Data management and Reproducibility

DESY Summer student program

2025, September 1

Gernot Maier

HELMHOLTZ RESEARCH FOR GRAND CHALLENGES

DESY.

“Wissenschaftler”.

“knowledge creators…”

- **create**
- **distribute, share, publish**
- **reproduce**
- **attribute**
- **re-use**

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Knowledge does not exist until you make it accessible
(publish & make it reproducible)

Knowledge as Research Objects

- **Publications / Notes / Presentations**
- **Data (raw, derived, processed)**
- **Software**
- **Algorithms**
- **Simulations**
- **Videos**
- **….**

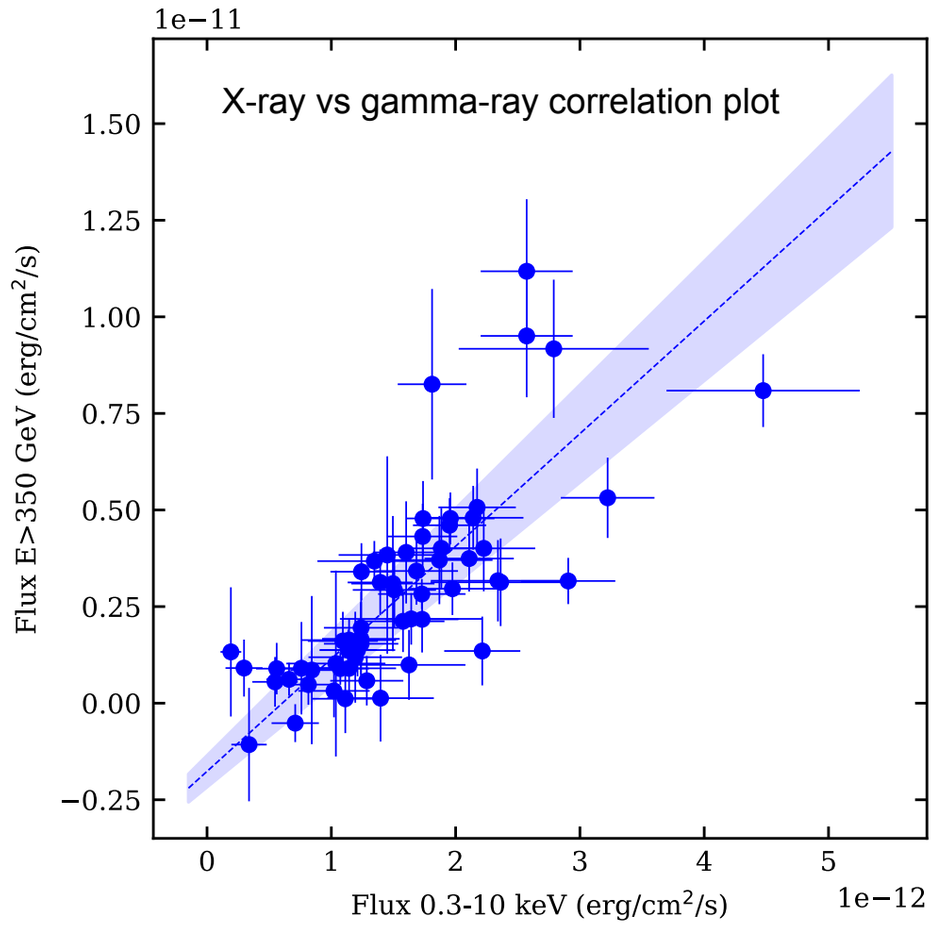
Publication consisting of paper + data + software + environment:
“dynamic and executable publications”

“Research Data Management”

Why is research data management important?

Example

Would we be able to reproduce
this figure in 5 years?
5 months? Ever struggled to redo
a plot?



Data as plotted (flux points), units, high-level analysis, fit results, event lists, instrument response functions, reconstruction code with all options, raw data files,

Re-run, Repeat, Reproduce, Reuse, Replicate

- Re-runnable (R^1): have you ever tried to re-run a program you wrote a few years ago?
- Repeatable (R^2): do you get the same result when running your code twice?
- Reproducible (R^3): can your collegue take your data and software and reproduce the result?
- Reusable (R^4): can your collegue make use of your data, algorithms, or software?
- Replicable (R^5): can your collegue take your data, writes his own software and come to the same conclusion? Are the algorithms applied documented?

see Benureau et al (2018)

Example (2)

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- “Could we have the data used for figure 11 in paper X?”
  “*Yes of course - wait, not sure if it is in final_data.dat, final_data_v1.dat, final_data_really_final.dat, final_more_final.dat, final_most_final.dat …*”
  “Yes - here is a link to the original data in my google drive. What, it doesn’t exist anymore?”
  “Yes, here are the files. It is saved as (....).”*

(*) a file format which you have never heard off, and for which only a reader for Windows 95 exist

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- “Let’s update the dark matter analysis published 5 years ago. Could we first look again at what data, software, algorithms were used?”
  “*Hmm, that was done by the PhD Student N, who graduated and left science. All data / software is on her laptop”*
  “No idea which software version was used? Does someone has the run list?”

Example (3)

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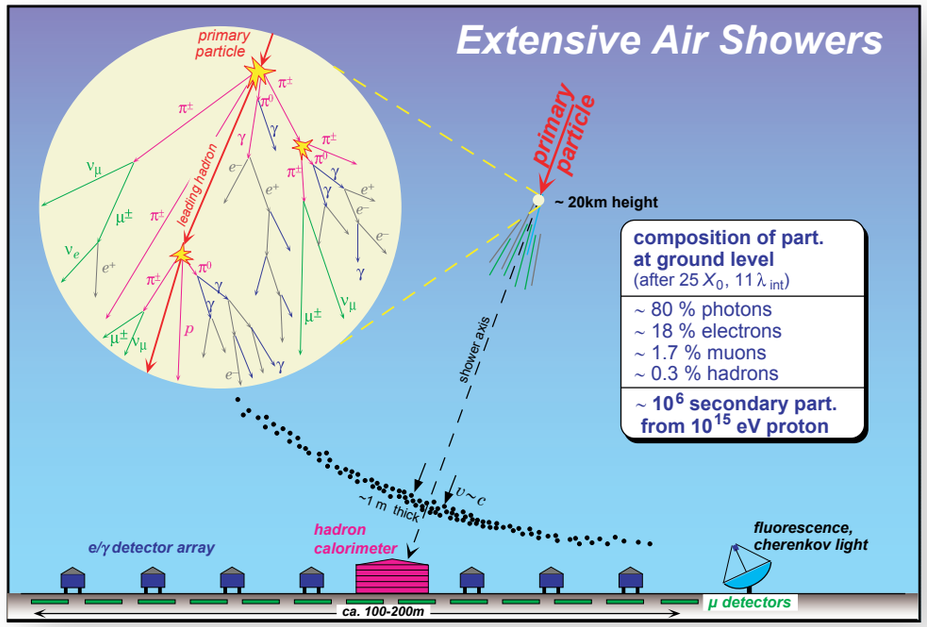
- “Very nice summary plot let’s use it in our publication”

  “Wait - who did it?
  I found them on the web, can we use it?”

  (note there is something like copyright)



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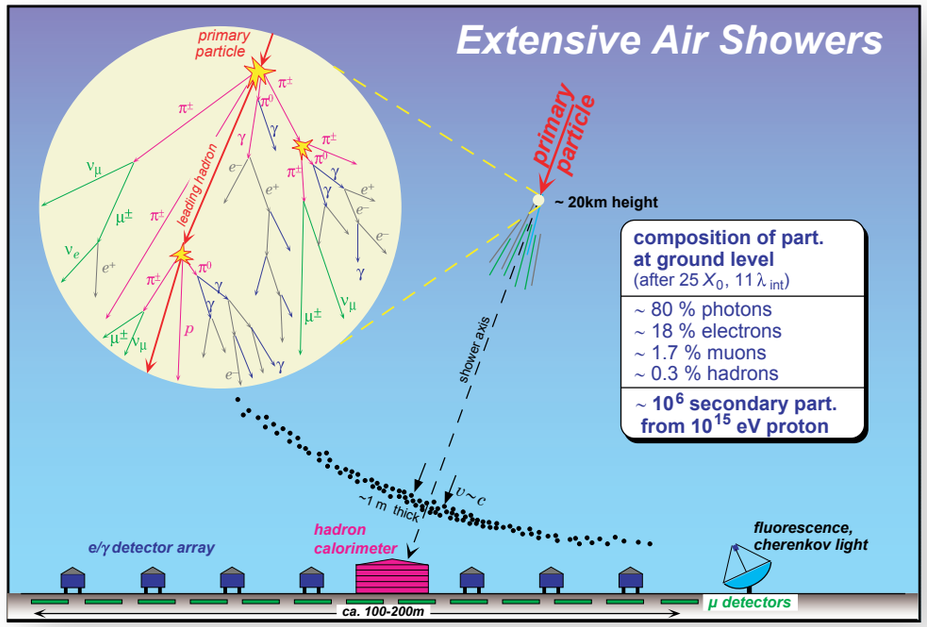
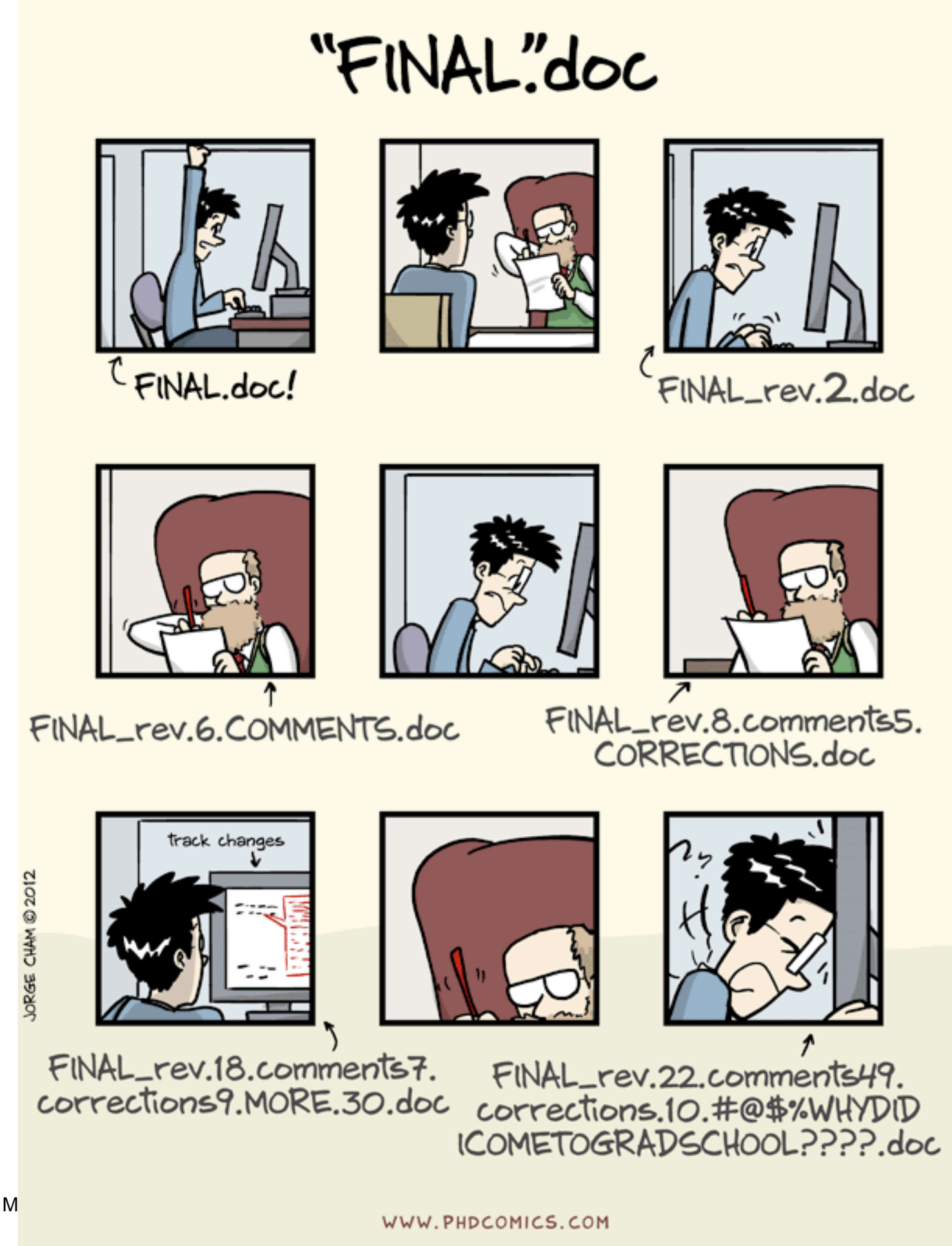


- “Let’s query all published spectra of object type X and search for feature Y”
  “Can’t find them, need to digitise them, …”

Obvious (maybe good?) advices.

- document now (today) what you do (not tomorrow)
- add README files everywhere
  “love letters to your future self”
- describe your data
  (how was it derived; when; units; …, Metadata)
- assume whatever you do, it will be wrong / full of mistakes
- assume that anything you do, you will have to do again (write scripts and document it)
- assume that of any document, program, data set there will be different versions
- assume that what you do is useful for others


"FINAL".doc
FINAL.doc!
FINAL_rev.2.doc
FINAL_rev.6.COMMENTS.doc
FINAL_rev.8.comments5.
CORRECTIONS.doc
track changes
FINAL_rev.18.comments7.
corrections9.MORE.30.doc
FINAL_rev.22.comments49.
corrections.10.#@$%WHYDID
ICOMETOGRADSCHOOL????.doc
JORGE CHAM © 2012
WWW.PHDCOMICS.COM

Version Control - git.

Update LAT-000023-2-lc.ecsv — Browse files

changed the unit for LAT flux from m-2 s-1 to cm-2 s-1

main (#213)
v0.8.0

qi-feng committed 11 days ago Verified — 1 parent 97f00ec commit bc71321a12d1b0b35df3dec1252f132be15b60d3

Showing **1 changed file** with **2 additions** and **2 deletions**. Split | Unified

4 2022/2022ApJ...932..129A/LAT-000023-2-lc.ecsv

```
@@ -3,8 +3,8 @@
  # datatype:
  # - {name: e_min, unit: MeV, datatype: float64}
  # - {name: time, unit: MJD, datatype: float64}
- # - {name: flux, unit: 1e-7 m-2 s-1, datatype: float64}
- # - {name: flux_err, unit: 1.e-7 m-2 s-1, datatype: float64}
+ # - {name: flux, unit: 1e-7 cm-2 s-1, datatype: float64}
+ # - {name: flux_err, unit: 1.e-7 cm-2 s-1, datatype: float64}
  # meta: !!omap
  # - data_type: lc
  # - source_id: 23
```

0 comments on commit bc71321 — Lock conversation

You need to be familiar with git.

Good research practice

Code of Conduct

Guidelines for Safeguarding Good Research Practice

Code of Conduct

DFG

Guideline 12: Documentation

- Researchers document all information relevant to the production of a research result as clearly as is required by and is appropriate for the relevant subject area to allow the result to be reviewed and assessed. In general, this also includes documenting individual results that do not support the research hypothesis. The selection of results must be avoided. Where subject-specific recommendations exist for review and assessment, researchers create documentation in accordance with these guidelines. If the documentation does not satisfy these requirements, the constraints and the reasons for them are clearly explained. Documentation and research results must not be manipulated; they are protected as effectively as possible against manipulation.

Explanations:

An important basis for enabling replication is to make available the information necessary to understand the research (including the research data used or generated, the methodological, evaluation and analytical steps taken, and, if relevant, the development of the hypothesis), to ensure that citations are clear, and, as far as possible, to enable third parties to access this information. Where research software is being developed, the source code is documented.

There is something similar in your country.
Look for it and read it!

Scientific Misconduct

“Research misconduct is defined as fabrication, falsification, or plagiarism in proposing, performing, or reviewing research, or in reporting research results. (...)
Research misconduct does not include honest error or honest differences of opinion.”

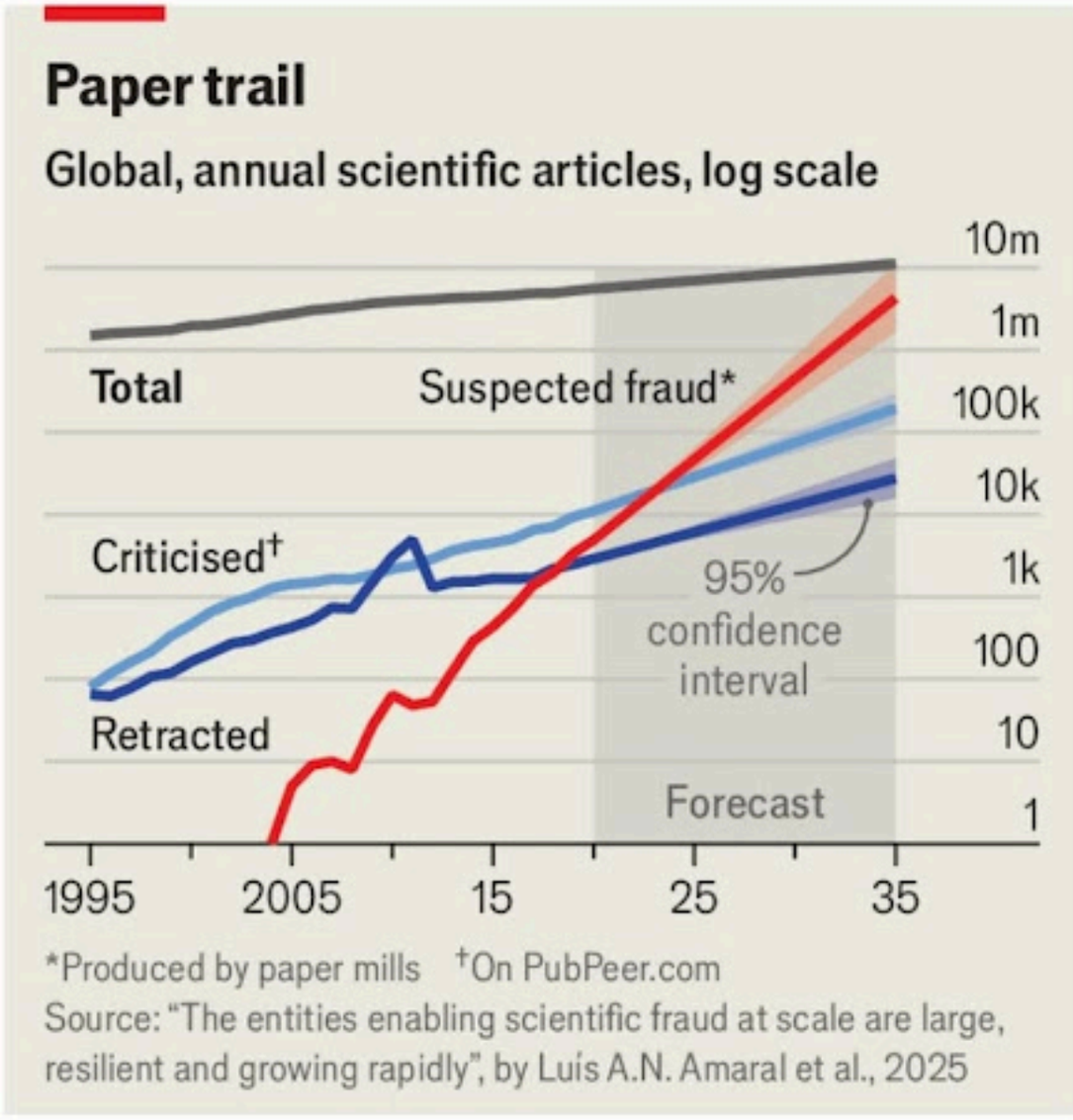
OECD Global Science Forum

Science & technology | Inside job

Fraudulent scientific papers are booming

A subset of journal editors may be partly responsible

IMAGE: BEN DENZER



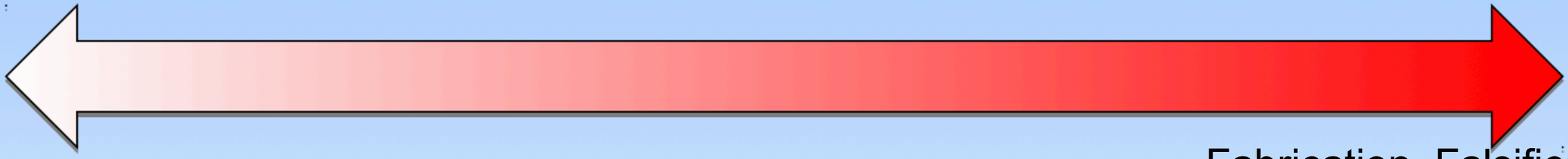
Aug 6th 2025 (updated Aug 7th 2025) · 5 min read

Listen 7:02

SCIENTIFIC JOURNALS exist to do one thing: provide accurate, peer-reviewed reports of new research to an interested audience. But

Degrees of Scientific Misconduct

Sloppy work	Questionable practice	Severe misconduct
Carelessness	Bad statistics	FFP
Mislabelling	Salami slicing	Sabotage
Bad lab book	Intransparency	Destroying data
	Using expired chemicals	Data theft
	Hiding “negative” results	Ethics violation
		Fake authors
		Bad lab book



Fabrication, Falsification and Plagiarism

Dr. Julia Verse Team Scientific Integrity www.scientificintegrity.de

Scientific Misconduct

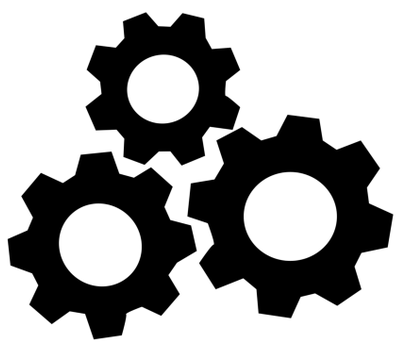
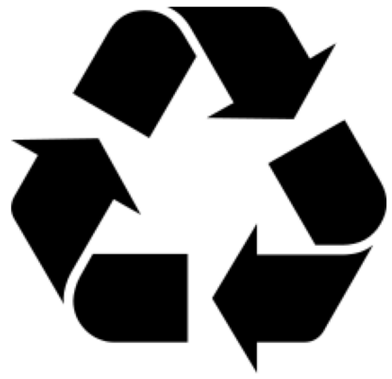
"The published reports on scientific misconduct are full of accounts of vanished original data and of the circumstances under which they had reputedly been lost. This, if nothing else, shows the importance of the following statement:

The disappearance of primary data from a laboratory is an infraction of basic principles of careful scientific practice and justifies a prima facie assumption of dishonesty or gross negligence."

DFG Recommendations 2013, p. 75f

Findable Accessible Interoperable Reusable



A set of principles in data management that ensures that data is made available in a way that enables and stimulated reuse by humans and machines

Comes from life science - but today adopted for all data

Mark D. Wilkinson *et al.*[#] https://www.nature.com/articles/sdata201618

Sharing.

SPRINGER NATURE

Findable Accessible Interoperable Reusable

Box 2 | The FAIR Guiding Principles

To be 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 it describes
F4. (meta)data are registered or indexed in a searchable resource

To be Accessible:
A1. (meta)data are retrievable by their identifier using a standardized communications protocol
A1.1 the protocol is open, free, and universally implementable
A1.2 the protocol allows for an authentication and authorization procedure, where necessary
A2. metadata are accessible, even when the data are no longer available

To be 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

To be 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

assigned a persistent identifier and described by detailed metadata

Clear access conditions; machine access

Standardised formats and vocabulary

Well-defined licence; clear provenance

Wilkinson et al 2015

Persistent Identifiers

an organisation made a promise to keep it alive

globally unique string of characters

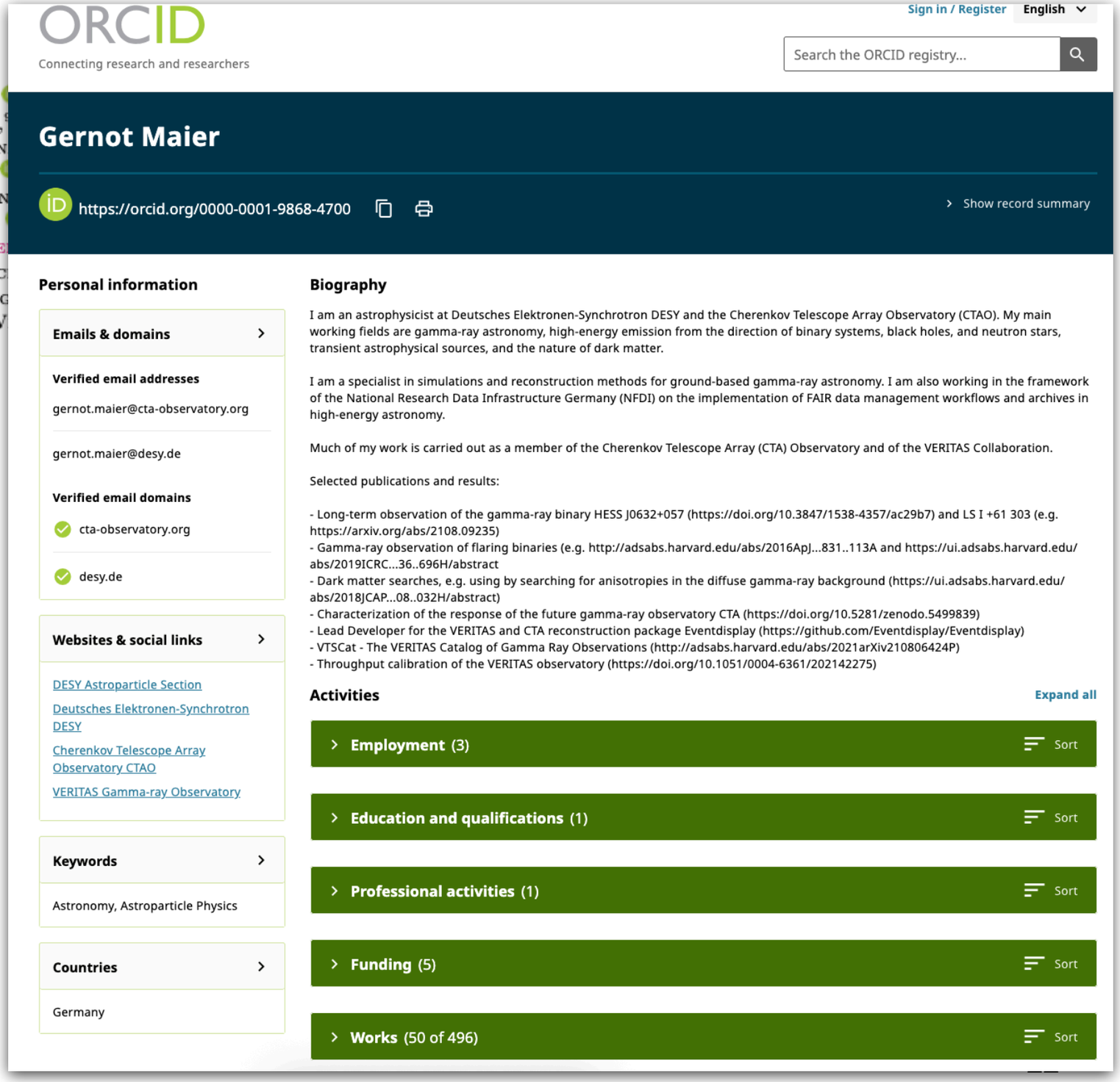
- **DOI - digital object identifier**
- **ORCID - identify a person**
- **ROR - research organisation registry**
- **(similar: ISBNs from books)**

Do you have an ORCID?

- **O**pen **R**esearcher and **C**ontributor **ID**

C. B. Adams,[1] W. Benbow,[2] A. Brill,[1] J. H. Buckley,[3] M. Capasso
A. Falcone,[6] K. A Farrell,[7] Q. Feng,[4] J. P. Finley,[8] G. M Foote,
A. Gent,[12] G. H. Gillanders,[13] C. Giuri,[14] O. Gueta,[14] D. Hann
J. Holder,[9] B. Hona,[17] T. B. Humensky,[1] W. Jin,[18] P. Kaaret
T. K Kleiner,[14] F. Krennrich,[5] S. Kumar,[15] M. J. Lang,[13] M. Lun
P. Moriarty,[13] R. Mukherjee,[4] D. Nieto,[21] M. Nievas-Rosillo
A. N. Otte,[12] N. Park,[23] S. Patel,[19] K. Pfrang,[14] A. Piche
J. Quinn,[7] K. Ragan,[15] P. T. Reynolds,[26] D. Ribeiro,[1] E. Roac
M. Santander,[18] S. Schlenstedt,[27] G. H. Sembroski,[8] R. Shang
A. Weinstein,[5] D. A. Williams,[16] T. J W
(The VERITAS Collaboration)

orcid.org

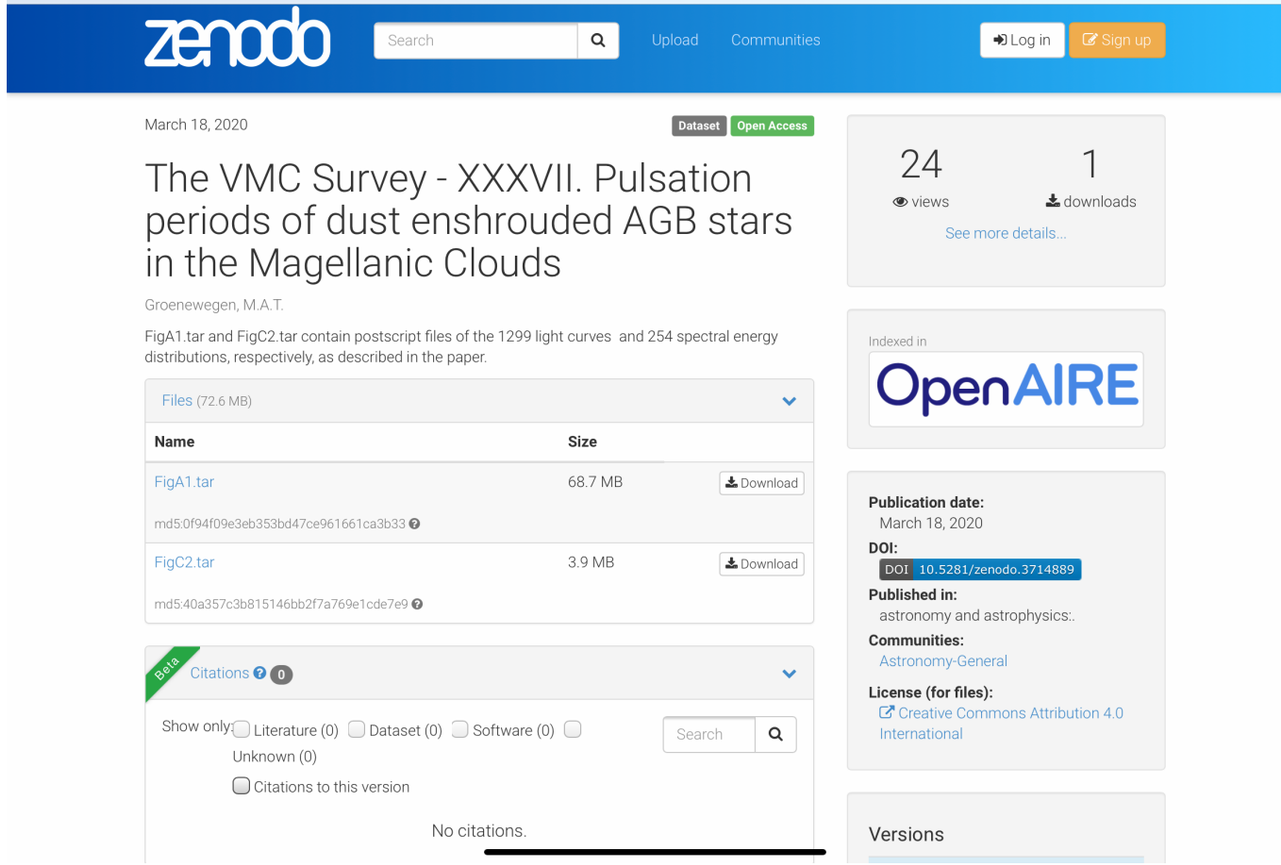


Findable data

Findable **A**ccessible **I**nteroperable **R**eusable

- Deposit your data in a repository with metadata and a persistent identifier
  - e.g., online archives like zenodo+github
- Machine readable metadata that describes the datasets
  - Contextual information, title, author, keywords, when, what purpose, size, standards, ...
- **D**igital**O**bject**I**dentifiers

Data is **not findable on your laptop**

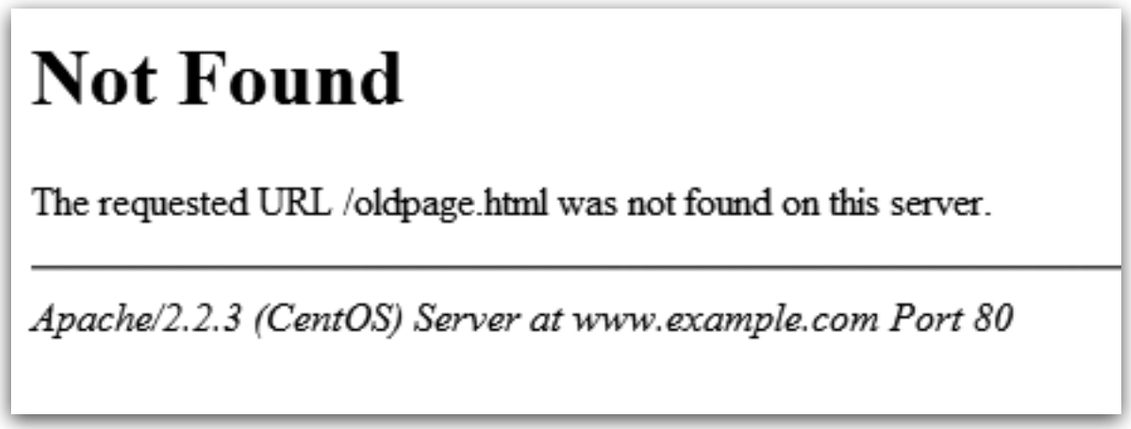


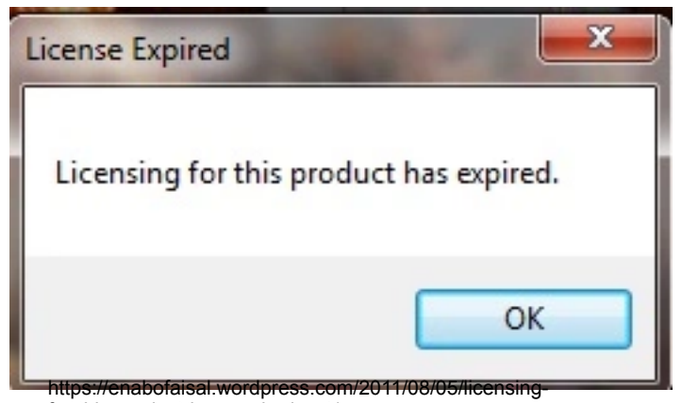
Accessible data

Findable **Accessible** Interoperable Reusable

- Can be open (but not necessarily)
- If not open: clear authentication and authorization
- Human and machine accessibility
  - (Your laptop is not machine accessible; neither tapes on a shelf; or some printouts)

- Open and free protocol



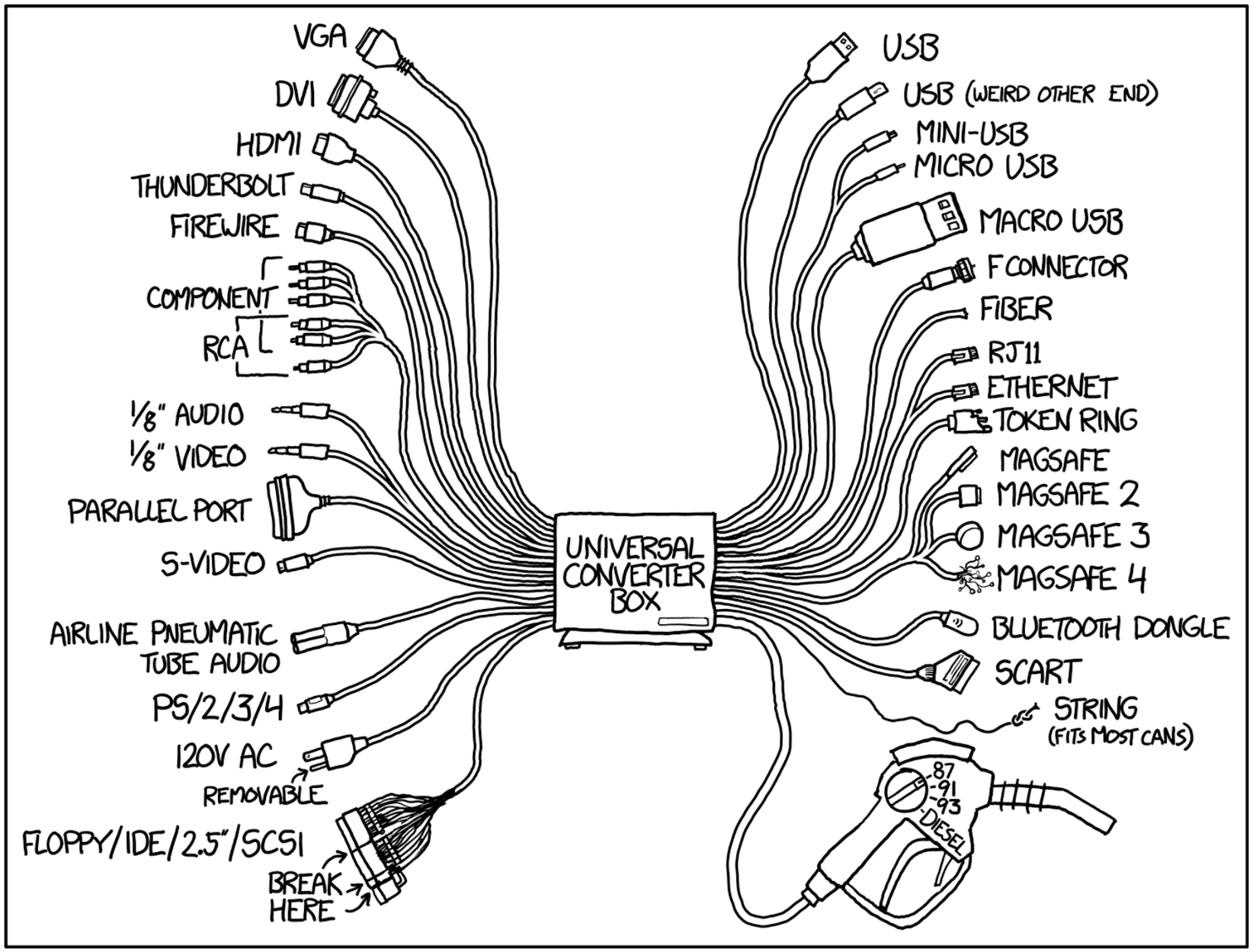


https://enabofaisal.wordpress.com/2011/08/05/licensing-for-this-product-has-expired-cs4/

Interoperable data

Findable Accessible **Interoperable** Reusable

Use a standard that can be mapped to others



https://xkcd.com/1406/

Interoperable data

Findable Accessible **Interoperable** Reusable

- Datasets are Interoperable if they are
  - machine readable (metadata)
  - specific formats (open/common)
  - specific language and vocabularies

Example: FITS data format + FITS headers

- Formats should be:
  - Community agreed, open, suitable for long-term preservation

- Metadata should use community agreed standards and vocabularies
  - e.g., if the whole field talks about telescopes, don’t use the expression ‘antenna’

Reusable data

Findable Accessible Interoperable **Reusable**

- Does your data include relevant provenance data?
  - Data is only reusable if it is known how it was obtained (e.g., software versions, IRF versions, etc)
  - Documentation, documentation, documentation
- Licensing - clearly stated re-use rights
  - (this is a tough topic for scientists)

- (You might want to get familiar with containers (e.g. run by Podman or docker))

AI tools

- use them - especially for routine task
  - text, code, …
- learn how to write good prompts
- challenge for reproducibility
  (no clear path on how this is solved)
- supports the importance of sharing data, software, knowledge (as public sources are used for training)

Conclusions - simple rules

(after Goodman A, Pepe A, Blocker AW, Borgman CL, Cranmer K, et al. (2014) Ten Simple Rules for the Care and Feeding of Scientific Data. PLoS Comput Biol 10(4): e1003542. doi:10.1371/journal.pcbi.1003542)

- **love your data, help others to love it**
- **share your data with a permanent identifier**
- **conduct science with reuse in mind**
- **publish workflows, methods, context**
- **link your data to your publications**
- **publish your code**
- **give credit and state how you want to get credit**
- **use data repositories**

Websites

- www.orcid.org
- zenodo.org
- github.com gitlab.desy.de …
  - https://docs.github.com/en/repositories/archiving-a-github-repository/referencing-and-citing-content