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PHYSICAL SCIENCES
DATA INFRASTRUCTURE

Promoting Open & Transparent Research Practices in the Physical Sciences through PSDI

Keele University Open Research Network
10th April 2024

Dr Samantha Pearman-Kanza & Dr Nicola Knight
University of Southampton

https://www.psdi.ac.uk/

Presentation Outline

- About Us & PSDI
- A Grand Vision of Process Recording
- Current Barriers & Challenges to Open & Transparent Digital Research
- Producing FAIR Data & Research
- PSDI Initiatives to help with this

THE MOST COMMON OPENING LINES OF A PRESENTATION
THANKS FOR COMING TO MY TALK...
OH IT'S NOT SHOWING, HANG ON A SECOND
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About Us

Dr Samantha Pearman-Kanza

- Senior Enterprise Fellow at University of Southampton
- Pathfinder Lead & Researcher for PSDI
- Research Interests: Semantic Web Technologies, RDM, Metadata, Process Recording, Interoperability
- Twitter: @samikanza

Dr Nicola Knight

- Senior Enterprise Fellow at University of Southampton
- Project Coordinator for PSDI
- Research Interests: Chemical data management, connected lab technologies, RDM
- Twitter: @njkknight

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About PSDI

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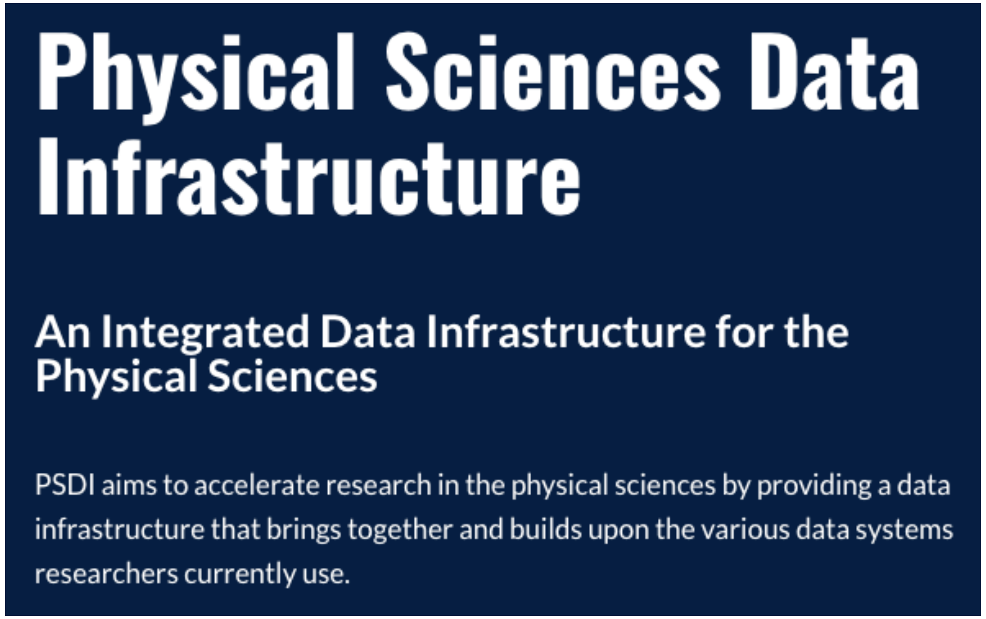


Physical Sciences Data Infrastructure

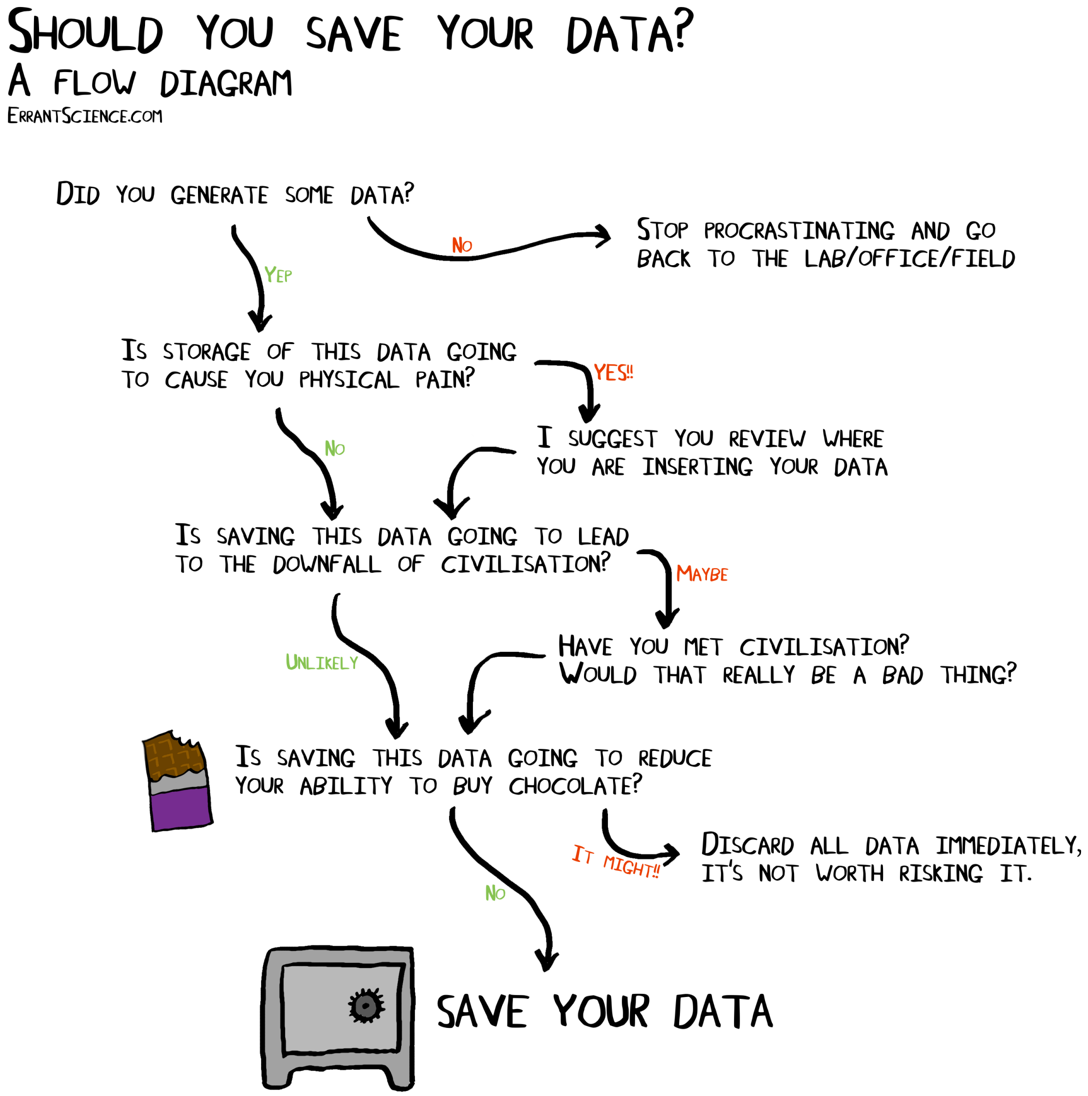
An Integrated Data Infrastructure for the Physical Sciences

PSDI aims to accelerate research in the physical sciences by providing a data infrastructure that brings together and builds upon the various data systems researchers currently use.

Through PSDI researchers will be able to:

- Find and Access to reference quality data from commercial and open sources
- Combine data from different sources
- Share data, software and models including experimental and simulation data
- Use AI to explore data
- Learn how to make the results of their research open and FAIR

A grand vision


SHOULD YOU SAVE YOUR DATA?
A FLOW DIAGRAM
ERRANTSCIENCE.COM
DID YOU GENERATE SOME DATA?
NO
STOP PROCRASTINATING AND GO BACK TO THE LAB/OFFICE/FIELD
YEP
IS STORAGE OF THIS DATA GOING TO CAUSE YOU PHYSICAL PAIN?
YES!!
I SUGGEST YOU REVIEW WHERE YOU ARE INSERTING YOUR DATA
NO
IS SAVING THIS DATA GOING TO LEAD TO THE DOWNFALL OF CIVILISATION?
MAYBE
HAVE YOU MET CIVILISATION? WOULD THAT REALLY BE A BAD THING?
UNLIKELY
IS SAVING THIS DATA GOING TO REDUCE YOUR ABILITY TO BUY CHOCOLATE?
IT MIGHT!!
DISCARD ALL DATA IMMEDIATELY, IT'S NOT WORTH RISKING IT.
NO
SAVE YOUR DATA

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A wonderful world of researchers capturing and sharing all their data, code, and methods in a re-useable way

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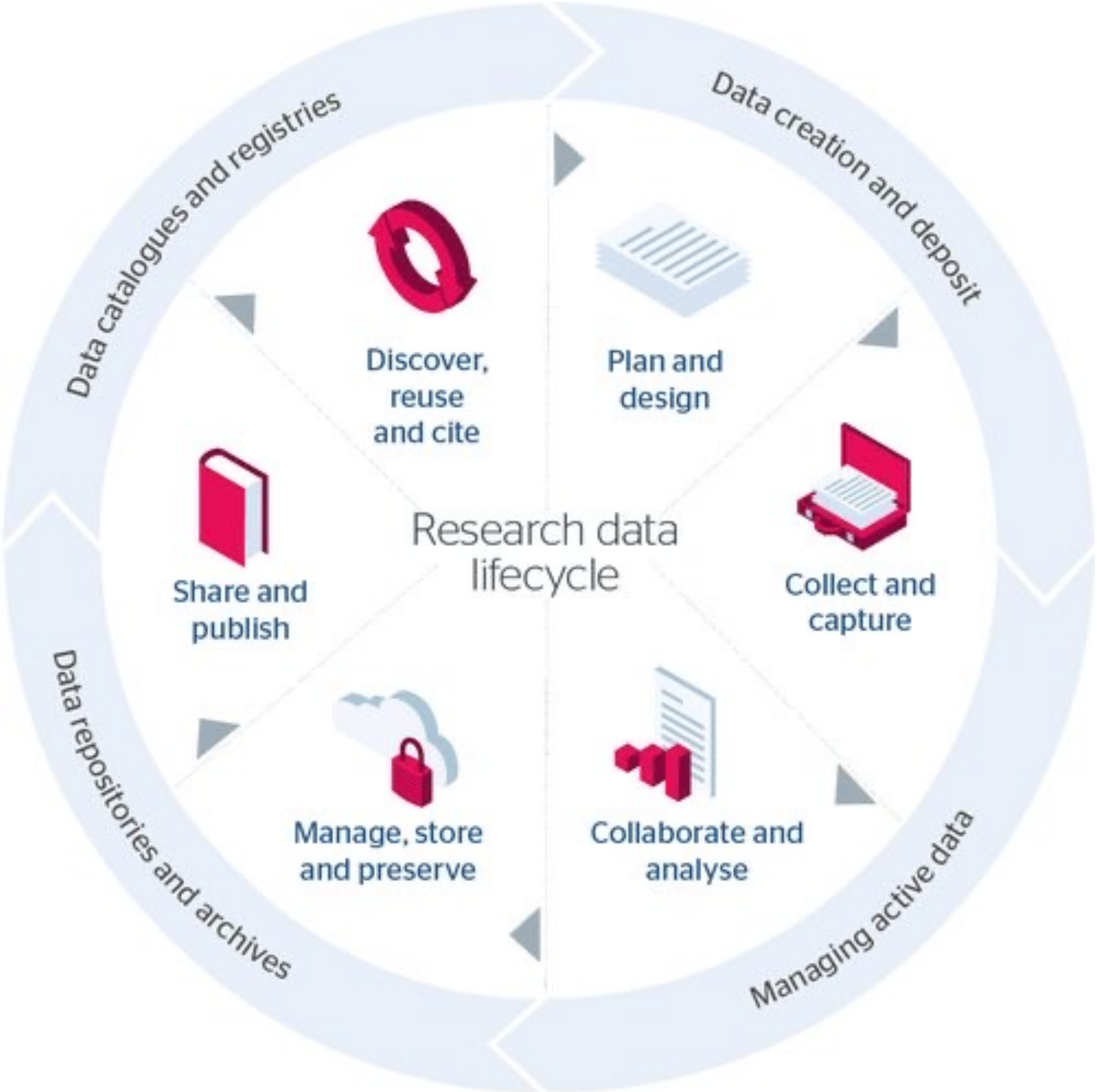
Research Data Lifecycle



JISC Research data lifecycle model - (CC BY-NC-ND) https://www.jisc.ac.uk/guides/research-data-management-toolkit

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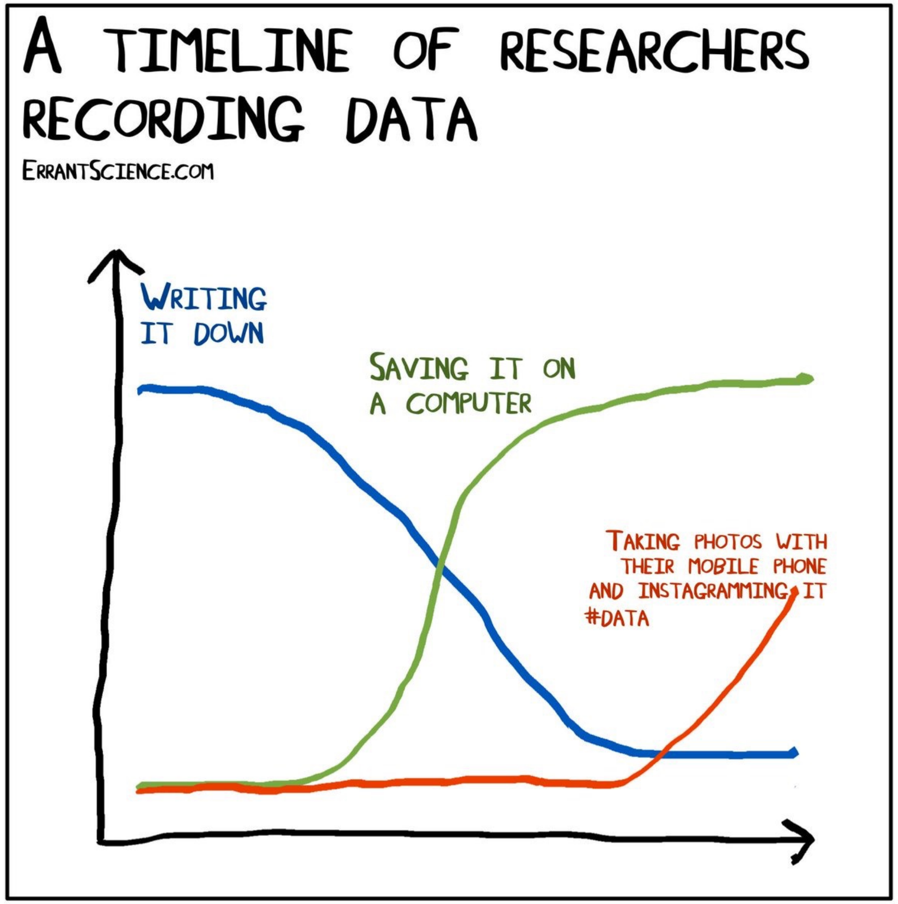
Process Recording


A TIMELINE OF RESEARCHERS RECORDING DATA
ERRANTSCIENCE.COM
WRITING IT DOWN
SAVING IT ON A COMPUTER
TAKING PHOTOS WITH THEIR MOBILE PHONE AND INSTAGRAMMING IT #DATA

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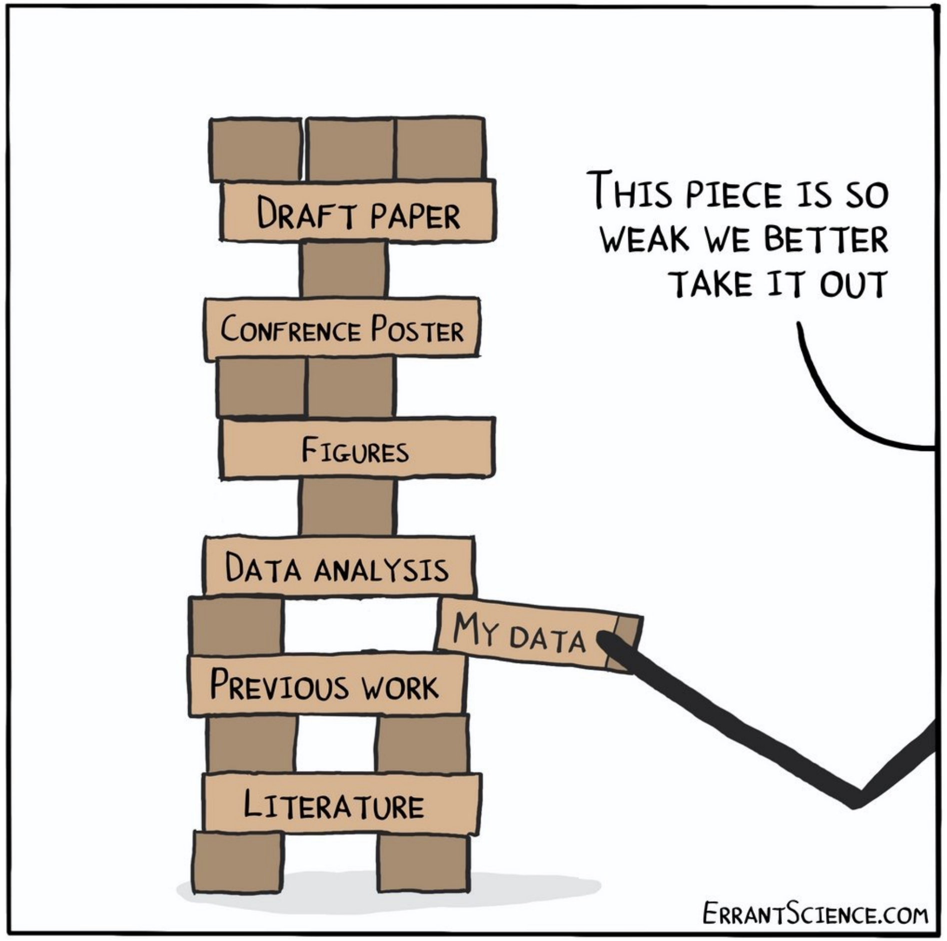
- It is vital that we capture our data and processes throughout our research so that:
  - Our future selves can find it and understand it
  - We can share it alongside our publications and others can ACTUALLY USE IT

So why haven’t we achieved this already?

Current Barriers & Challenges to Open and Transparent Digital Research



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- Data
- Standards
- Software
- Hardware
- Cost
- Time
- Trust
- People / Adoption

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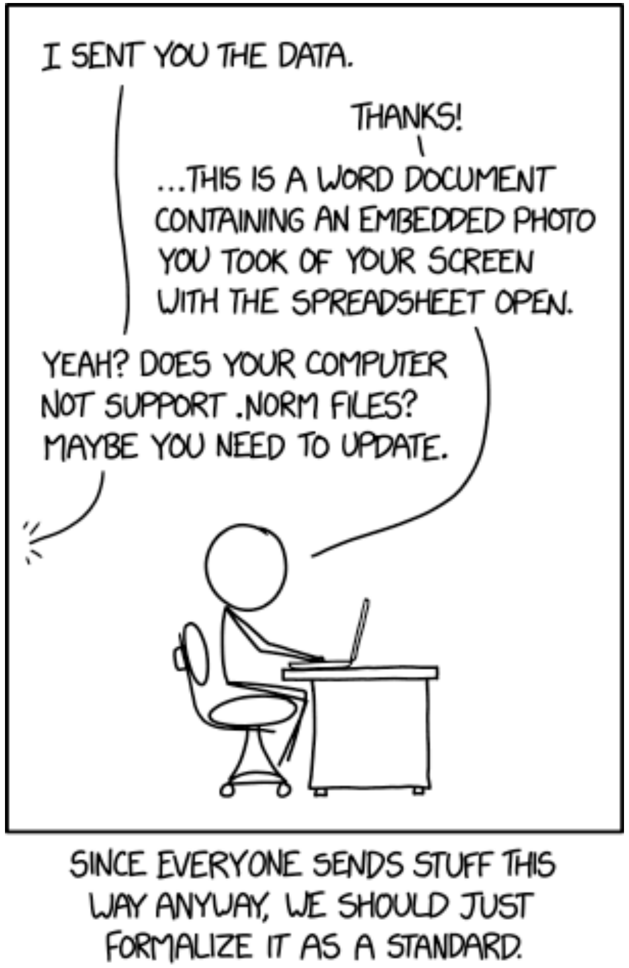
People/Adoption Barriers

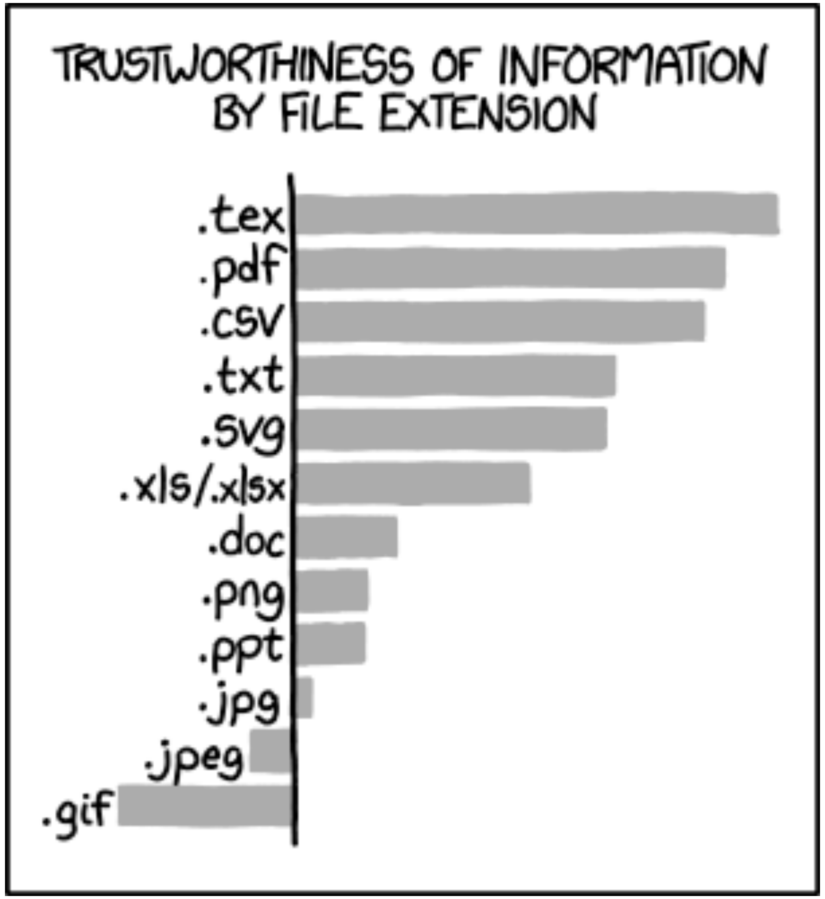
- People are arguably one of the biggest barriers
- Top-down influence can make or break this
- Concerns about changing processes
- Hard to persuade people to embark on a journey with a lot of front-loaded work, unless they really understand the benefits


I SENT YOU THE DATA.
THANKS!
...THIS IS A WORD DOCUMENT CONTAINING AN EMBEDDED PHOTO YOU TOOK OF YOUR SCREEN WITH THE SPREADSHEET OPEN.
YEAH? DOES YOUR COMPUTER NOT SUPPORT .NORM FILES? MAYBE YOU NEED TO UPDATE.
SINCE EVERYONE SENDS STUFF THIS WAY ANYWAY, WE SHOULD JUST FORMALIZE IT AS A STANDARD.

"NORM Normal File Format" by XKCD is licensed under CC BY-NC 2.5

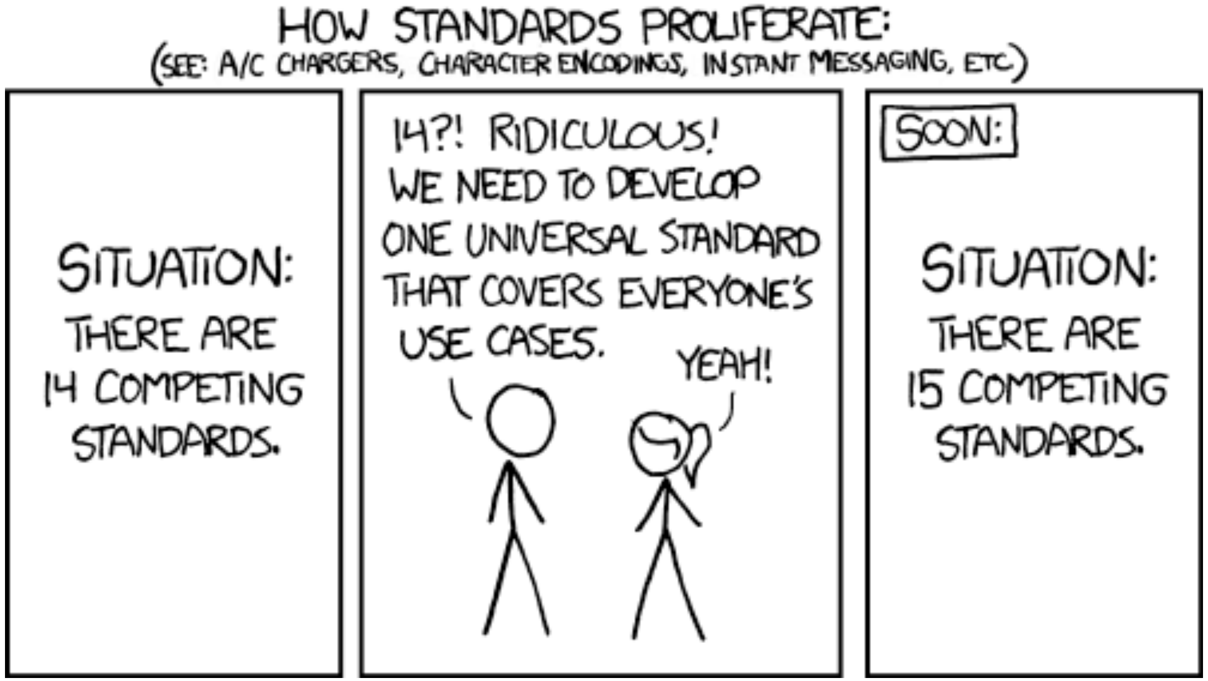
Data Barriers

- Un-FAIR Data
  - Much data doesn't adhere to FAIR standards. Data isn't findable, accessible, interoperable or re-useable
- Metadata/Provenance
  - Data often lacks context
  - Time consuming to capture metadata
  - Leads to not being able to trace the provenance of research
- Data Size
  - Scientists frequently work with large datasets that are harder to store and share



"File Extensions" by XKCD is licensed under CC BY-NC 2.5

Standards Barriers



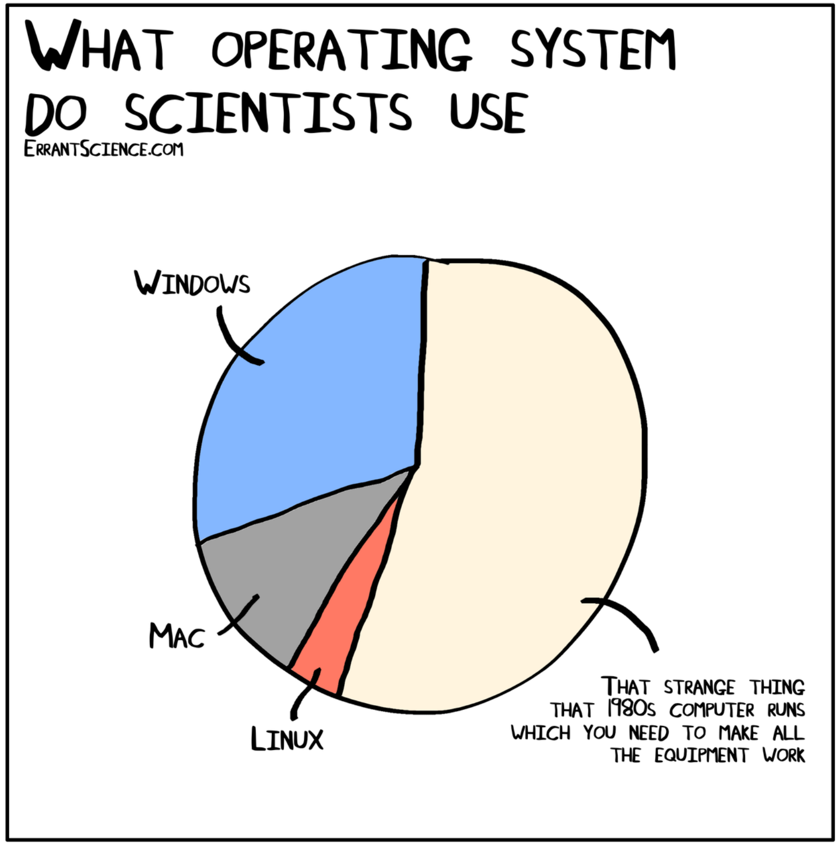
HOW STANDARDS PROLIFERATE:
(SEE: A/C CHARGERS, CHARACTER ENCODINGS, INSTANT MESSAGING, ETC)
SITUATION: THERE ARE 14 COMPETING STANDARDS.
14?! RIDICULOUS! WE NEED TO DEVELOP ONE UNIVERSAL STANDARD THAT COVERS EVERYONE'S USE CASES.
YEAH!
SOON:
SITUATION: THERE ARE 15 COMPETING STANDARDS.

"Standards" by XKCD is licensed under CC BY-NC 2.5

- Too many Standards
  - We are drowning in standards, and yet still lack them in many areas
- Proprietary Formats
  - Lots of software uses proprietary formats that won't work with other software to lock vendors in
- Lack of Interoperability
  - There are many formats that won't work across multiple pieces of software

Software Barriers

- Software Overload
  - There are so many different pieces of software for capturing data and research digitally, how on earth can we choose?
- Software Compatibility
  - Software often doesn't play well together, which makes having an overarching digital ecosystem challenging
- Software Quality
  - Software often isn't at a high enough quality for users to want to engage with it
- Online Software
  - Online Software is great, until the internet stops working


WHAT OPERATING SYSTEM DO SCIENTISTS USE
ERRANTSCIENCE.COM
WINDOWS
MAC
LINUX
THAT STRANGE THING THAT 1980s COMPUTER RUNS WHICH YOU NEED TO MAKE ALL THE EQUIPMENT WORK

"Scientists Computer Use" by ErrantScience.com is licensed under CC-BY-NC

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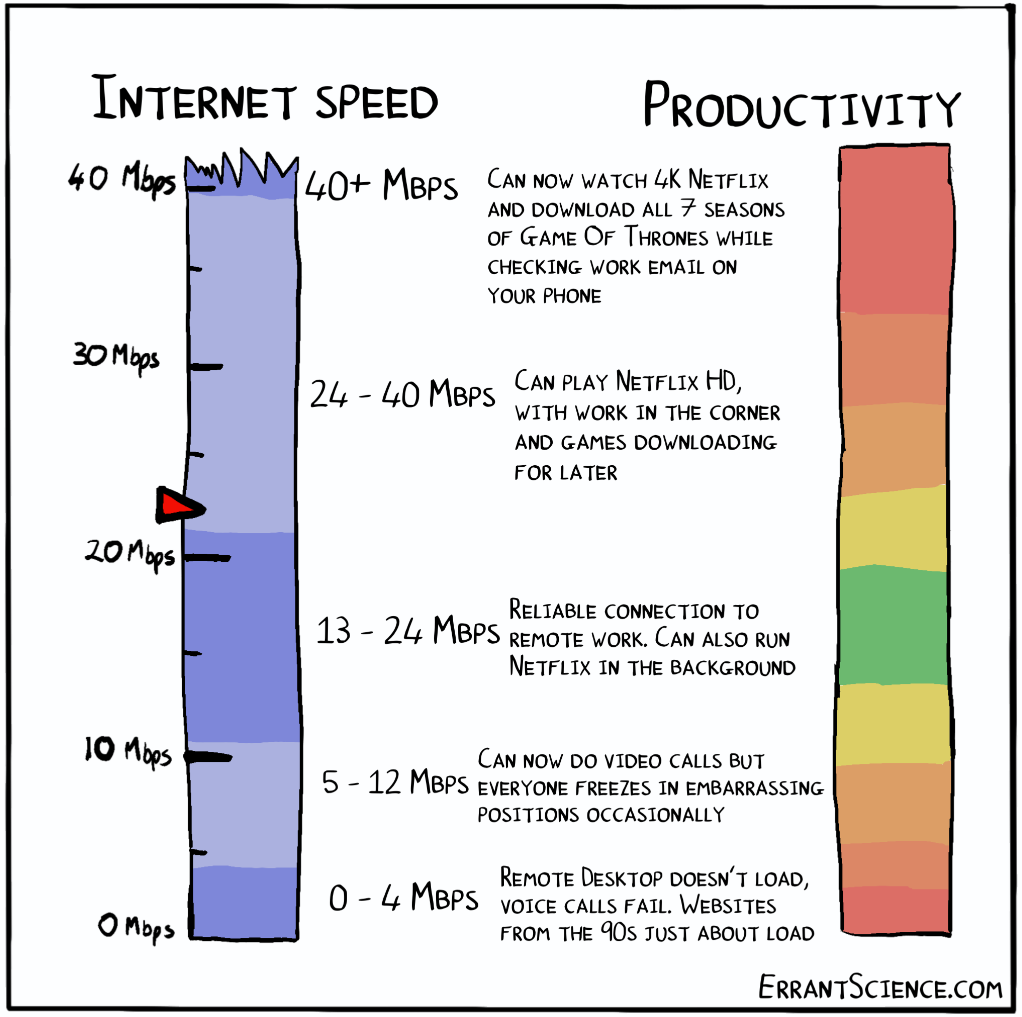
Hardware Barriers


INTERNET SPEED
PRODUCTIVITY
40 Mbps
30 Mbps
20 Mbps
10 Mbps
0 Mbps
40+ MBPS
CAN NOW WATCH 4K NETFLIX AND DOWNLOAD ALL 7 SEASONS OF GAME OF THRONES WHILE CHECKING WORK EMAIL ON YOUR PHONE
24 - 40 MBPS
CAN PLAY NETFLIX HD, WITH WORK IN THE CORNER AND GAMES DOWNLOADING FOR LATER
13 - 24 MBPS
RELIABLE CONNECTION TO REMOTE WORK. CAN ALSO RUN NETFLIX IN THE BACKGROUND
5 - 12 MBPS
CAN NOW DO VIDEO CALLS BUT EVERYONE FREEZES IN EMBARRASSING POSITIONS OCCASIONALLY
0 - 4 MBPS
REMOTE DESKTOP DOESN'T LOAD, VOICE CALLS FAIL. WEBSITES FROM THE 90S JUST ABOUT LOAD
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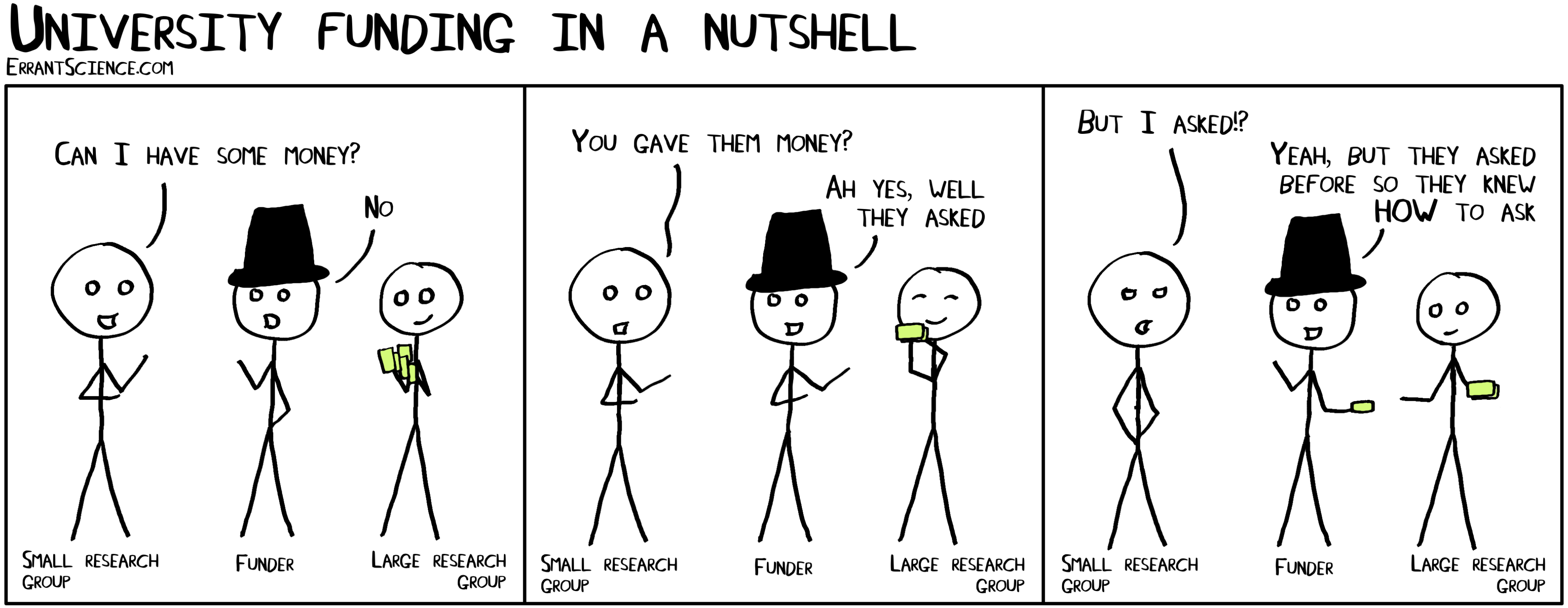
- Data Storage Capabilities
  - Many scientists say they do not have sufficient data storage capabilities
- Clunky Hardware
  - Often researchers struggle to gain access to hardware that will run their digital tools well – which then leads to them not wanting to use them at all
- Legacy Equipment
  - Many laboratories use legacy equipment which requires legacy software and outdated data formats
- Hardware Cross Contamination
  - Where digital tools are required in the lab, we need dedicated hardware to run these tools otherwise there are contamination risks moving computers/laptops in and out of the lab

Cost Barriers

- Cost
  - Funding, Research, Software, Hardware, Publishing



"University Funding in a Nutshell" by ErrantScience.com is licensed under CC-BY-NC

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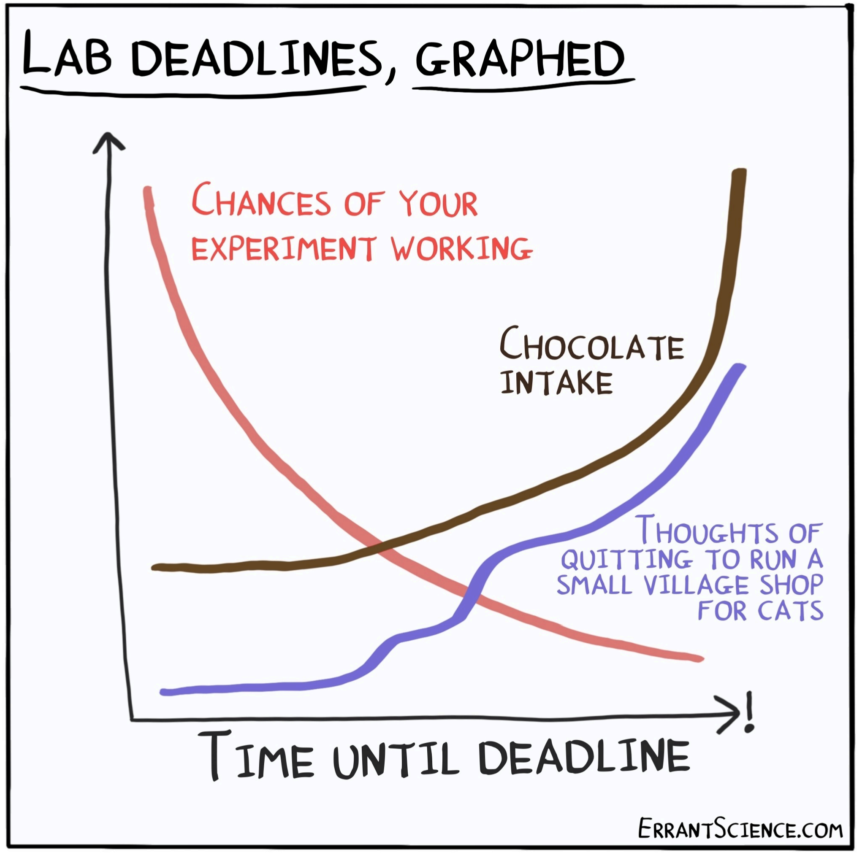
Time Barriers

- Lack of time for projects
- Time taken to learn and use new systems
- Time to do research data management PROPERLY
- Current systems in place make digitizing data and capturing research in a transparent way very time consuming


LAB DEADLINES, GRAPHED
CHANCES OF YOUR EXPERIMENT WORKING
CHOCOLATE INTAKE
THOUGHTS OF QUITTING TO RUN A SMALL VILLAGE SHOP FOR CATS
TIME UNTIL DEADLINE
!
ERRANTSCIENCE.COM

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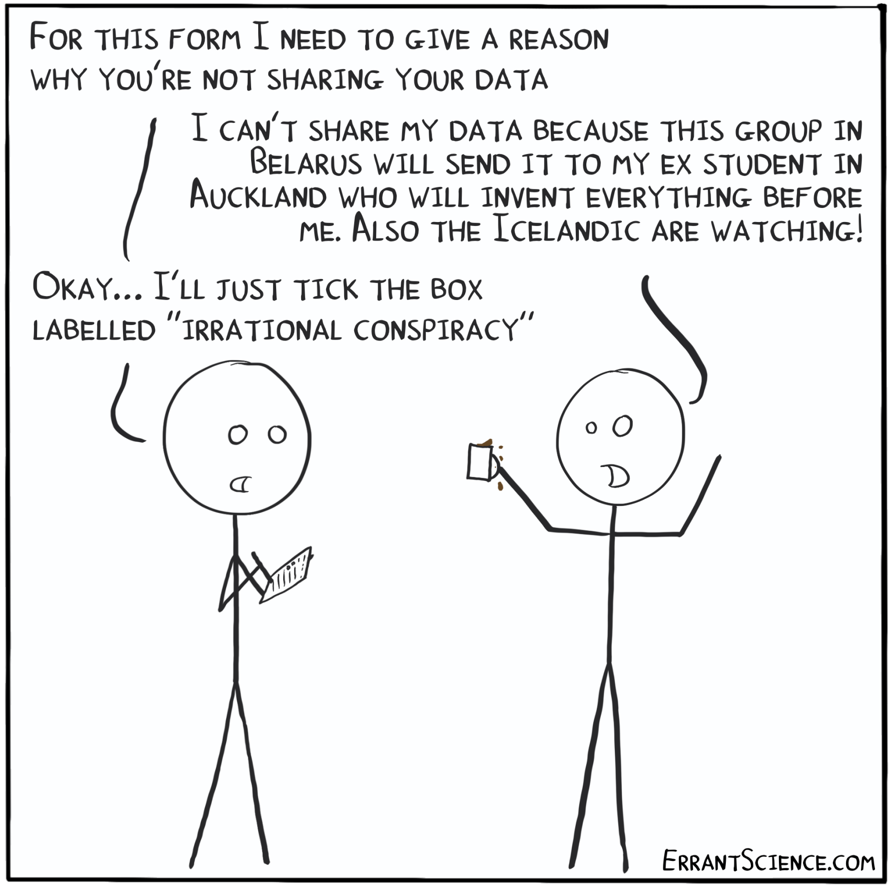
Trust Barriers


FOR THIS FORM I NEED TO GIVE A REASON WHY YOU'RE NOT SHARING YOUR DATA
I CAN'T SHARE MY DATA BECAUSE THIS GROUP IN BELARUS WILL SEND IT TO MY EX STUDENT IN AUCKLAND WHO WILL INVENT EVERYTHING BEFORE ME. ALSO THE ICELANDIC ARE WATCHING!
OKAY... I'LL JUST TICK THE BOX LABELLED "IRRATIONAL CONSPIRACY"
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- Many researchers do not trust storing the data/research online
- There are many concerns to consider:
  - Data privacy (Sharing/Hacking)
  - Software using proprietary formats
  - Lack of cohesive data exit strategy

So how do we overcome these barriers?

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Lets talk about FAIR

From ‘The FAIR Guiding Principles for scientific data management and stewardship’[1]

- F – Findable
- A – Accessible
- I – Interoperable
- R – Reusable

Image created using imgflip.com

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

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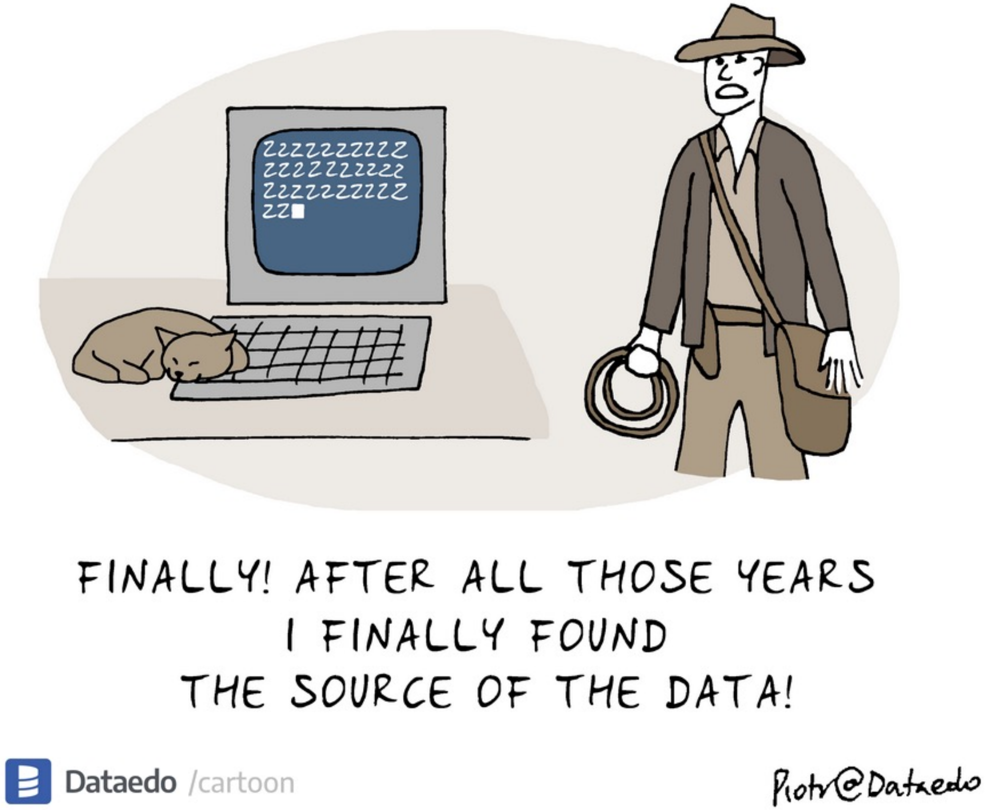
F is for Findable

- To be Findable:
  - It needs to exist
  - But existing != findable
  - Provide your users with pointers!

- **Are all your code/data/lab book/notes actually there?**


ZZZZZZZZZZ ZZZZZZZZZZ ZZZZZZZZZZ ZZ
FINALLY! AFTER ALL THOSE YEARS I FINALLY FOUND THE SOURCE OF THE DATA!
Dataedo /cartoon
Piotr@Dataedo

CC BY-ND 3.0 Dataedo - https://dataedo.com/cartoon/

A is for Accessible

- What should and shouldn’t be accessible?
- What is the use case?
- If access is restricted or complex, have you provided relevant information?

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Technically accessible != Easily accessible

I is for Interoperable

- Consider your data standards
- Use Common and Shared Vocabularies
  - For Data and Metadata
- Use Ontologies/Knowledge Graphs to the best of their potential

Michael J. Swart https://michaeljswart.com/2011/06/meta-aggregate/

Even standards need standards

R is for Re-useable

- This isn't JUST about the data! You need to consider:
  - Data, Tools, Code, Methods, Context
  - How could/would your work be re-used, replicated, reproduced or repurposed
    - Re-use – re-use the data (or run the software) in the same manner
    - Replicate – repeat entire research from scratch including data collection and analysis
    - Reproduce – reanalyse the existing data in the same manner
    - Repurpose – use existing data or software for a new purpose

This is only the tip of the "R" Iceberg

My funder expects me to upload the data supporting my paper to the repository...
ESRC DMP
I'm employed to do research not manage data! This extra work is a waste of my valuable time!
Sharing research data increases reproducibility for others and visibility for you!
OSC DATA TEAM

Claire Trowell - (CC BY-NC-ND) https://www.data.cam.ac.uk/intro-data-champions/data-champions-cartoons

FAIR Details

Data

- Do your data file names make sense
- Do your data headings make sense?
- Are your files understandable?

Code

- Do your code files make sense
- Is your code all there?
- Is it commented?

Lab Books

- Does your lab book fully detail your reagents, samples, experiment parameters?

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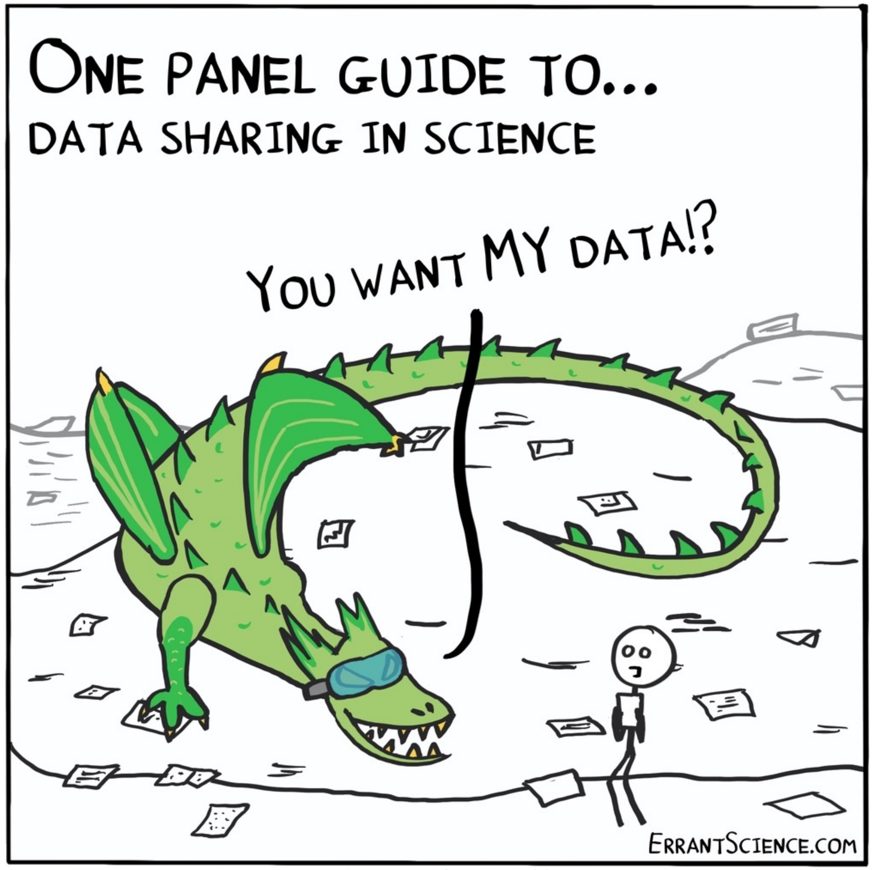
FAIR Pre-requisites

- Performing any of our ‘R’ operations on data or software is complex
- Data
  - Is this stored on outdated media?
  - What tools/software/dependencies do we need to use the data
- Databases
  - How do we use these? Are there database dumps? Schemas? Instructions?
- Software
  - What coding libraries are required?
  - Are there dependencies?
  - What installations and drivers are required?
  - Is all the underlying data included and accessible
- Lab Books
  - What were the experimental conditions?
  - What was the experimental setup?
  - What context exists for the experiment that you haven’t recorded?



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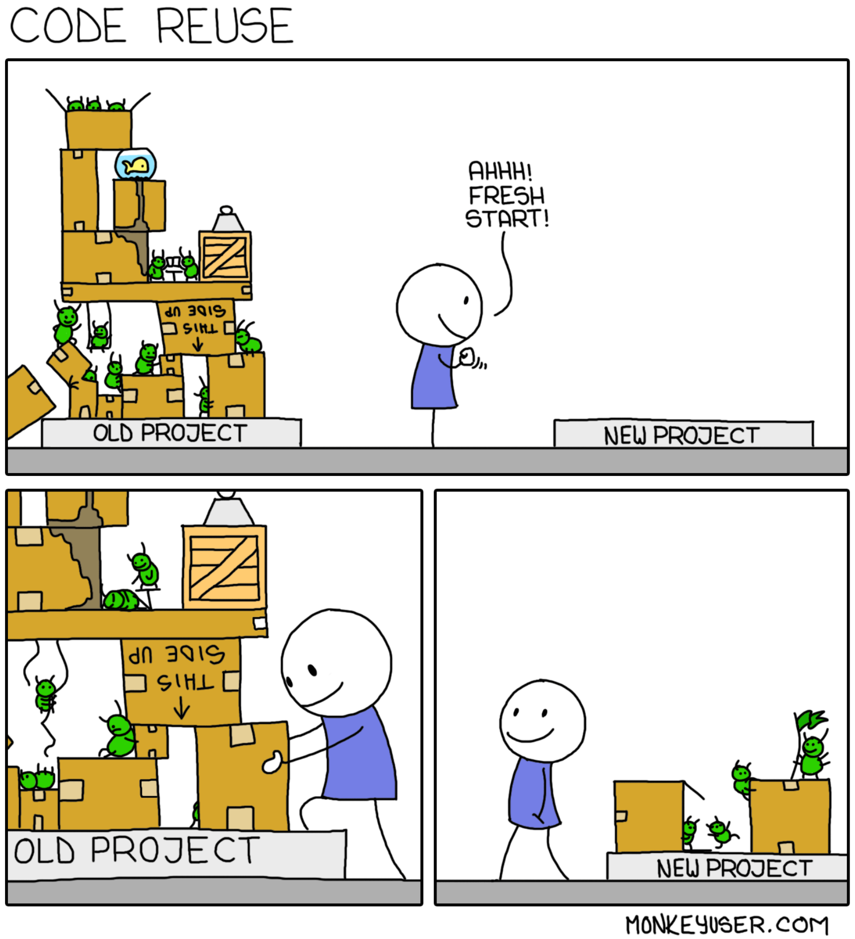
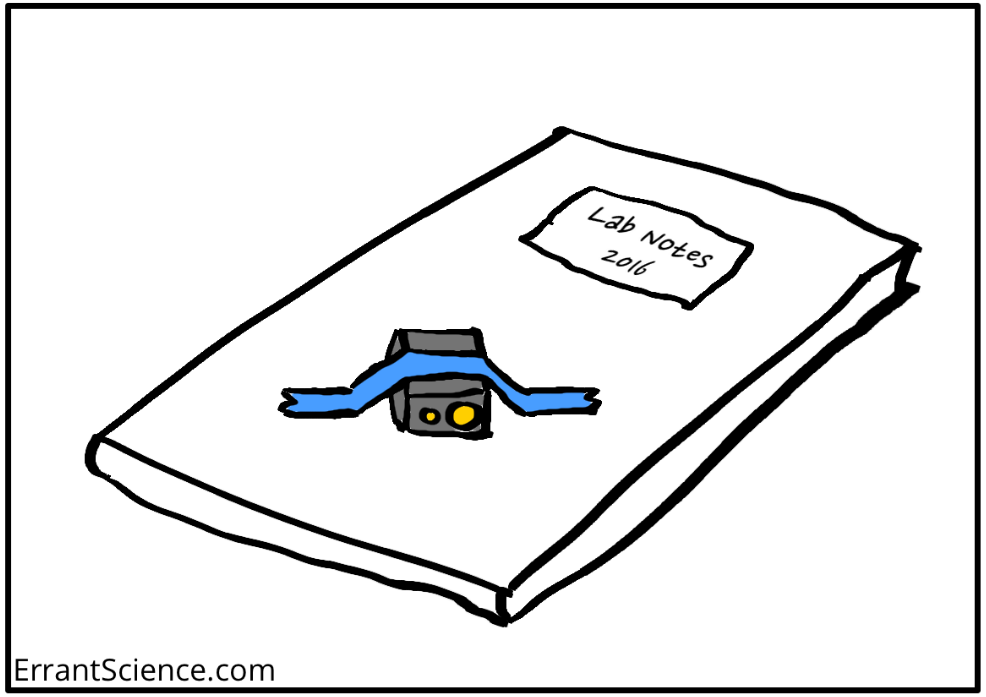
FAIR Instructions

- Be clear
- Do not assume prior knowledge
- Include all steps from start to finish (which means documenting as you go along)
- How was the data collected?
- What scripts/parameters were used?
- How did you get your database to interface with your code?
- How do you access the data?
- How do you run the software locally?
- If someone had your lab book and all your data could they re-run your experiment?
- Could someone else really re-use, reproduce, replicate or repurpose this?



FAIR Considerations for Selecting Digital Tools

- What data are you currently recording?
- How are you recording it?
- Where are you recording it?
- Is there extra data that you should be capturing?
- Who needs to access the data?
- What tools are people already using, and why?



If your electronic lab book looks like this, you're doing it wrong

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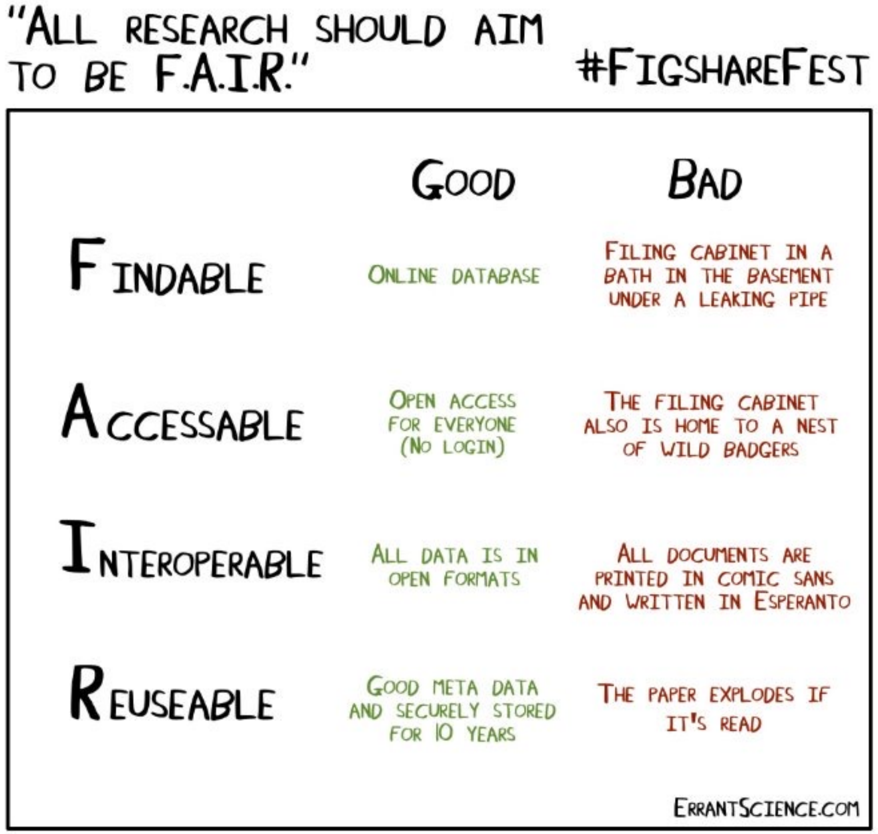
Further FAIR Considerations

- Investment through people and finance are imperative
- We are the problem so we can be the solution
- Investing in the relevant hardware and software tools will make these processes easier
- Should be considered early in the project, not just at the end



"ALL RESEARCH SHOULD AIM TO BE F.A.I.R." #FIGSHAREFEST

	GOOD	BAD
FINDABLE	ONLINE DATABASE	FILING CABINET IN A BATH IN THE BASEMENT UNDER A LEAKING PIPE
ACCESSABLE	OPEN ACCESS FOR EVERYONE (NO LOGIN)	THE FILING CABINET ALSO IS HOME TO A NEST OF WILD BADGERS
INTEROPERABLE	ALL DATA IS IN OPEN FORMATS	ALL DOCUMENTS ARE PRINTED IN COMIC SANS AND WRITTEN IN ESPERANTO
REUSEABLE	GOOD META DATA AND SECURELY STORED FOR 10 YEARS	THE PAPER EXPLODES IF IT'S READ

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What is PSDI working on to help this?

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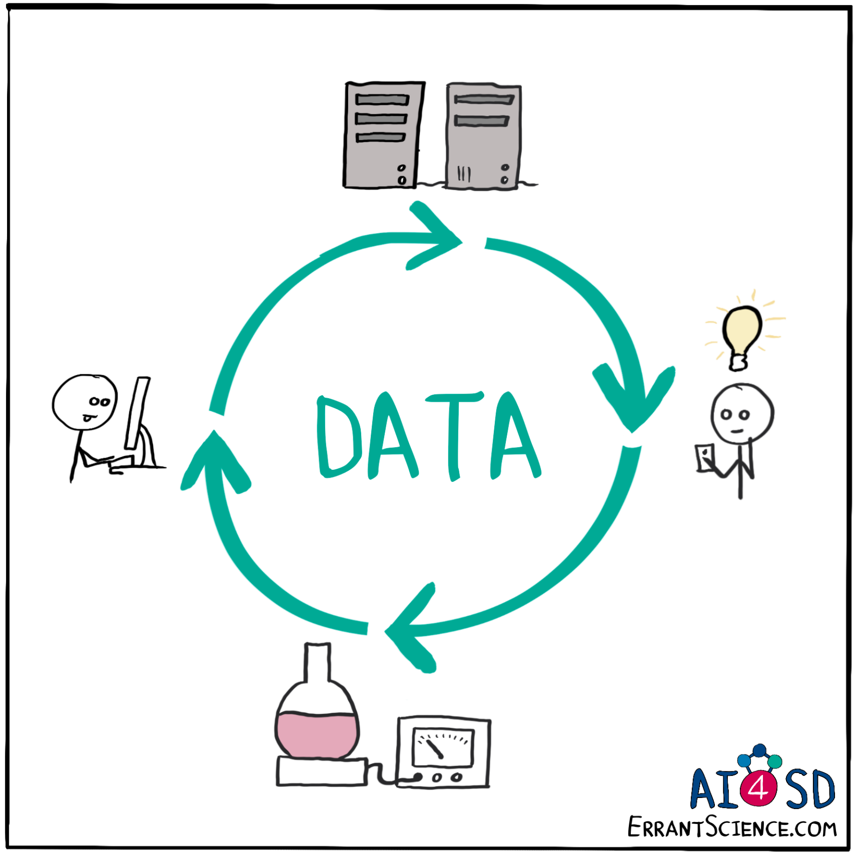
PSDI Focus Areas

Our current (but growing) focus is on:

- Process Recording
- Metadata
- DMPs
- Access to trusted data resources



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Domain Exemplars:

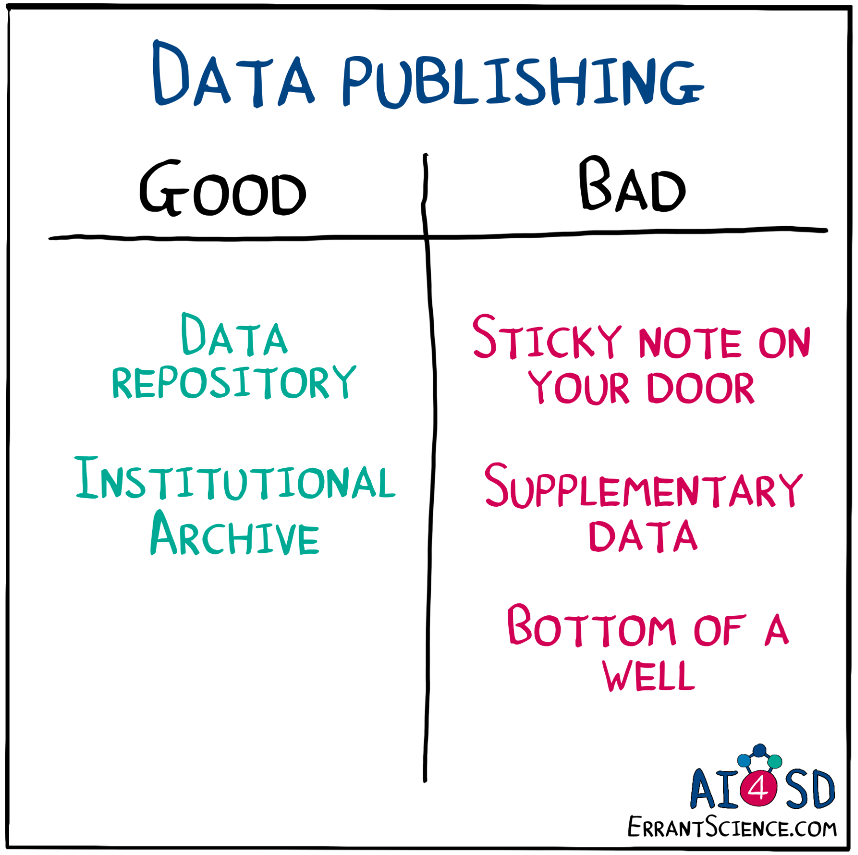
- Biomolecular simulation
- Catalysis
- Machine learnt interatomic-potentials
- Materials
- NMR Crystallography

Tools to help researchers (in development)

- Recording workflows for reproducibility
  - Developing tools in both AiiDA and Galaxy to enable easy and thorough recording of the steps taken in computational processes
- Data Conversion
  - Lookup and conversion between data formats to enable interoperability
- Data Revival
  - Scan in paper lab books and get data back in a machine-readable form
- Metadata Generation
  - Generate semantically rich metadata records, template READ-ME’s, license files
- Toolkits for creating better structured data / databases

Training & Guidance

- DMPs
- FAIR data publication
- Skills4Scientists
  - Technical skills
  - Soft skills
- Metadata creation
- Tool selection (e.g. picking the right process recording tool, implementing tools in teaching / research environments)
- Software guides (for PSDI developed tools)



Data Publishing

Good	Bad
Data Repository	Sticky note on your door
Institutional Archive	Supplementary data
	Bottom of a well

AI4SD

ErrantScience.com

How to get involved

- User focus groups
- Come to our webinars
- Send us an email

Townhall

- Add the other things here…

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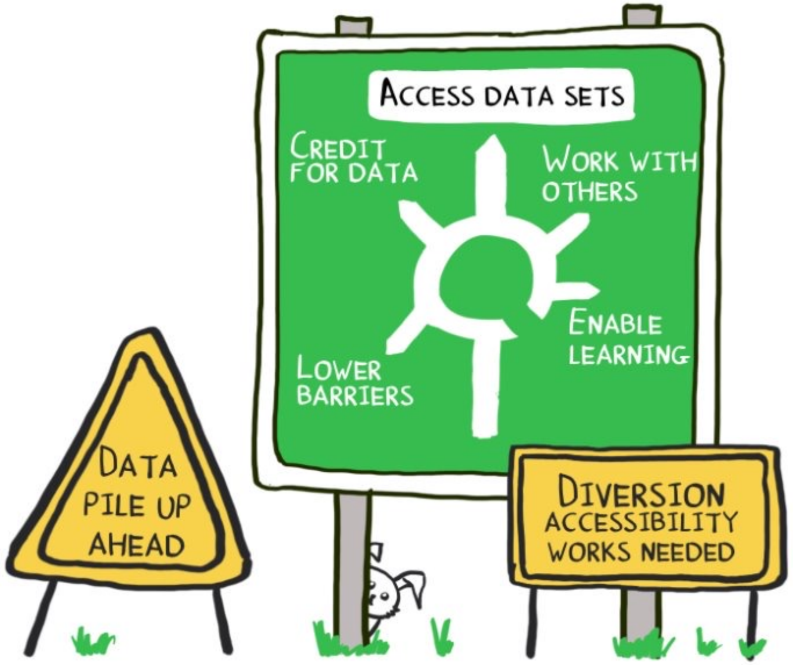
Conclusions

- There are still many barriers to overcome
- But PSDI is working towards solutions
- We need to remember the following:
    - Ask the right questions, about your data, your tools, your situation
    - FAIR is a FOUR letter word, but it has many many nuances
    - Collaboration is key - This is as much a human endeavor as a software/data one
    - We must all strive to be better



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To the well organised FAIR dataset, re-use, replication, reproduction and repurpose are but the next great adventure

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Relevant Talks

- Kanza, S. (2022, June 7). The effects of COVID-19 on the digitisation of Scientific Research - Presentation at Future Labs Live 2022. Future Labs Live 2022 (FLL2022), Basel. Zenodo. https://doi.org/10.5281/zenodo.10118139
- Kanza, S. (2022, October 4). To Digitisation And Beyond! The Digitisation Requirements Of A 21st Century Scientist - Presentation at Drug Discovery World 2022. Drug Discovery World 2022 (DDW2022), London. Zenodo. https://doi.org/10.5281/zenodo.10142544
- Kanza, S. (2022, December 6). Technical and Data Requirements of Digitalising Scientific Research - Presentation at Smart Labs & Automation 2022. Smart Labs & Automation, London. Zenodo. https://doi.org/10.5281/zenodo.10142749
- Kanza, S. (2023, January 25). The Digitisation of Scientific Research: Requirements, Barriers and Logistics - Presentation at Lab of the Future 2023. Lab of the Future 2023, Online. Zenodo. https://doi.org/10.5281/zenodo.10142604
- Kanza, S. & Knight, N. (2023, March 29). Process recording and digitisation requirements for the 21st century scientist - Presentation for ACS Spring 2023. ACS SPRING 2023 Crossroads of Chemistry (ACS SPRING 2023), Indianapolis, IN & Hybrid. Zenodo. https://doi.org/10.5281/zenodo.10144147
- Kanza, S. (2023, May 31). ELNs are Dead! Long Live ELNs! - Presentation at Future Labs Live 2023. Future Labs Live 2023 (FLL2023), Basel. Zenodo. https://doi.org/10.5281/zenodo.10138225
- Kanza, S. (2023, August 13). We don't talk about Semantic Web Technologies - Presentation at ACS Fall 2023. ACS FALL 2023 Harnessing the Power of Data (ACS FALL 2023), San Francisco, CA & Hybrid. Zenodo. https://doi.org/10.5281/zenodo.10149599
- Kanza, S. (2023, August 14). Electronic Lab Notebooks and Beyond! The evolution of process recording tools for scientific research - Presentation at ACS Fall 2023. ACS FALL 2023 Harnessing the Power of Data (ACS FALL 2023). Zenodo. https://doi.org/10.5281/zenodo.10149499
- Pearman-Kanza, S. (2023, November 1). To the well organised FAIR dataset, re-use is but the next great adventure - Presentation at Lab Innovations 2023. Lab Innovations 2023, NEC, Birmingham. Zenodo. https://doi.org/10.5281/zenodo.10119611
- Pearman-Kanza, S. (2023, December 7). How can we combat heterogeneous, unfair and disparate data in digital chemistry? Presentation at the ChemSpider Webinar Series. ChemSpider Webinar Series: Challenges and opportunities for digital chemistry data, Online. Zenodo. https://doi.org/10.5281/zenodo.10417786
- Pearman-Kanza, S. (2024, March 13) Electronic Lab Notebooks and Beyond! The evolution of process recording tools for scientific research’. RSC Historical Group Open Meeting, Zenodo https://doi.org/10.5281/zenodo.10818945

Relevant Publications

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