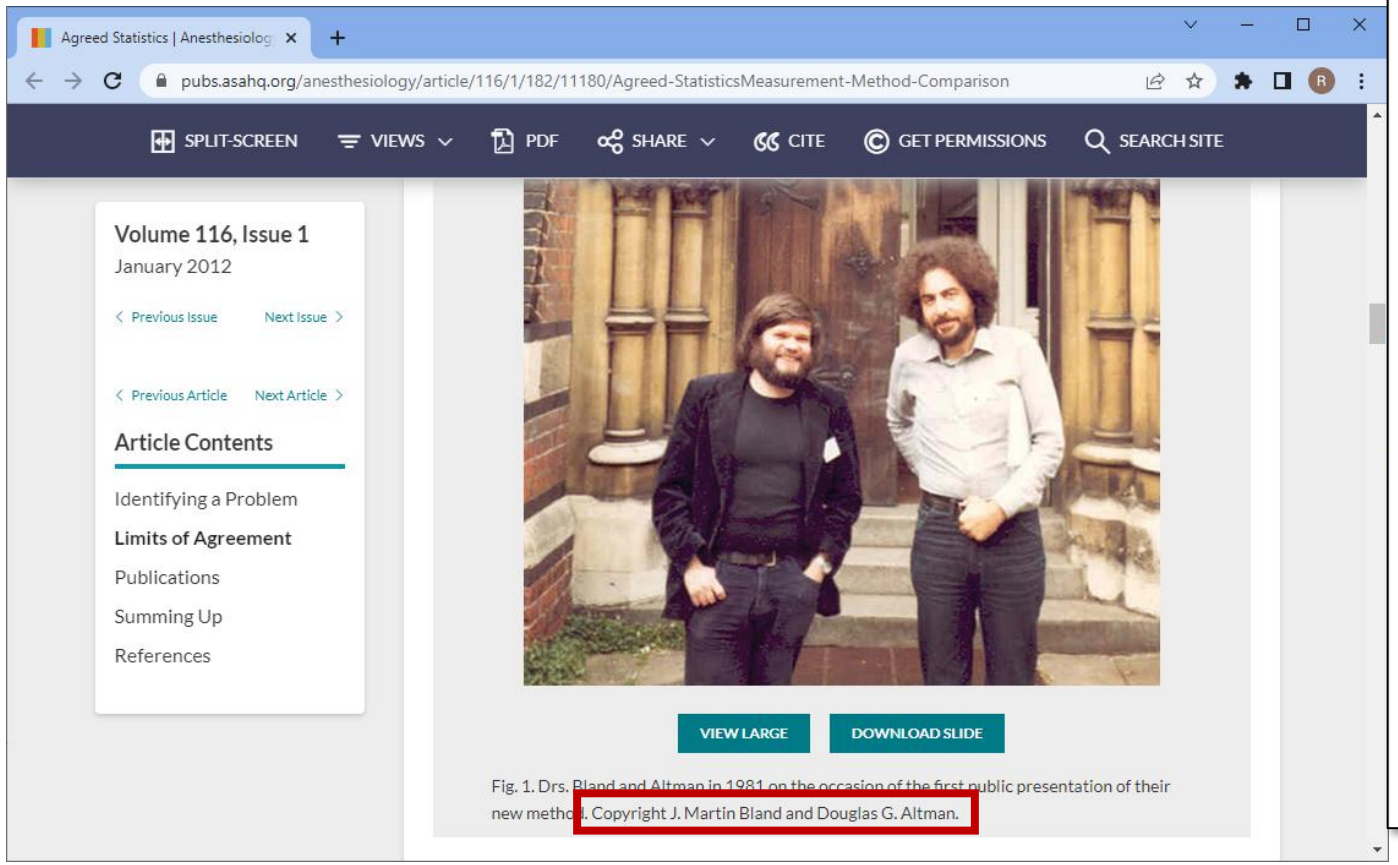
Example

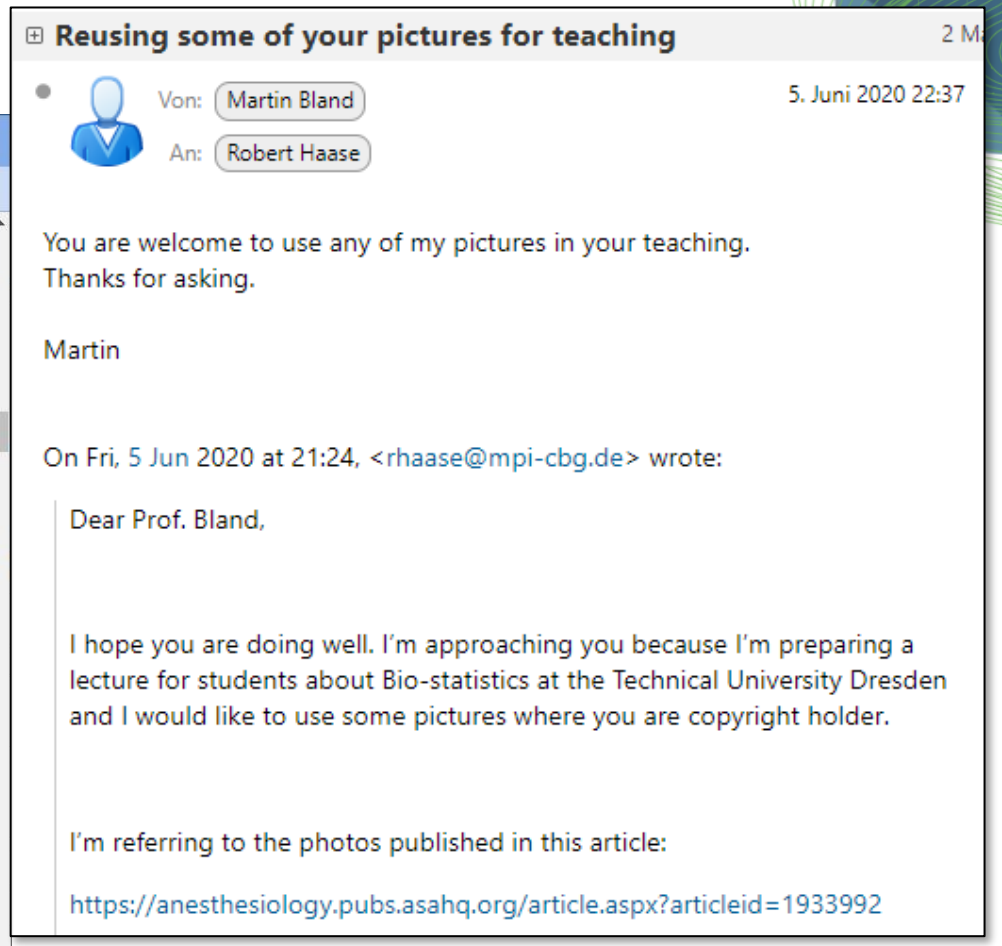


The issue is not so much paying 100 Eur, but the related administrative effort.

Licensing: Permissive versus restrictive

Example when you need to ask





Source: https://anesthesiology.pubs.asahq.org/article.aspx?articleid=1933992

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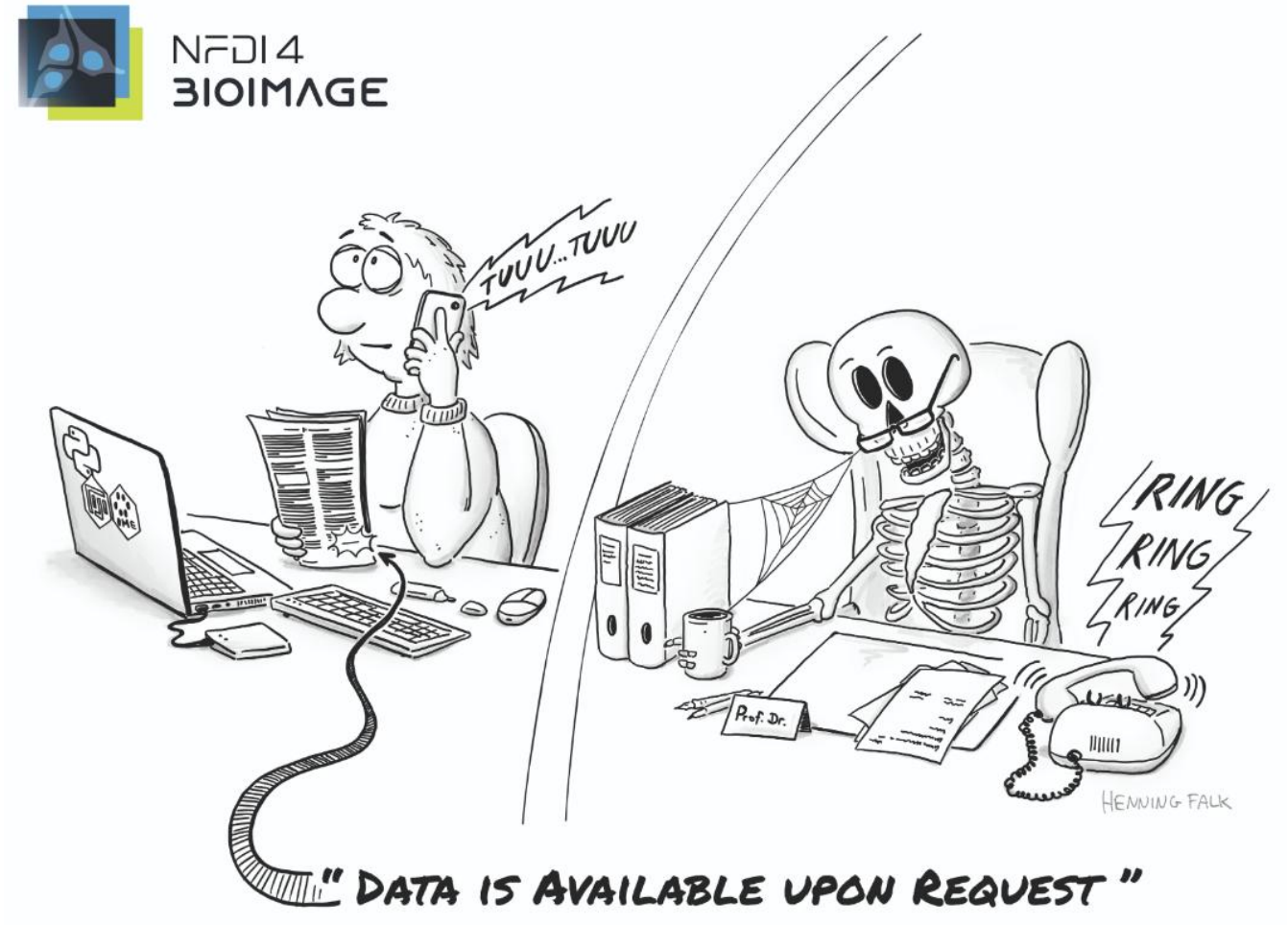


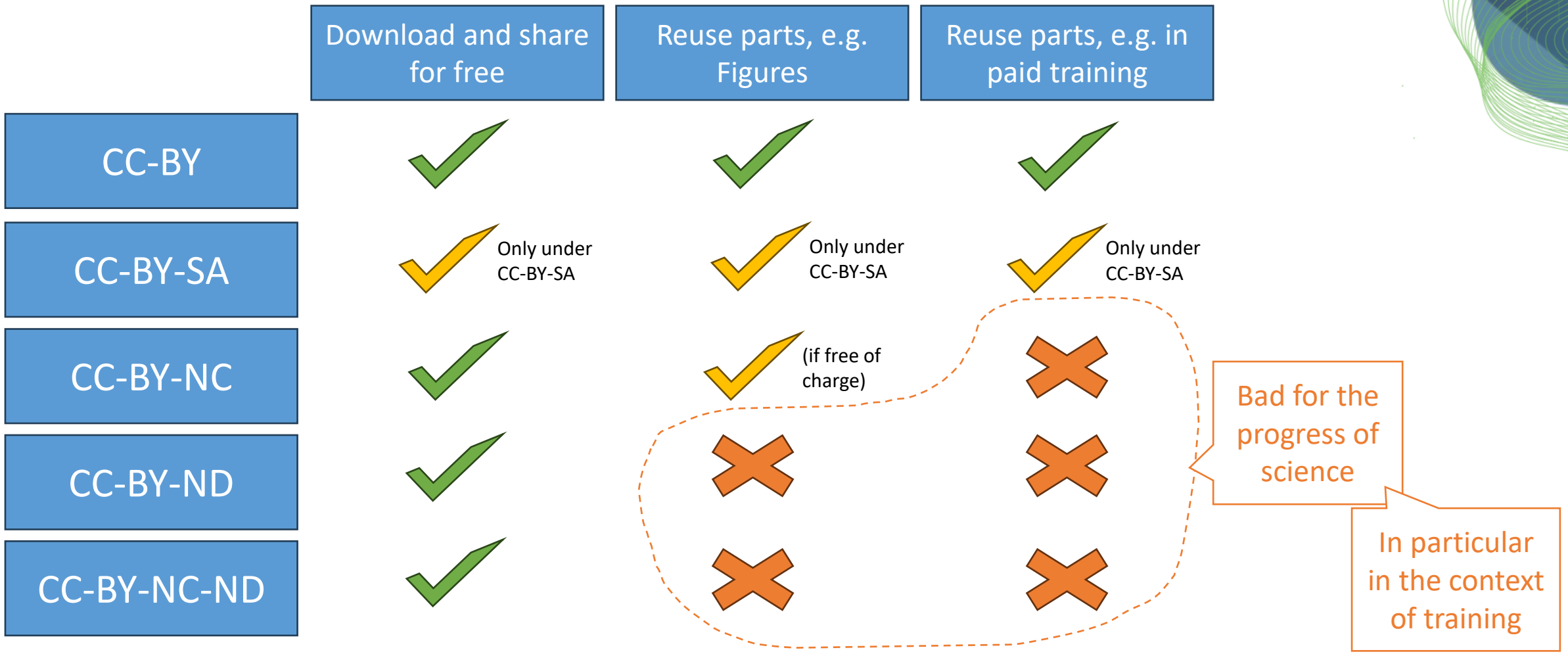
Licensing: Permissive versus restrictive

Restrictive licensing is
a community-wide issue.

I *presume* due to lack of awareness & training

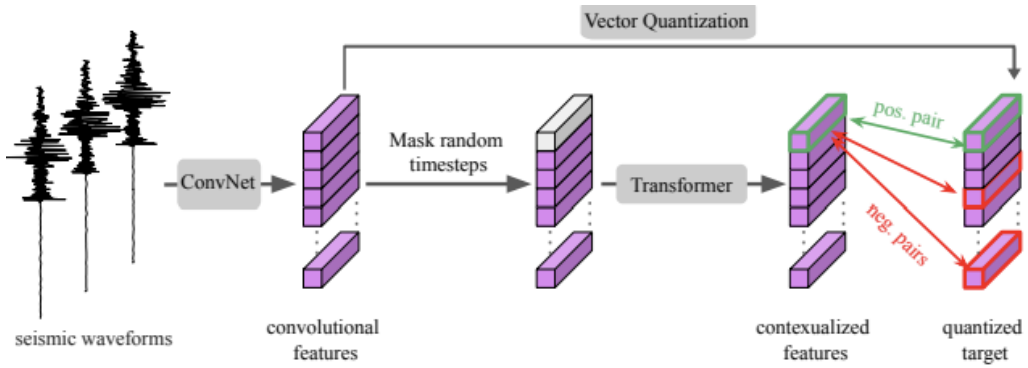
Train the trainers!

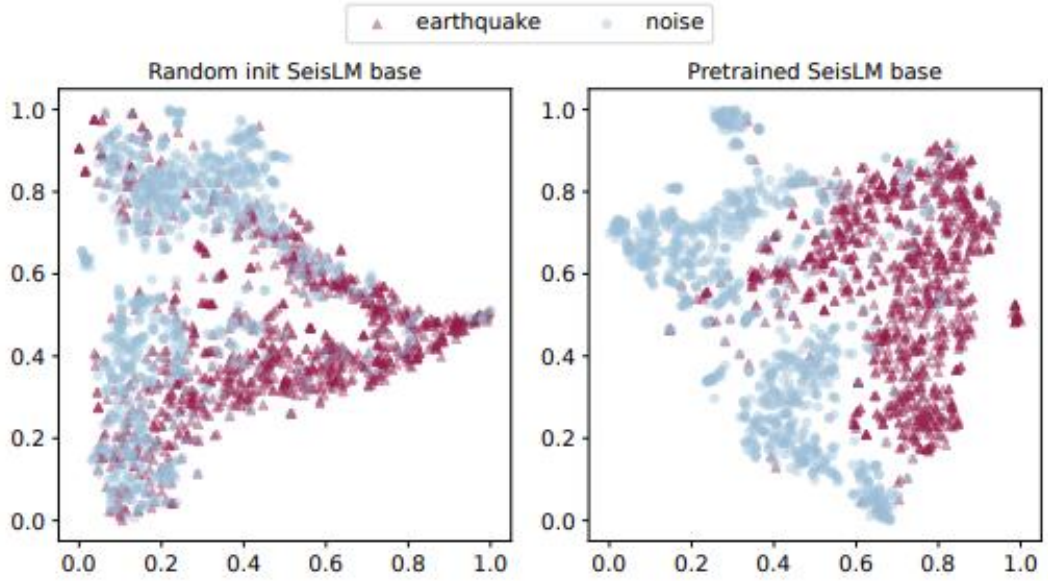
Licensing: Permissive versus restrictive



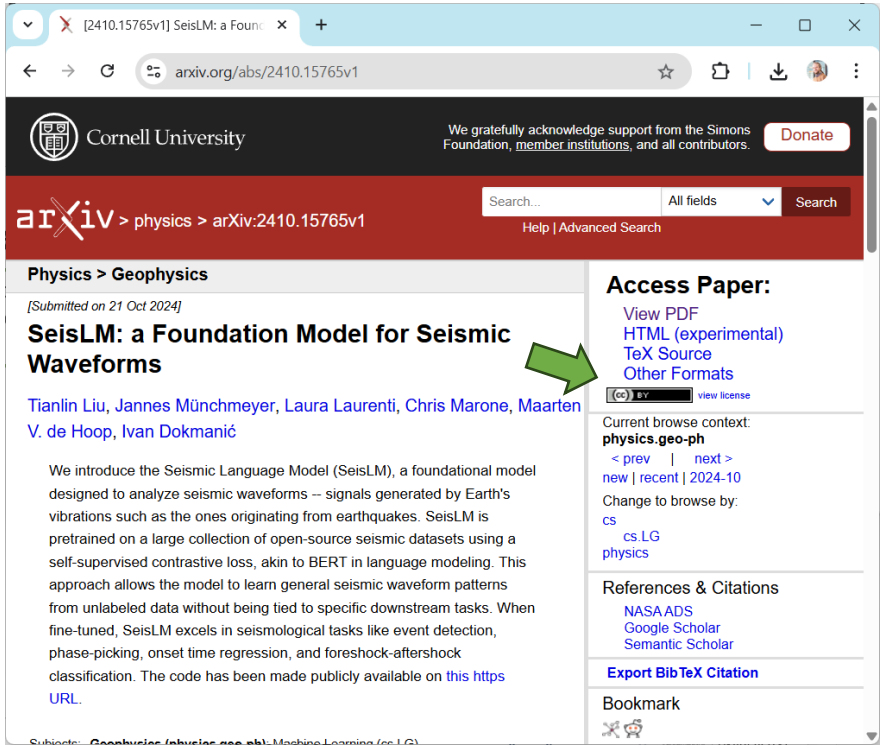
Licensing: Permissive versus restrictive

Example





Look at these great figures! They are from https://arxiv.org/abs/2410.15765v1 licensed CC-BY 4.0 by T. Liu et al.



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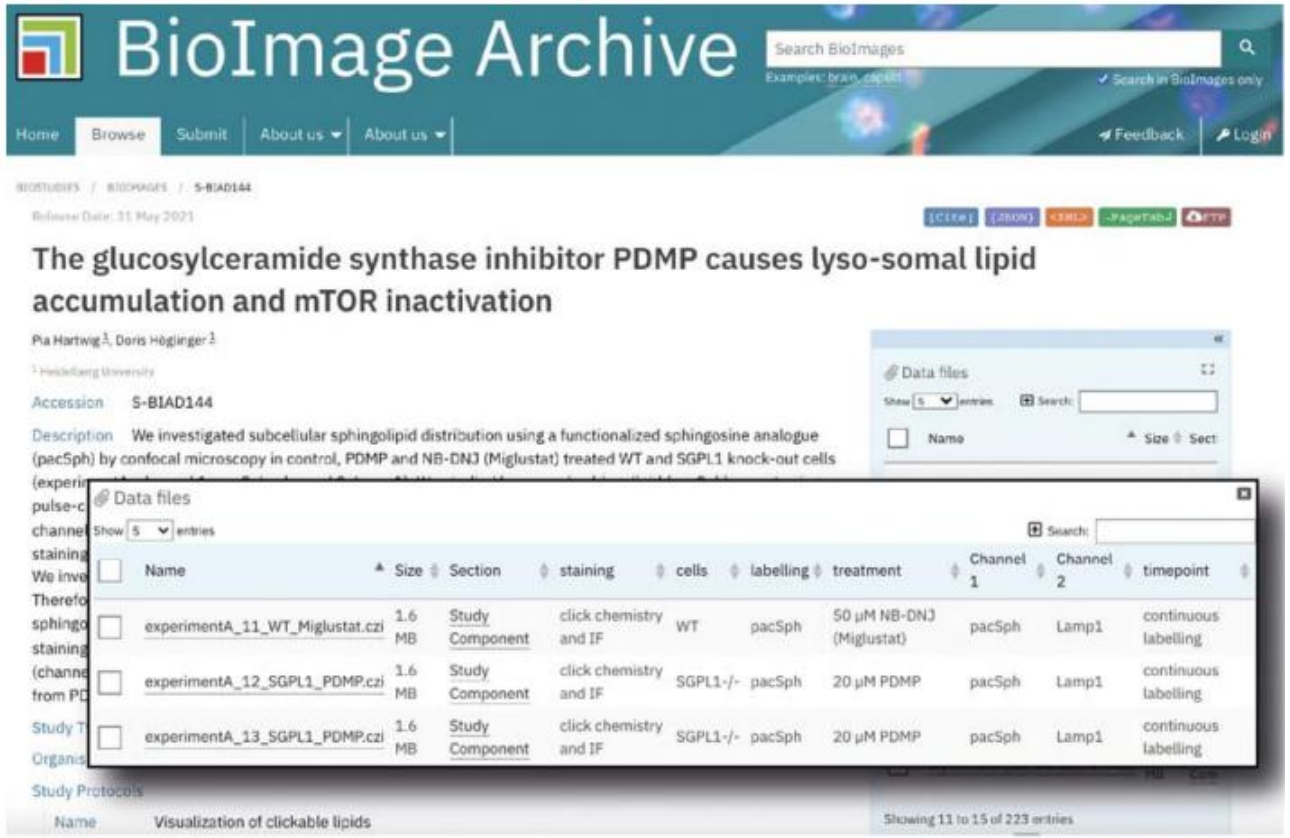
Example

Look at this great figure! It's taken from M. Hartley et al.



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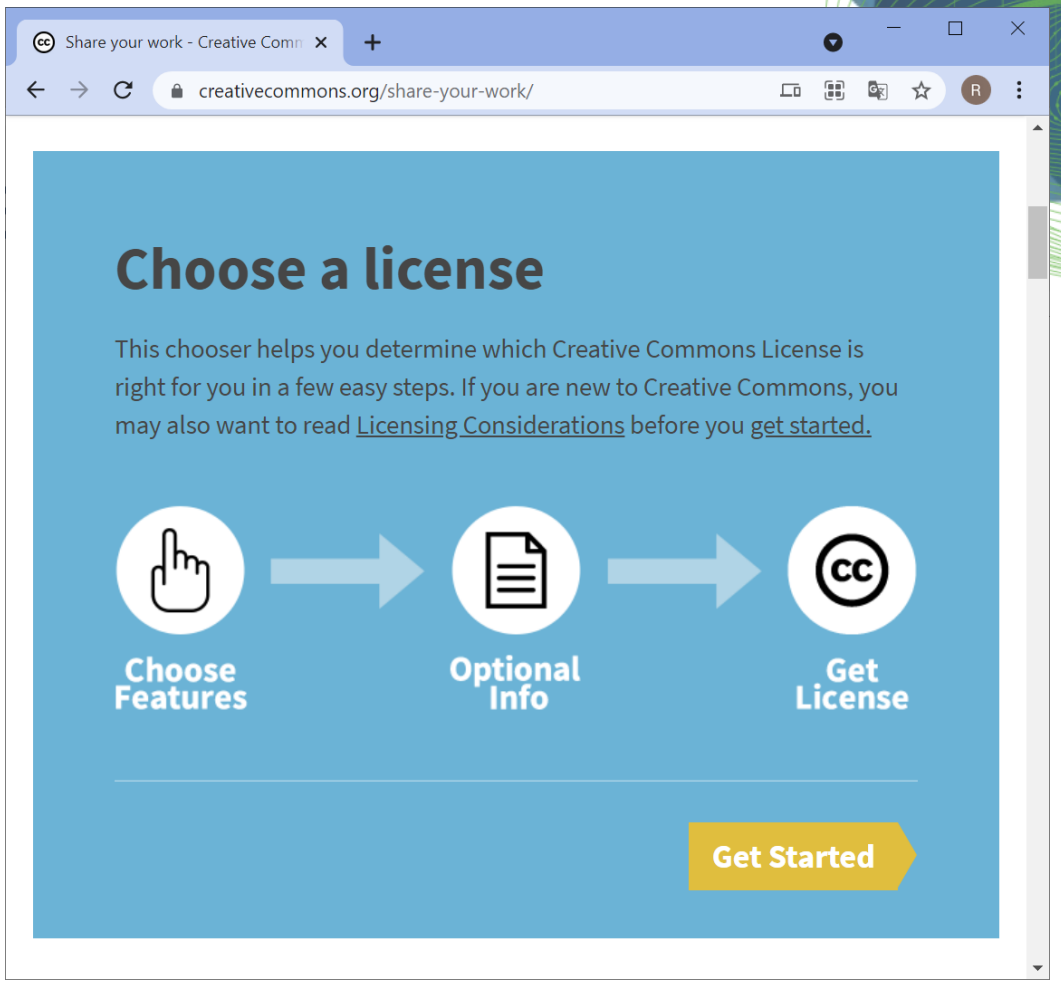
- Attribution ShareAlike Int. (CC-BY-SA)
- Attribution Non-Commercial Int. (CC-BY-NC)
- Attribution NoDerivatives Int. (CC-BY-ND)

+ Combinations, e.g. CC-BY-NC-ND



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Employers don't like this one because you give away the rights to *exploit* your work.

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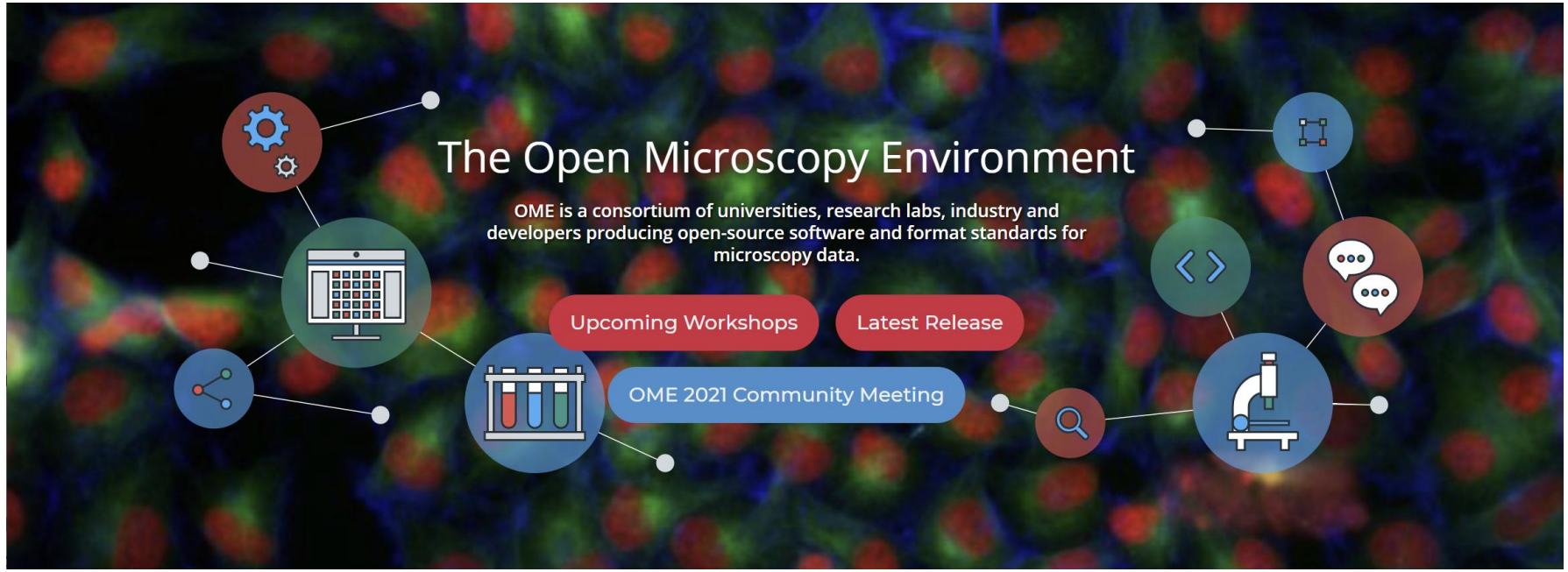
Example



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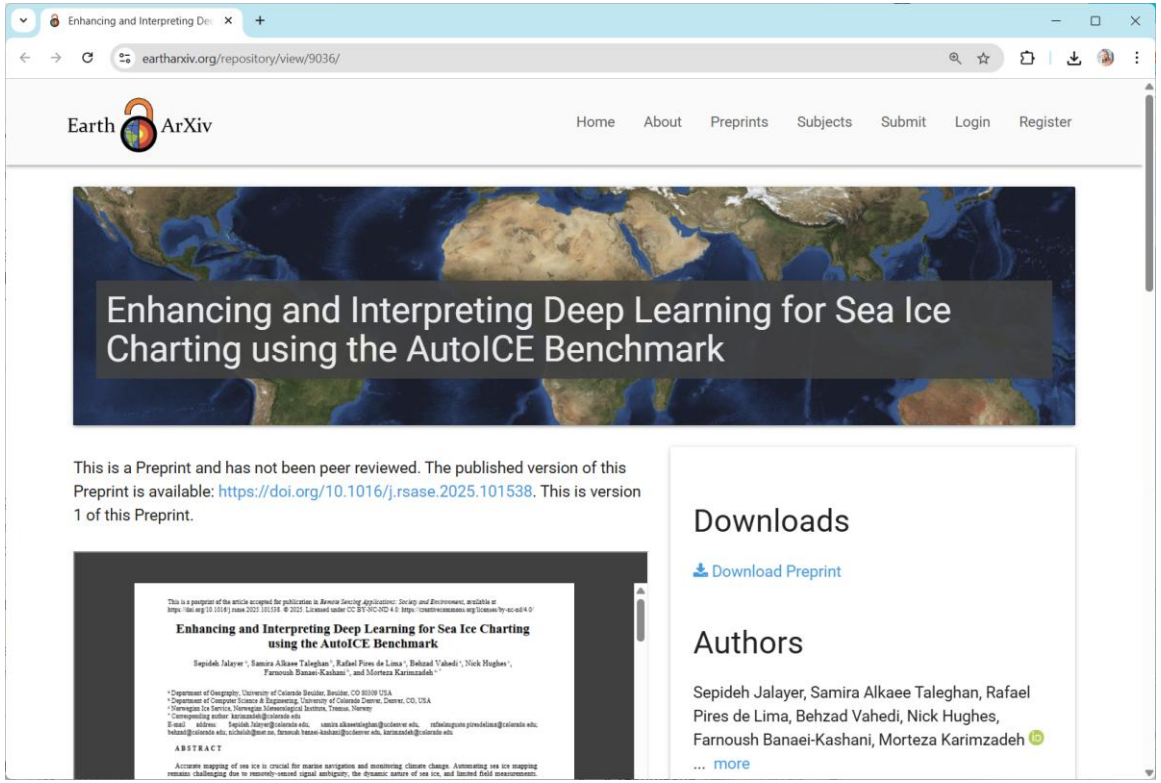

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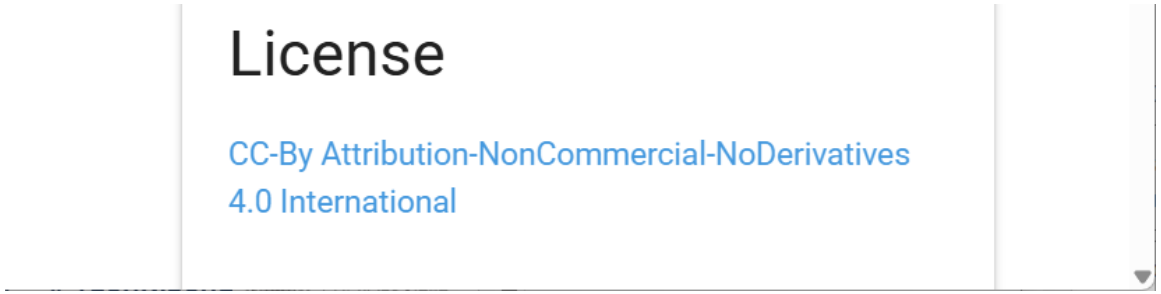

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Quiz

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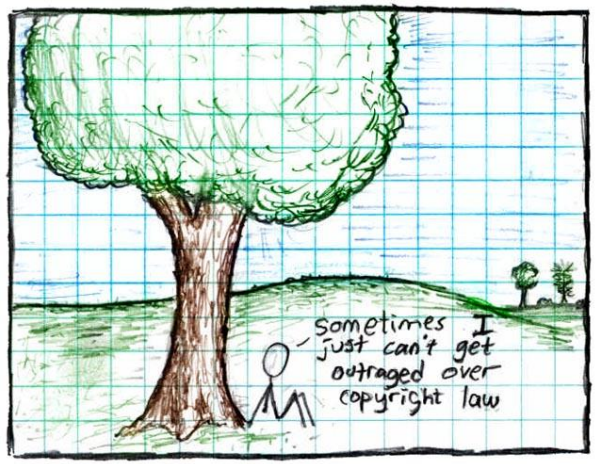

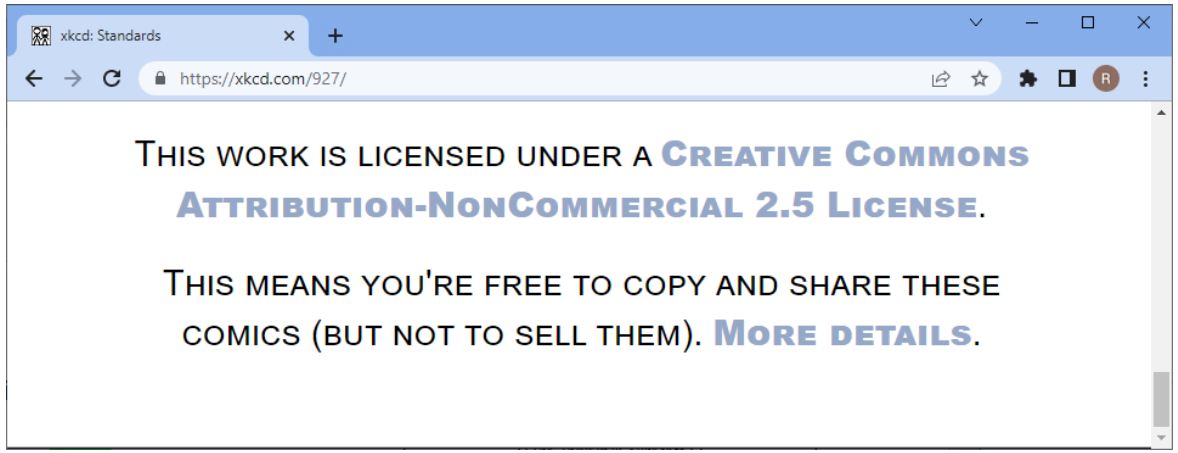

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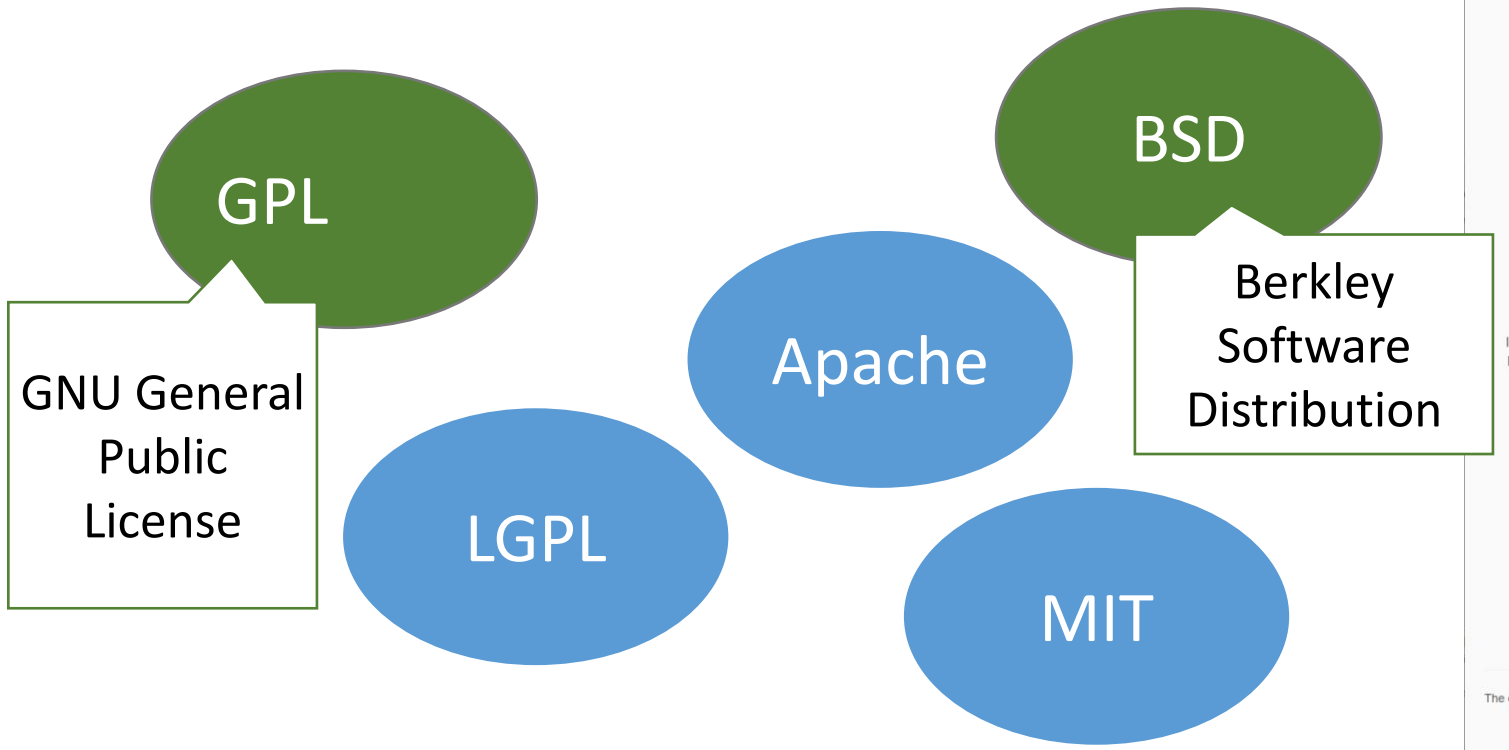

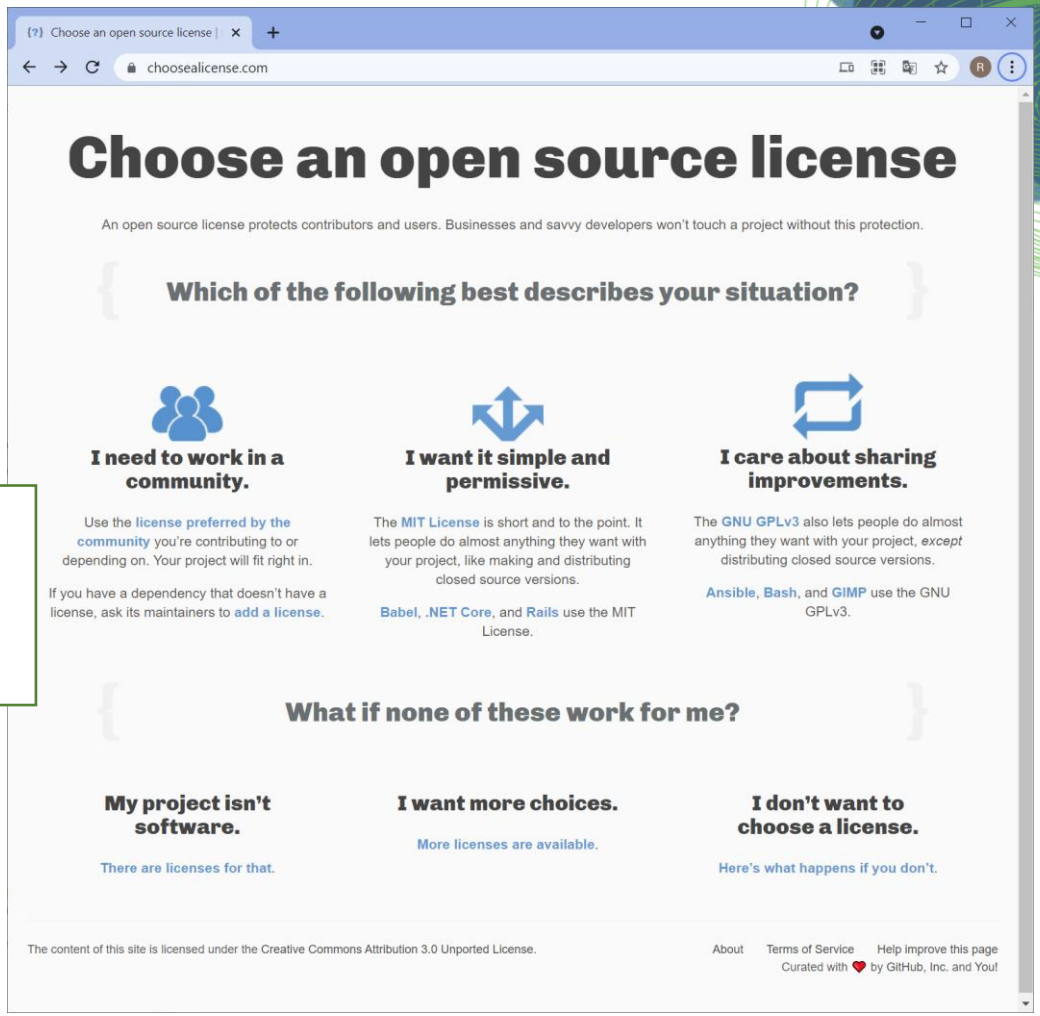

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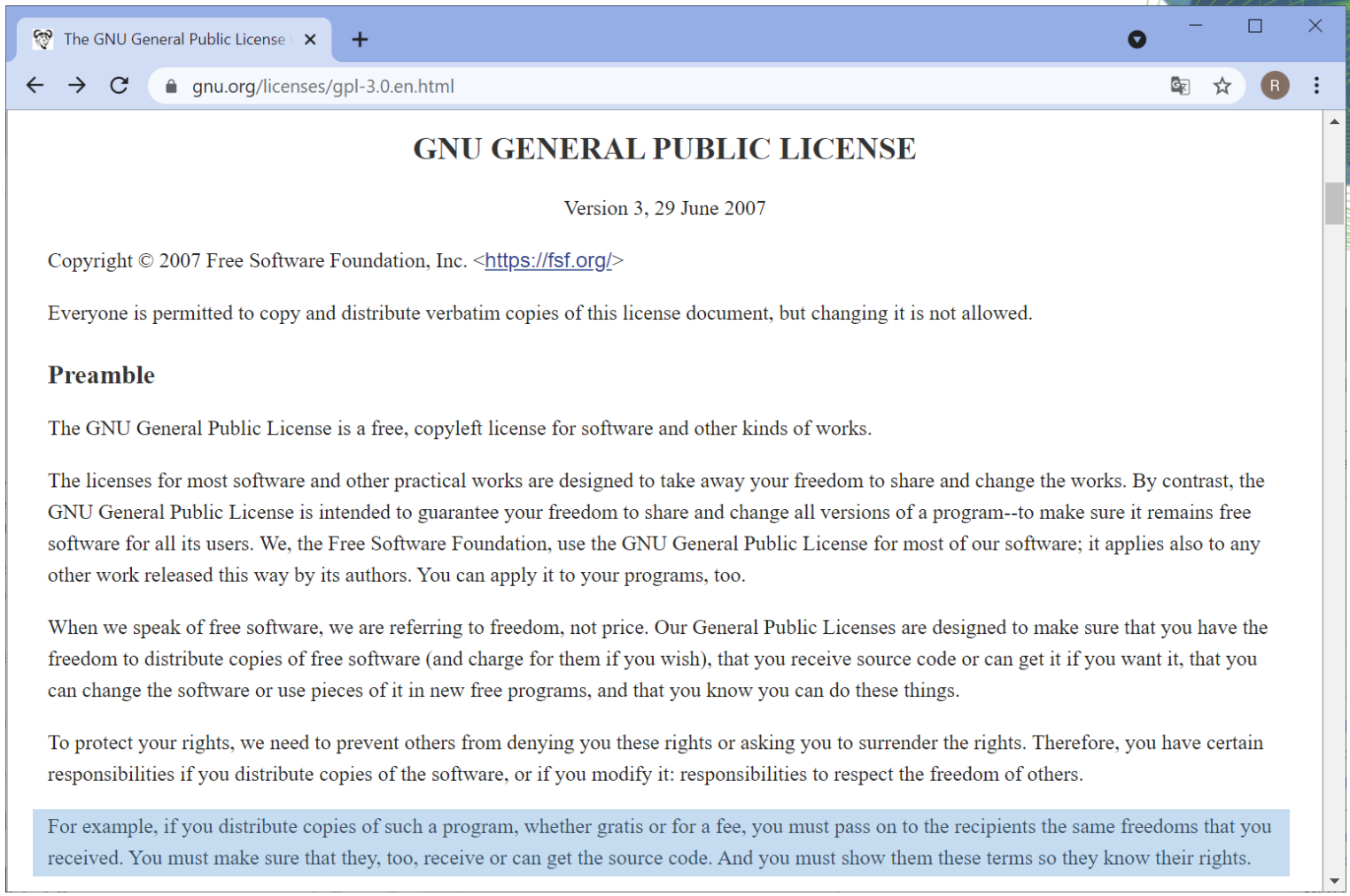

Quiz

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Yes

No

Do I have to release the code for this commercial product?

Yes

No

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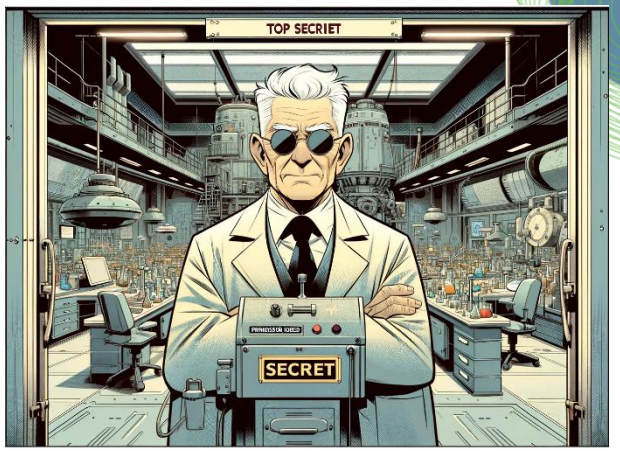

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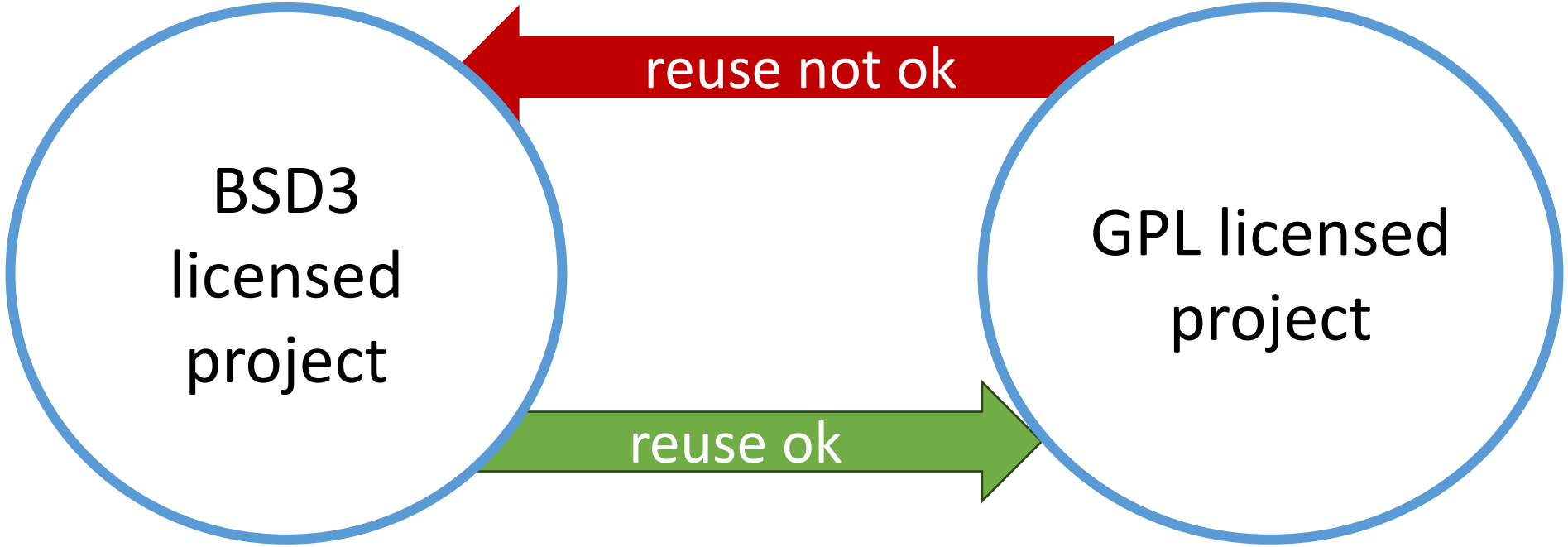

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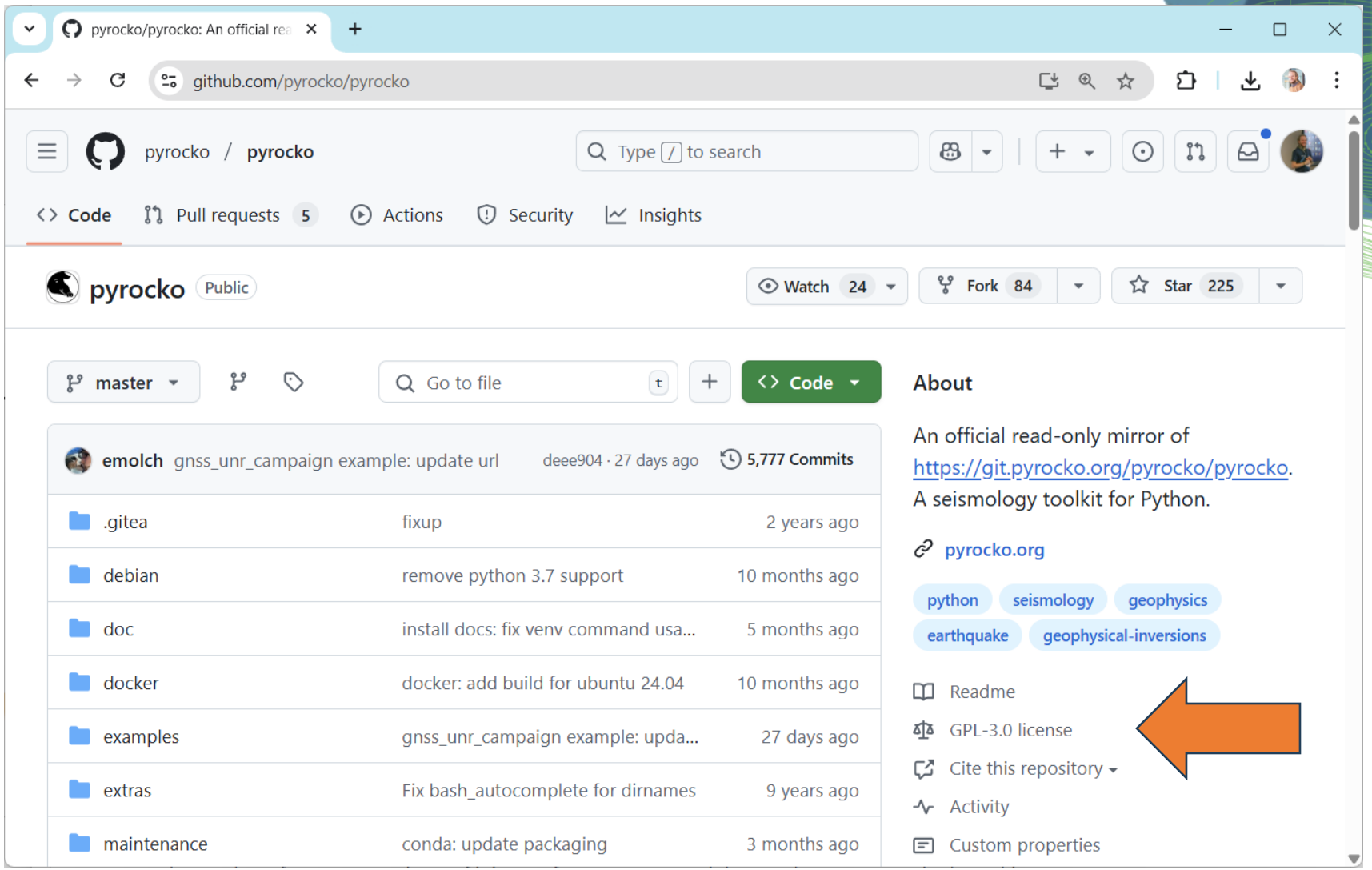

Quiz

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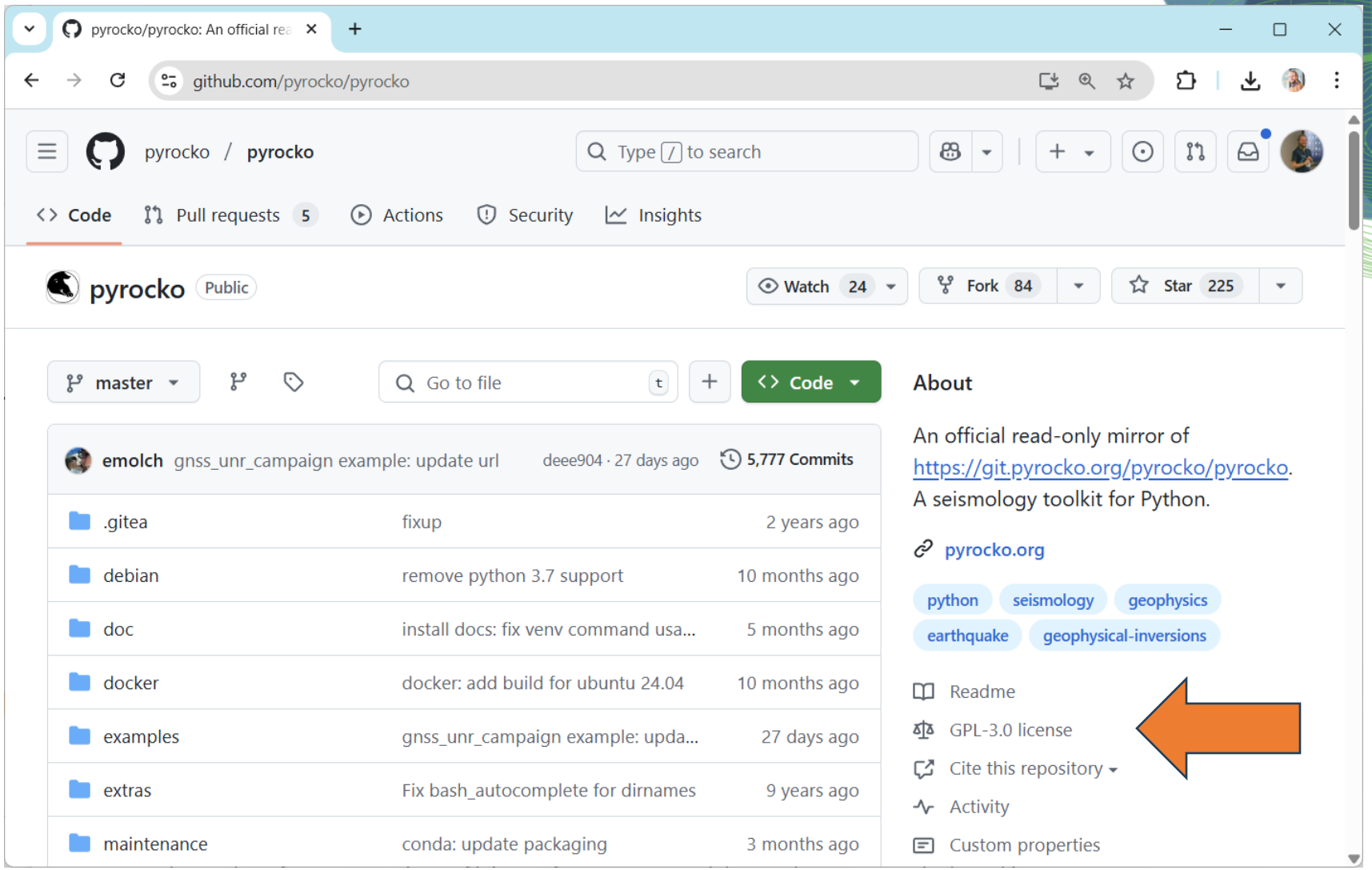

Quiz

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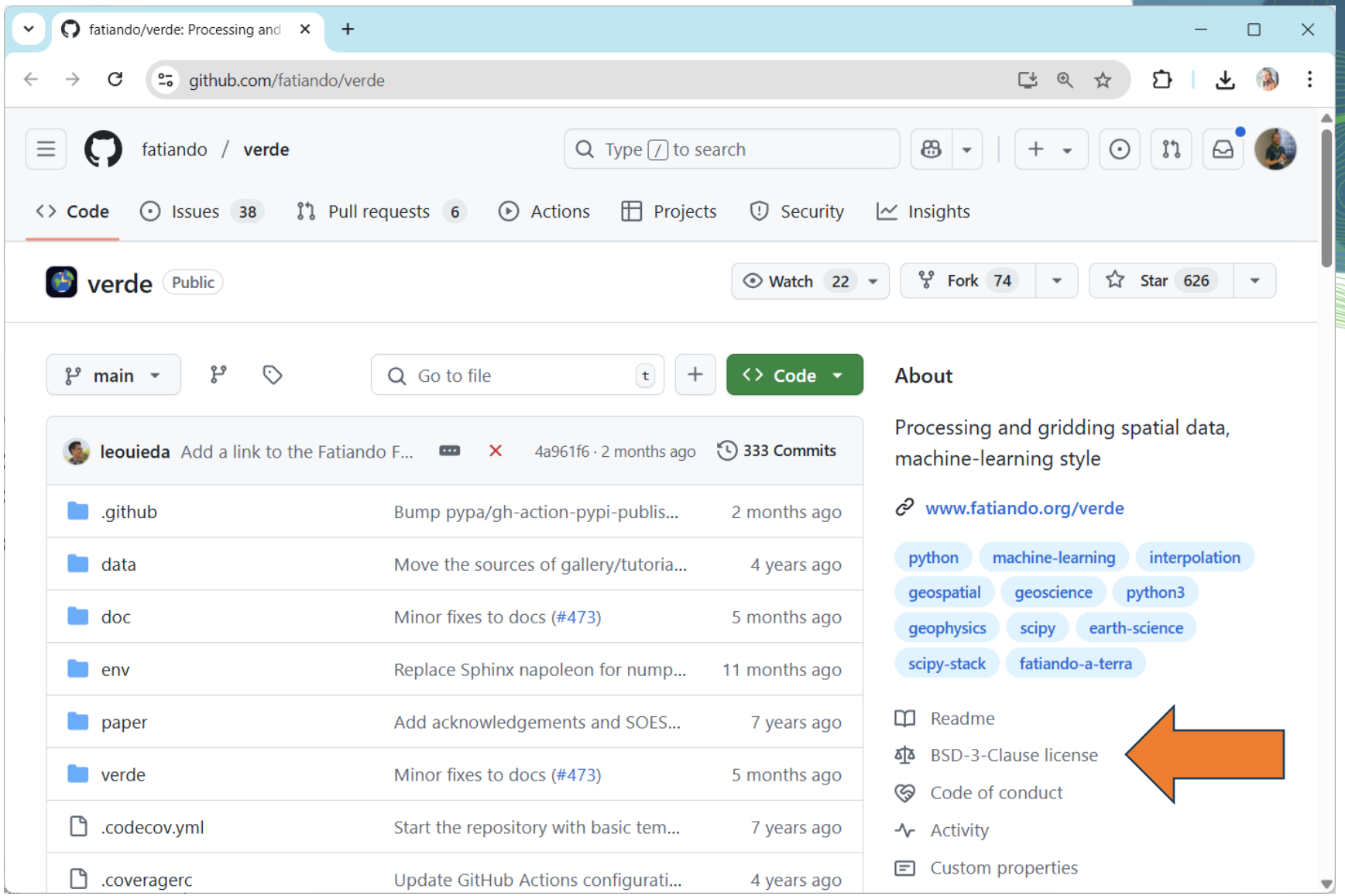

Take home message

If you share material (openly or not)

license it

and it'll be harder to steal it

Summary

- If you want to make your stuff reusable:
  - Use permissive licenses
  - Share it on community-wide platforms (preferably not institutional servers)
  - Register your data and software in search-indices
- Read more:
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