



# PSDI

PHYSICAL SCIENCES  
DATA INFRASTRUCTURE

## **The Bare Necessities: How to implement Electronic Lab Notebooks properly!**

**Lab Innovations 2024**

**30<sup>th</sup> October 2024**

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**University of Southampton**

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

# About Me



- ▶ Senior Enterprise Fellow at University of Southampton
- ▶ Pathfinder Lead on Process Recording for PSDI
- ▶ Researcher on Process Recording for PSDI & AIChemistry Hub
- ▶ Lab Horizons Columnist: CompSci Cat
- ▶ Advisory Boards/Committees: Future Labs Live, London Labs Live, MADICES, , Machines Learning Chemistry, RSC-CIAG, STRIX Award, KnowLedger: An Open Digital Research Notebook for Research Data Management
- ▶ Research Interests: FAIR Data, Semantic Web Technologies, IoT, Research Data Management, Digitisation, Lab of the Future, Paperless Labs, Re-use of Technology



# What is PSDI?



- ▶ UK funded project through the UKRI Digital Research Infrastructure theme (DRI) via EPSRC
- ▶ Developed out of a community statement of need
- ▶ Lead institutions: University of Southampton and Science and Technology Facilities Council (STFC)
- ▶ Still predominantly in requirements gathering and developing proof of concept
- ▶ Launch of resources in early 2025

## 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.

# Training & Guidance

We are collating together existing training materials and best practice guidance, and creating new resources where required

- ▶ Data Management Plans
- ▶ FAIR data publication
- ▶ Metadata creation
- ▶ Skills4Scientists
  - ▶ Technical skills
  - ▶ Research skills
  - ▶ Soft skills
- ▶ Tool selection (e.g. picking the right process recording tool, implementing tools in teaching / research environments)

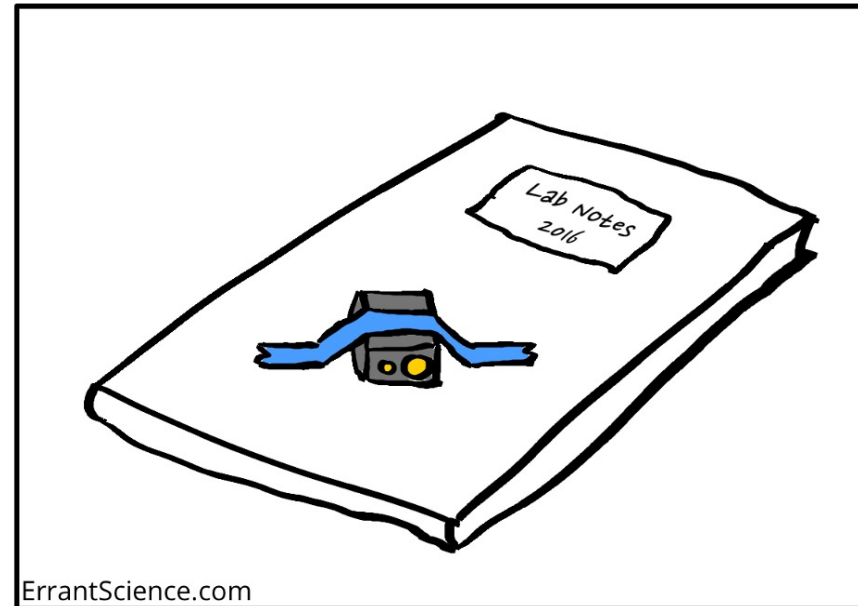
DATA PUBLISHING	
GOOD	BAD
DATA REPOSITORY	STICKY NOTE ON YOUR DOOR
INSTITUTIONAL ARCHIVE	SUPPLEMENTARY DATA
	BOTTOM OF A WELL

  
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# Process Recording

- ▶ Case studies of successful implementations
  - University of Nottingham - AI4Green in Undergrad & Postgrad Labs, and OneNote in Undergrad Labs
  - Wellington College – OneNote in School Labs
- ▶ Prototypes for digital notebook integration
  - University of Southampton - OneNote & Microsoft Ecosystem in Undergrad Labs
  - University of Southampton – Selecting and implementing an ELN for Chemistry Postgraduates
  - University of Southampton – Implementing LabTrove in the xray lab
- ▶ Contributing to ELNFinder (Resource to compare ELNs by a range of filter criteria)
- ▶ Data Revival Service to turn paper lab notebooks into machine readable data

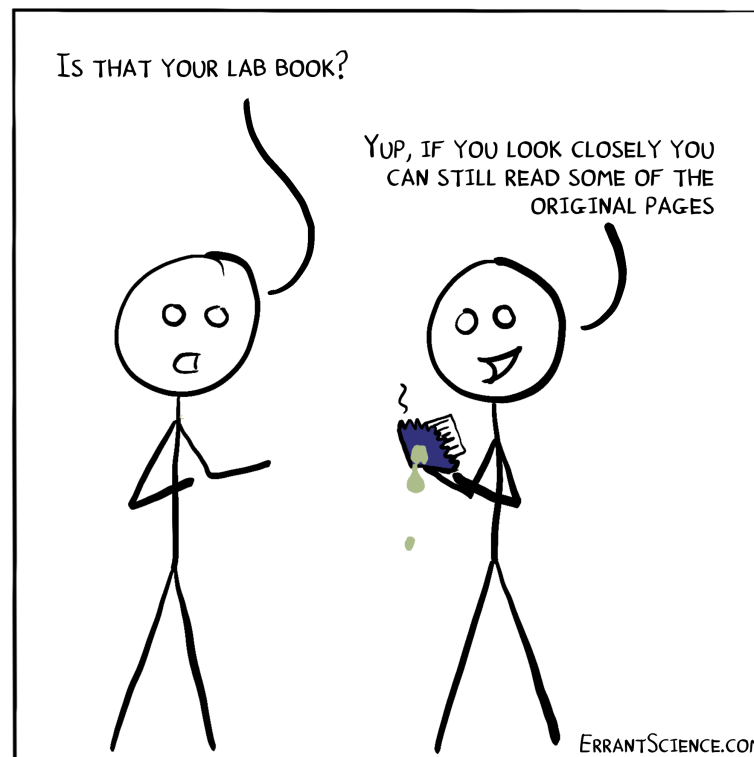


If your electronic lab book looks like this,  
you're doing it wrong

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# The Electronic Lab Notebook

- ▶ ELNs were originally created to serve as a direct replacement for the paper lab notebook
- ▶ Which sounds like a simple endeavour at first....!



# Active ELNs

There are now over 85 active ELNs on the market!

- ▶ ACAS
- ▶ Active LN
- ▶ AgiLab ELN
- ▶ Agilent SLIMS
- ▶ AI4Green
- ▶ Alchemy ELN
- ▶ Arxspan ELN
- ▶ Benchling ELN
- ▶ BioChemLab Solutions ELN
- ▶ BioRails
- ▶ Biovia Notebook
- ▶ Bookitlab
- ▶ CBIS E-Notebook
- ▶ CDD Vault ELN
- ▶ CERF 5.0
- ▶ ChemCart ELN
- ▶ Chemia
- ▶ Chemotion
- ▶ Colabra ELN
- ▶ CompuDrug ELN
- ▶ Dotmatics ELN
- ▶ E-WorkBook
- ▶ Ec-LabNote
- ▶ eLabFTW
- ▶ eLabJournal
- ▶ eLabNotes
- ▶ EmsoChemLab
- ▶ Espresso ELN
- ▶ eStudy
- ▶ eSystems
- ▶ Formulator
- ▶ Gene Inspector
- ▶ GenoFAB
- ▶ GOLims
- ▶ Herbie
- ▶ iLES Platform
- ▶ InELN
- ▶ iQ
- ▶ Kadi4Mat
- ▶ Lab Integrated Data (LabID)
- ▶ LabArchives
- ▶ LabCloud
- ▶ LabCollector ELN
- ▶ LabFolder
- ▶ Labguru ELN
- ▶ Labii
- ▶ LabKey ELN
- ▶ LabLog
- ▶ LabsForm
- ▶ LabSpace
- ▶ LabStep
- ▶ LabTrack ELN
- ▶ LabTrove
- ▶ LabVantage
- ▶ LabWare ELN
- ▶ Laby
- ▶ Limsophy LIMS
- ▶ LogBook
- ▶ Logilab
- ▶ LOGS-ELN
- ▶ Mbook
- ▶ MyLabBook
- ▶ NOMAD ELN
- ▶ NotebookMaker
- ▶ NuGenesis
- ▶ Online ELN Worksheet
- ▶ Open Enventory
- ▶ openBIS
- ▶ OpenText ELN
- ▶ PASTA-ELN
- ▶ PatentSafe ELN
- ▶ quattro/LJ
- ▶ RedFox
- ▶ Rspace
- ▶ SampleDB
- ▶ Sapio Seamless ELN
- ▶ SciCord ELN/LIMS
- ▶ Sciformation ELN
- ▶ Scilligence ELN
- ▶ SciNote
- ▶ Signals ELN
- ▶ Stackwave ELN
- ▶ STARLIMS ELN
- ▶ Studylog
- ▶ Sun Bio ELN
- ▶ Thermo Scientific Core ELN
- ▶ Unaccountable

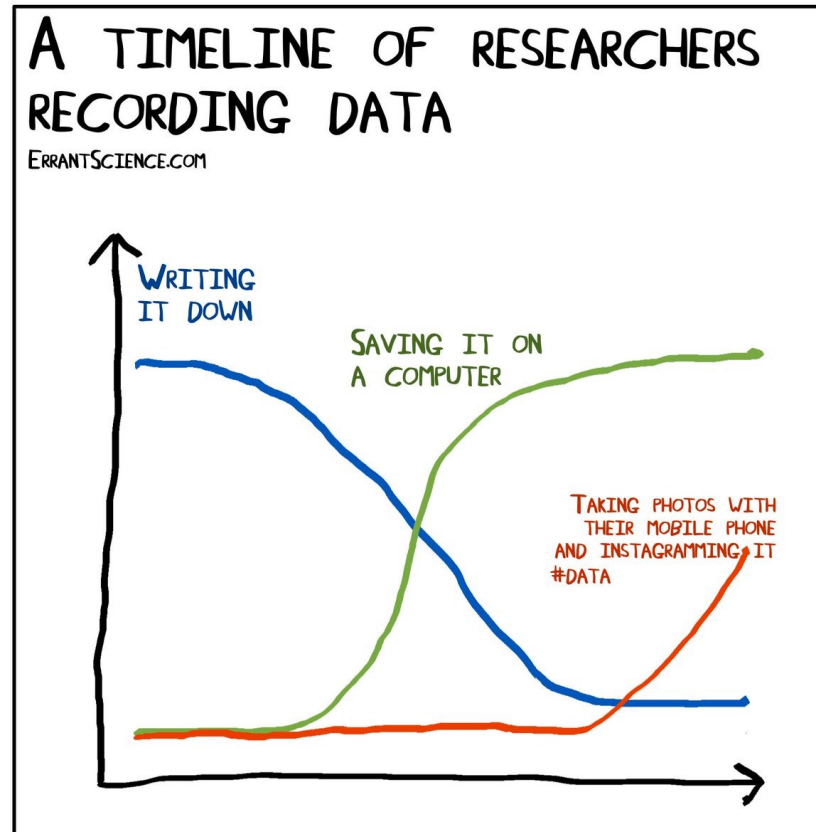
# Evolution of Tools





# Evolution of Tools

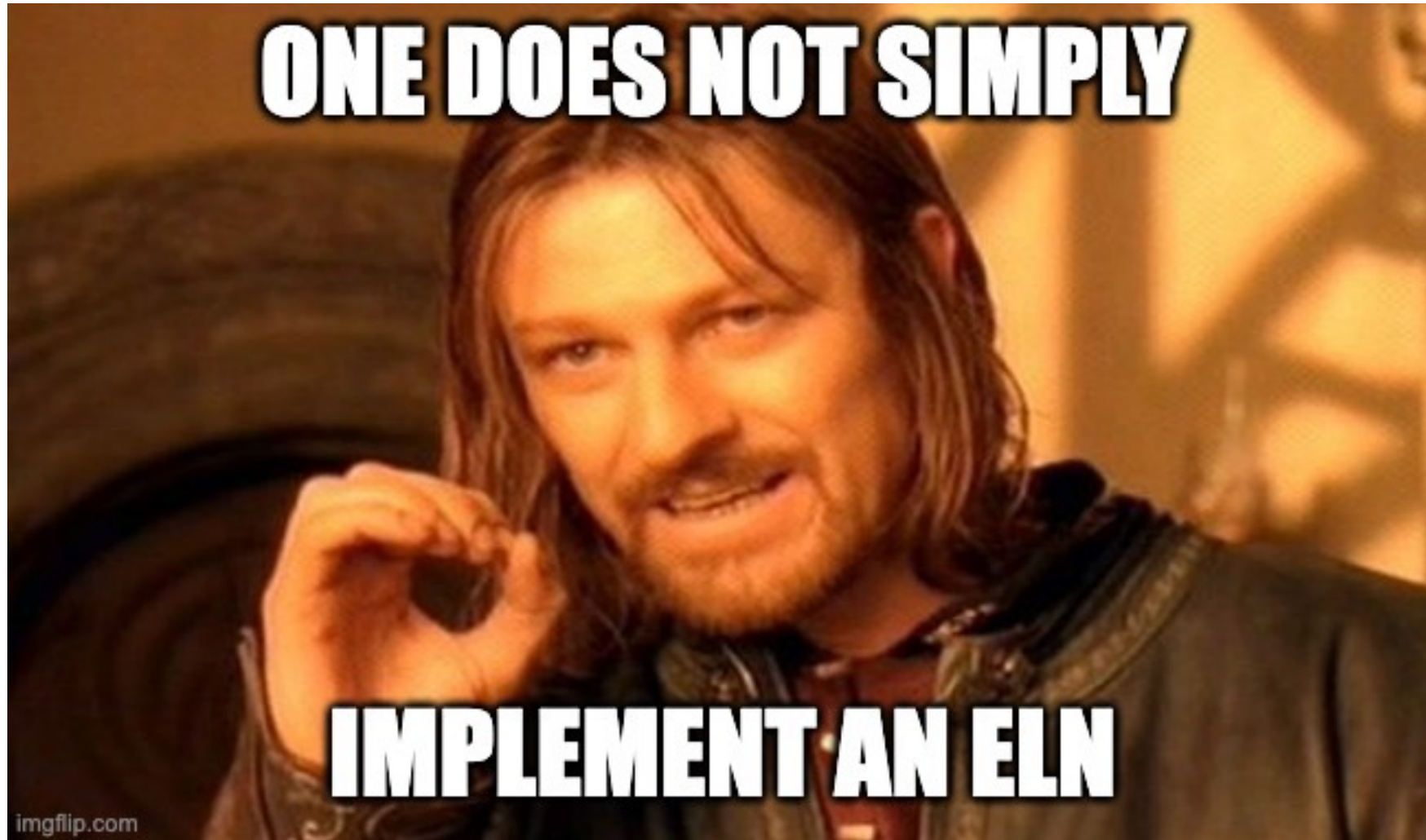
- ▶ Frequently these platforms encompass one of many of:
  - ▶ ELNs (Electronic Lab Notebooks)
  - ▶ LIMS (Laboratory Information Management System)
  - ▶ SDMS (Scientific Data Management System)
  - ▶ Inventory / Sample Management
  - ▶ Registry



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They are no longer **JUST A REPLACEMENT**

# So Lets talk about ELNs



# ELN Barriers

## ▶ People Barriers

- ▶ People still like paper
- ▶ Attitudes to ELNs
- ▶ Trust & Concerns about Data Security & Longevity
- ▶ Bureaucracy

## ▶ Technical Barriers

- ▶ Software
- ▶ Compatibility & Interoperability



Image created using <https://openart.ai/>

## ▶ Infrastructure/ Institutional Barriers

- ▶ Cost
- ▶ Time
- ▶ Lab Setup
- ▶ Hardware

## ▶ Data Barriers

- ▶ Compatibility & Interoperability
- ▶ Data Storage

# Implementation Considerations

- ▶ People Considerations
- ▶ Technical Considerations
- ▶ Data Considerations
- ▶ Infrastructure/Institutional Considerations



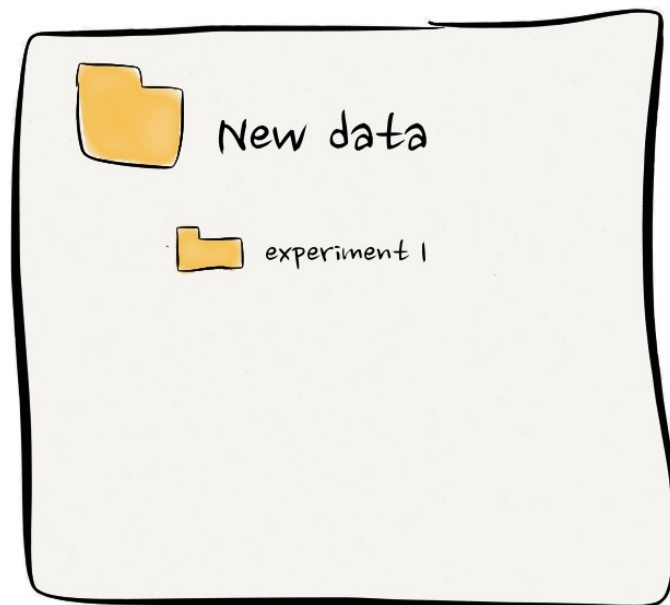
["Electronic Lab Notebooks are great, but not on vacation"](#) Cartoon by Phil Johnson for MIT.



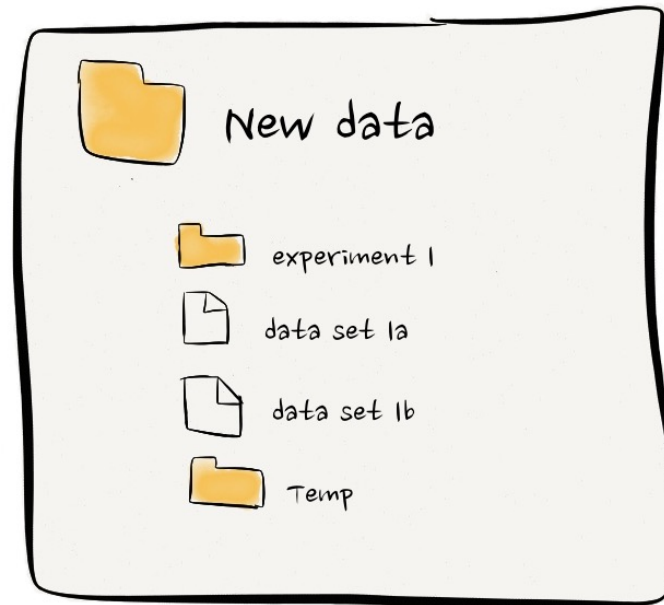
# People Considerations

- ▶ Career Level Consideration
- ▶ Domain Consideration

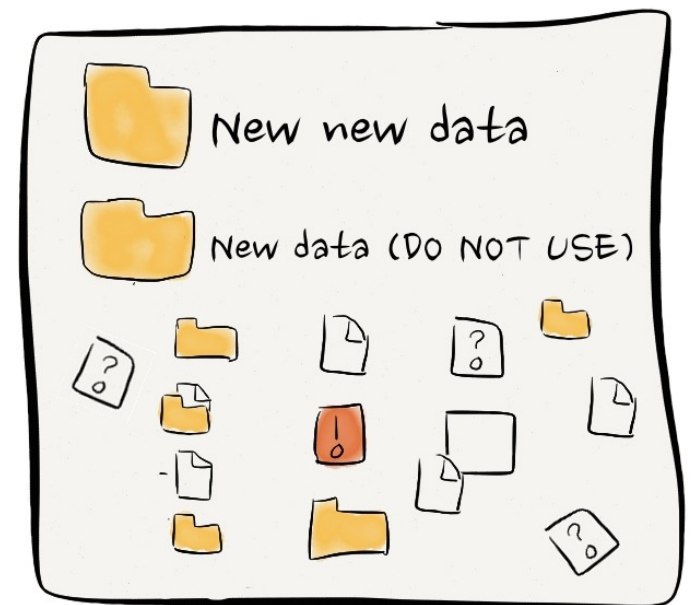
- ▶ Change Management / Adoption



**Day 1**



**Day 2**

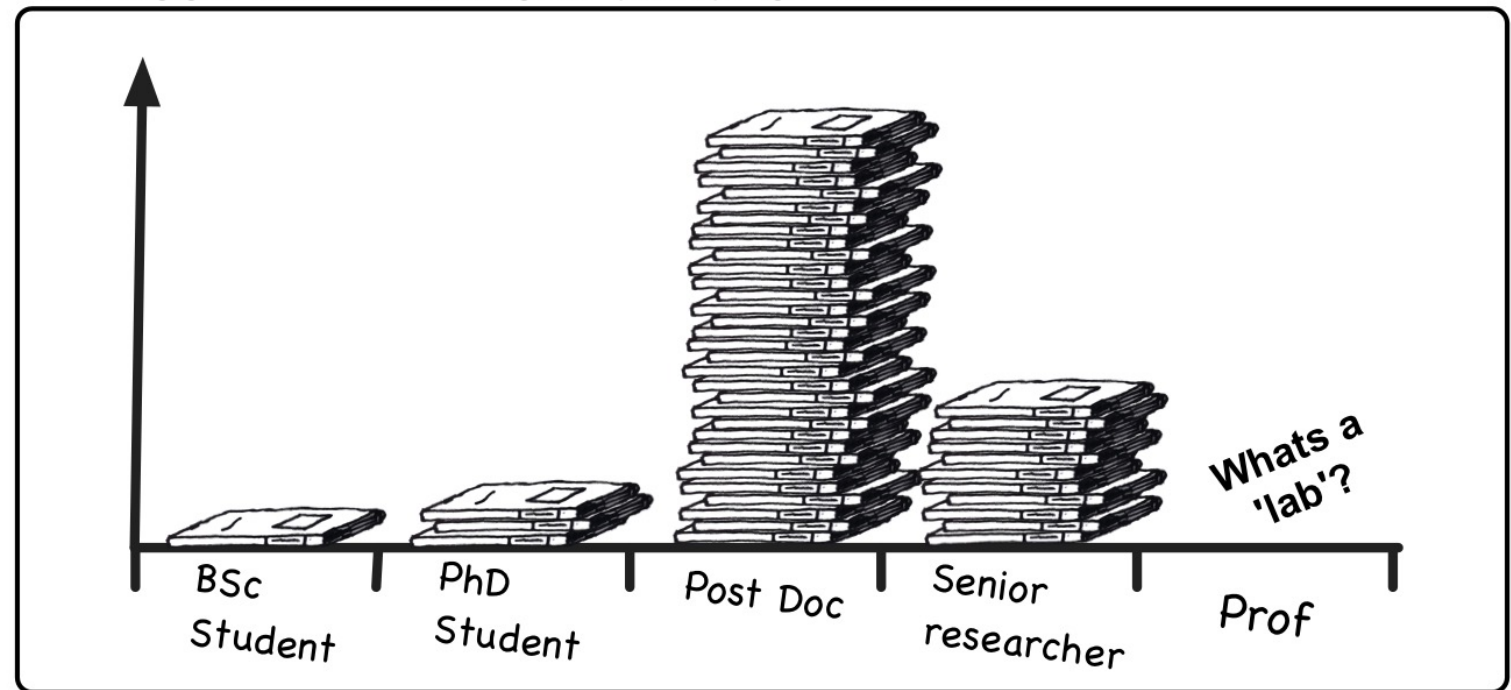


**Day 3**

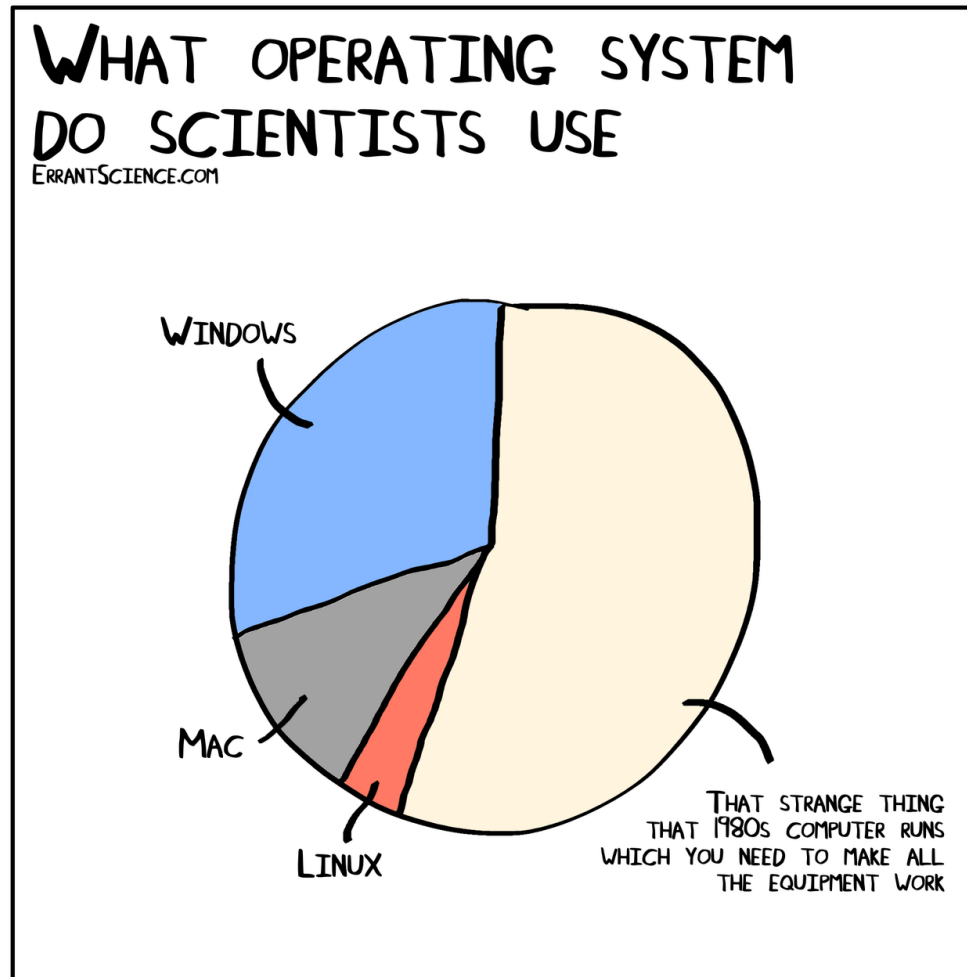
# Career Level Selection

- ▶ What career stage is this ELN aimed at? E.g. Undergraduate/Postgraduate?
- ▶ What is the primary aim for this career stage? E.g. Learning / Publishing
- ▶ Important question
  - ▶ How automated do you want/need this ELN to be?
  - ▶ Is a fully fledged ELN or a Generic Notebooking tool more appropriate?

Lab book use at various levels of academia



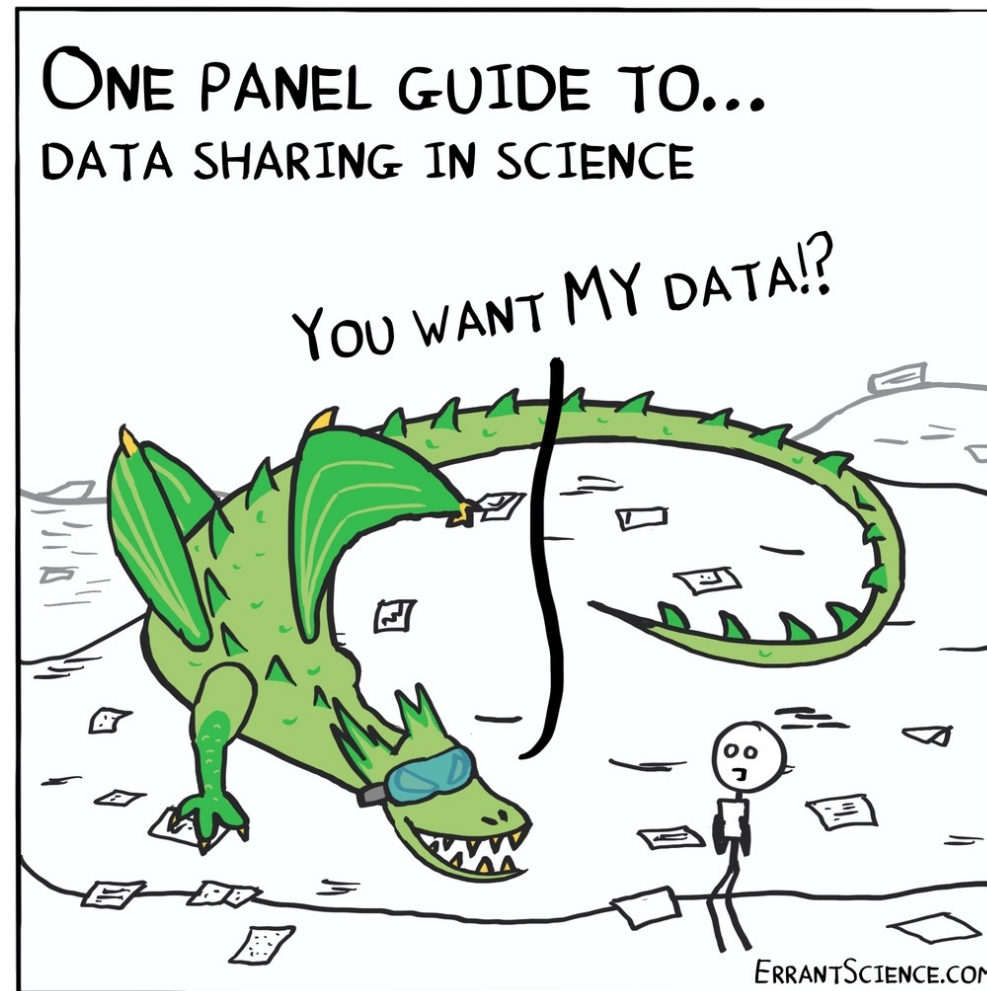
# Domain Selection



- ▶ Different domains have different requirements and data types
- ▶ Universities (and many companies) will need to cater for a variety of domains
- ▶ Is there specific domain-based software that this Digital Lab Notebook needs to integrate with?

# Change Management / Adoption

- ▶ People are arguably one of the biggest barriers
- ▶ Top-down influence can make or break this
- ▶ Need to get the whole group on board
- ▶ Identify keen early adopters and first years / new starters



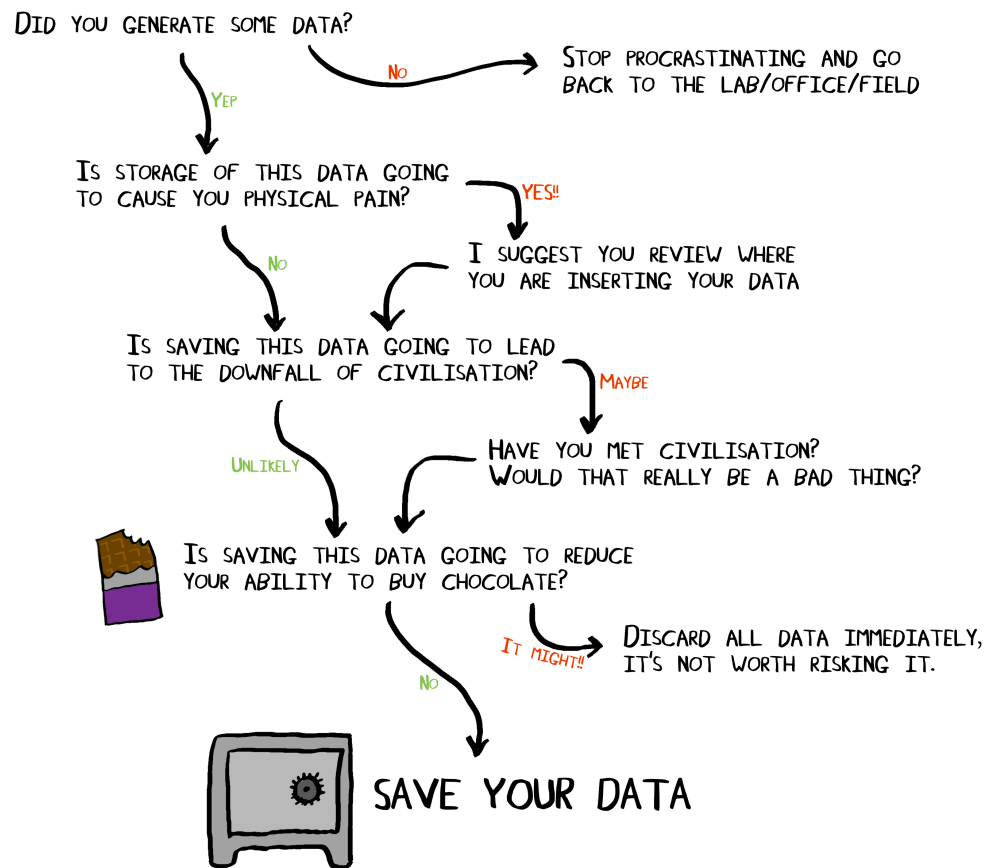


# Technical Considerations

## SHOULD YOU SAVE YOUR DATA?

A FLOW DIAGRAM

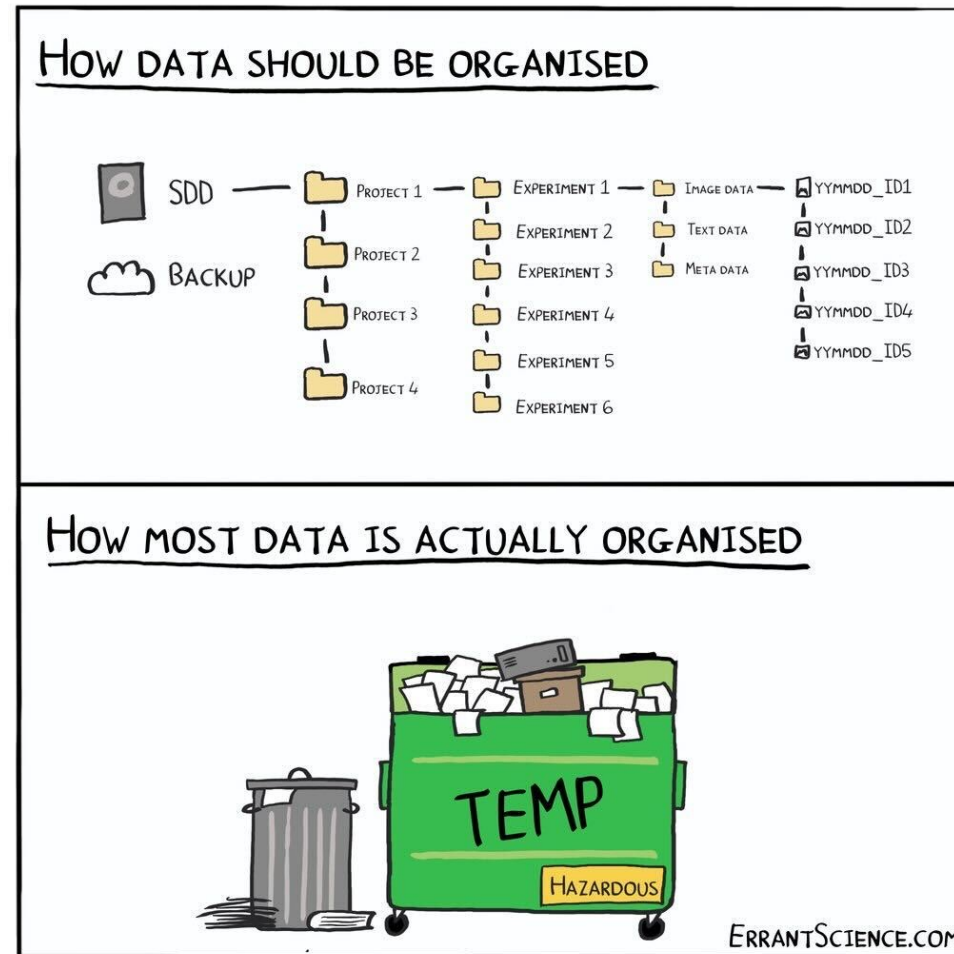
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- ▶ Pain Points - What are you trying to solve by implementing an ELN?
- ▶ Software Selection – How to even start choosing an ELN?

# Pain Points & What are you solving?

- ▶ Digitising is great, but **WHY** are you doing it?
- ▶ What are the actual pain points that you are trying to solve?
- ▶ Does the software align with what you are trying to achieve?
- ▶ ELN Implementation isn't just about the software, is your entire plan/setup moving towards your goal?



# Software Selection – ELNFinder I

<https://eln-finder.ulb.tu-darmstadt.de>

## ELN Finder

The ELN Finder helps you to search and select a suitable Electronic Lab Notebook (ELN) for your purposes.

- More than 40 filter criteria available.
- Filter criteria clearly divided into categories.
- Result list of the identified ELN tools displayed in an overview.
- Brief descriptions of the individual tools included.

 Find ELNs

**MAKE YOURS THE NEXT ONE!**

- ▶ Detailed hierarchical criteria catalogue created, defines and describes the metadata structure for the ELNs (Excel):
- ▶ > 40 criteria and associated values, attributes (e.g. name/URL).
- ▶ Summary of criteria in categories
- ▶ Fully functional first version developed on the basis of the open source software DSpace 7
- ▶ External ELN information collection created for individual ELNs
- ▶ Entering data from the information collection
- ▶ > 40 ELNs entered

# Software Selection – ELNFinder II

- ▶ APIs
- ▶ Automation
- ▶ Collaboration
- ▶ Compliance
- ▶ Controlled vocabulary
- ▶ Customizable user interface
- ▶ Data access
- ▶ Data export
- ▶ Data import (formats)
- ▶ Data import (method)
- ▶ Data input
- ▶ Data storage location
- ▶ Device connection
- ▶ Laboratory management functions
- ▶ Languages Support
- ▶ License
- ▶ Location of provider
- ▶ Offline functionalities
- ▶ Operating system
- ▶ Plug-Ins
- ▶ Preservation of evidence
- ▶ Pricing
- ▶ Project management tools
- ▶ Search functions
- ▶ Standard interfaces
- ▶ Subject
- ▶ Templates
- ▶ Usage option
- ▶ Usage statistics
- ▶ Versions
- ▶ Workflows

**Filter Criteria**



# Software Selection – Jisc Tender

Opportunity

## Electronic Research and Laboratory Notebook DPS

Jisc

Watch this notice

F02: Contract notice

Notice reference: 2024/S 000-030661

Published 25 September 2024, 4:19pm

### Contents

[I. Contracting authority](#)

[II. Object](#)

[IV. Procedure](#)

[VI. Complementary information](#)

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## Section I: Contracting authority

### I.1) Name and addresses

Jisc  
4 Portwall Lane  
Bristol  
BS1 6NB

### Contact

Chris Hallahan

### Email

[procurement@jisc.ac.uk](mailto:procurement@jisc.ac.uk)

### Country

United Kingdom

### NUTS code

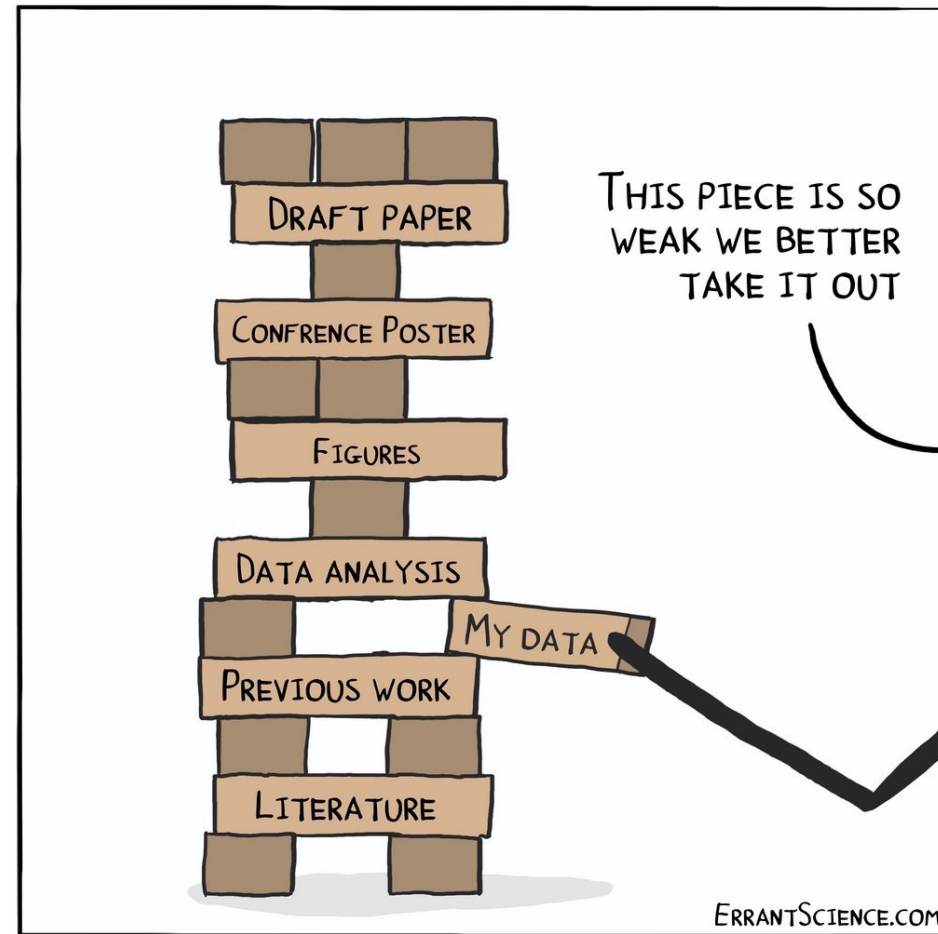
UK - United Kingdom

JSL is establishing a DPS that will enable Jisc and its customers to easily purchase value for money and technically sound Electronic Research and Laboratory Notebook solutions (ERNs).

<https://www.find-tender.service.gov.uk/Notice/030661-2024>

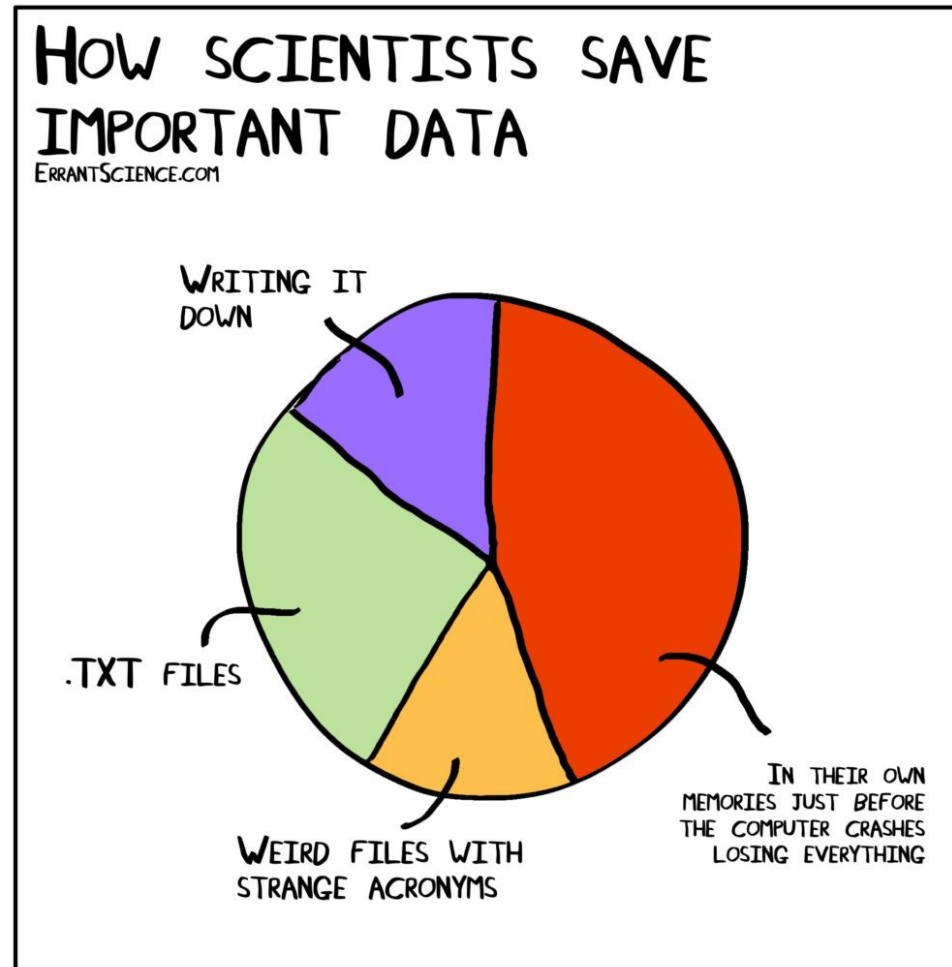
# Data Considerations

- ▶ Backup, Storage & Security
- ▶ Data Capture
- ▶ Experiment Templates
- ▶ FAIR Data
- ▶ Data Sharing
- ▶ Data Publishing



# Backup, Storage & Security

- ▶ Many researchers mistrust ELNs
- ▶ There are concerns about data exit strategies – need to make sure data is stored and backed up in a way that this is feasible
- ▶ Consider what export functionalities are available?
- ▶ Security measures and vulnerabilities need to be considered



# Data Capture / Templates




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- ▶ Different domains will require different levels of data capture
- ▶ What data formats need to be supported for import/export?
- ▶ Consider the different types of data that will be recorded and make templates to ensure that all the relevant data is captured
- ▶ Fewer templates are ideal, but need to cover the range of data

# Sharing / Publishing / FAIR Data

- ▶ A key reason to implement an ELN is to produce FAIRer Data for Publication – so your implementation plan needs to take this into account
- ▶ Another key reason is sharing data among colleagues/groups, its important to identify if people are finding it easier to locate relevant ELN entries to save time / inform

DATA PUBLISHING	
GOOD	BAD
DATA REPOSITORY	STICKY NOTE ON YOUR DOOR
INSTITUTIONAL ARCHIVE	SUPPLEMENTARY DATA
	BOTTOM OF A WELL

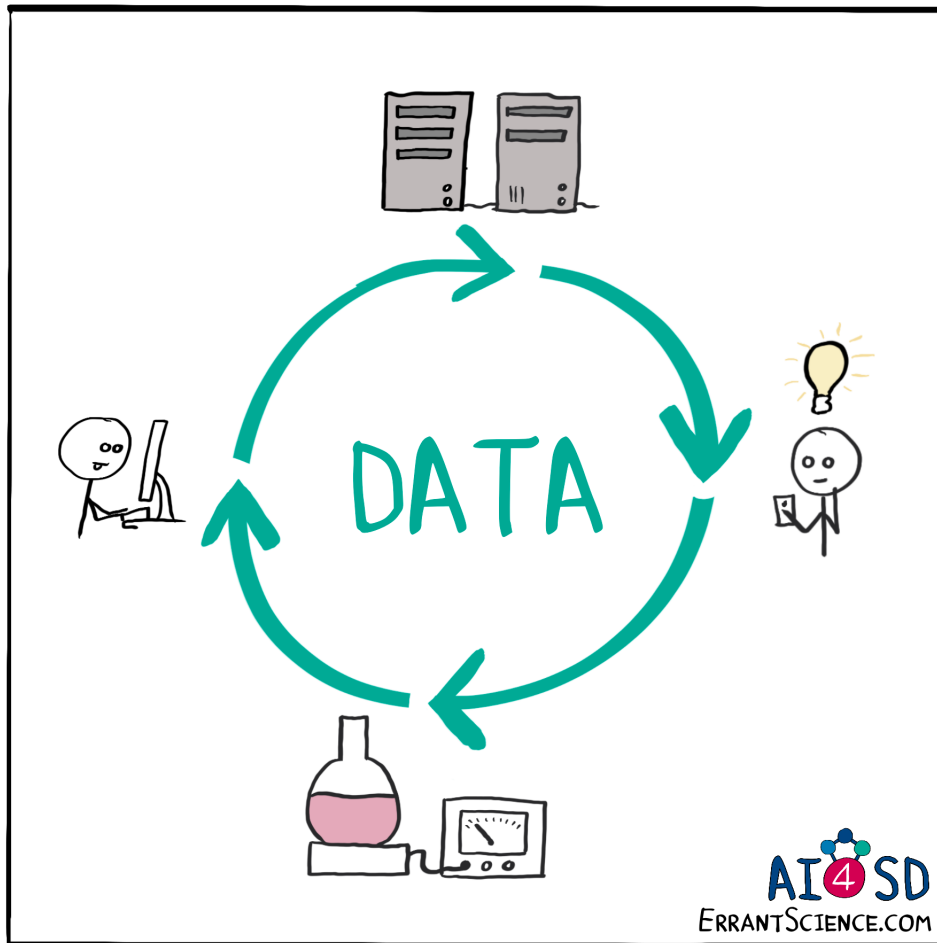


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# Infrastructure/Institutional Considerations



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- ▶ Lab Setup
  - ▶ Hardware
    - ▶ Power
    - ▶ Internet
- ▶ Infrastructure Setup
- ▶ Administration
- ▶ Finances
- ▶ Time



# Lab Setup (Hardware, Power, Internet)

## ▶ Hardware Devices

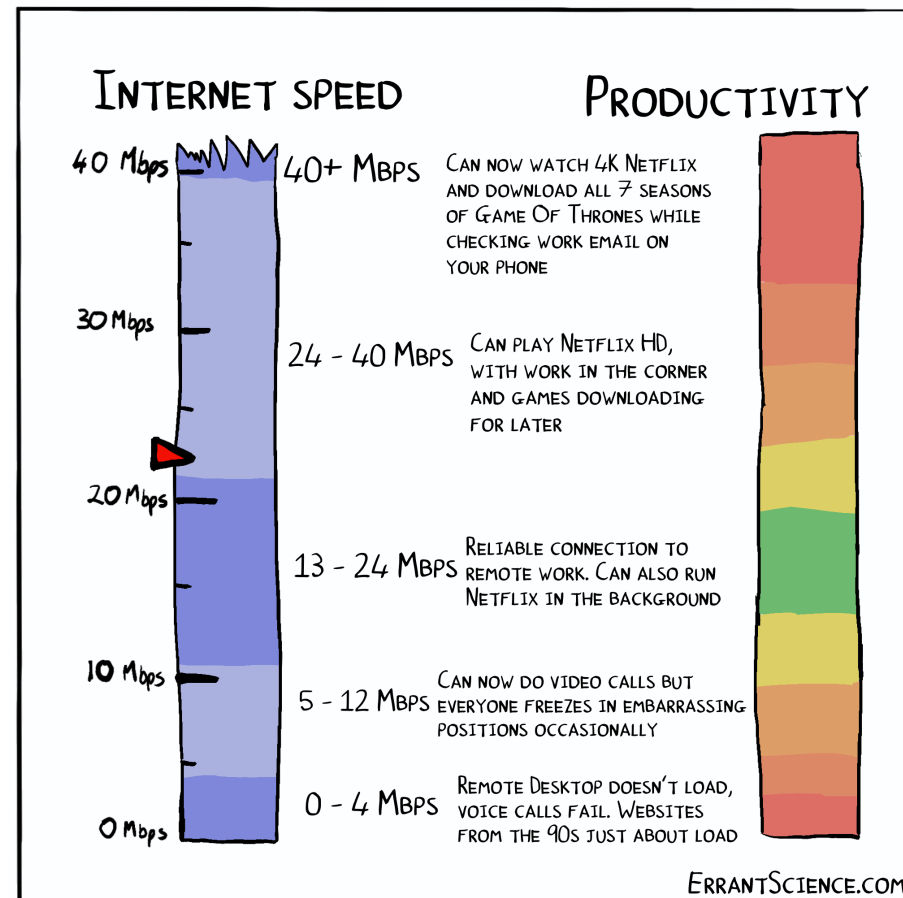
- ▶ What electronic devices are going to be used?
- ▶ Dedicated in-lab hardware is key to avoid cross contamination
- ▶ Where are the devices going to be placed?

## ▶ Power

- ▶ Need suitable power sockets to charge / power electronic devices

## ▶ Internet

- ▶ Need good quality WIFI or hardwired Internet cables/sockets



# Infrastructure / Administration



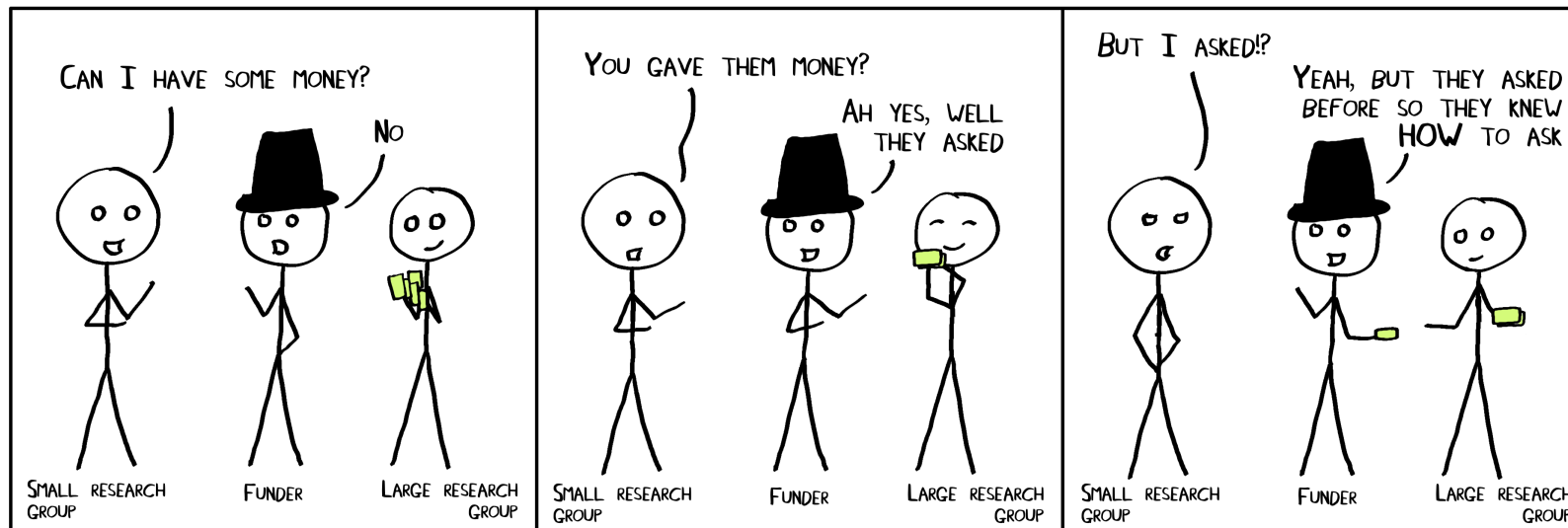
- ▶ ELN Implementation is more than just buying software licenses
- ▶ Administrators are required to manage Accounts/Roles/Groups
- ▶ Need to consider data owners after people move on

# Finances

- ▶ ELN Licensing costs
- ▶ Hardware costs - Replacing legacy equipment, Providing devices to use ELN on
- ▶ Lab renovation costs - Installing more power sockets/ethernet sockets / WIFI boosters
- ▶ Maintenance & Staffing costs
- ▶ Potential future development costs

## UNIVERSITY FUNDING IN A NUTSHELL

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# Time

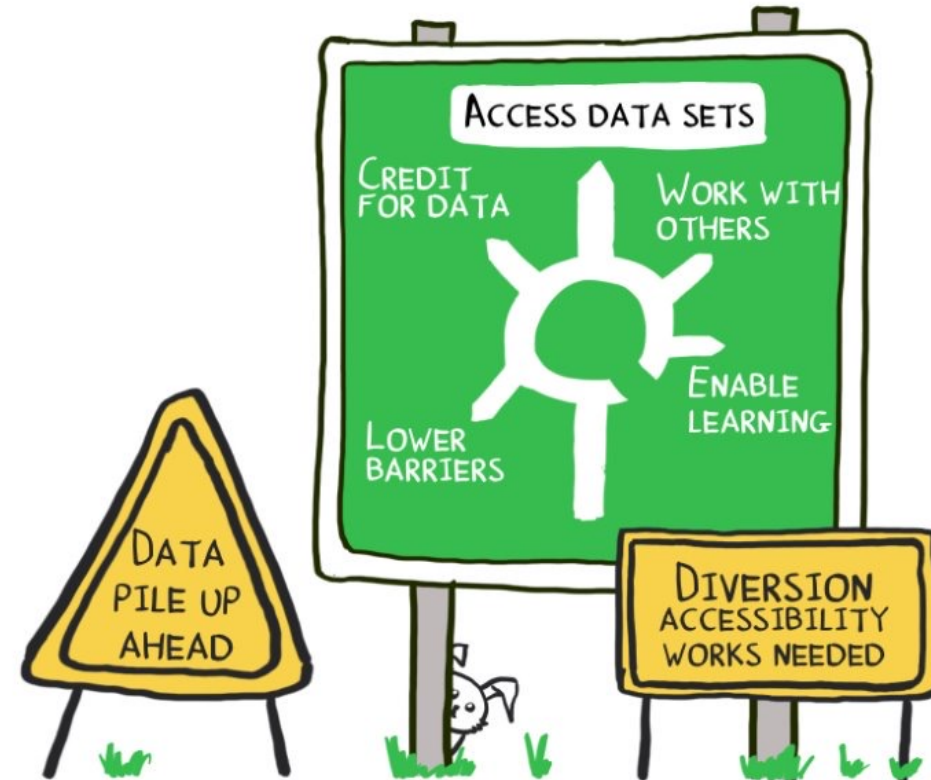


<https://www.pinterest.co.uk/pin/19281104642853801/>

- ▶ Implementing a new ELN takes considerable time
  - ▶ Time to convince people/institution
  - ▶ Select Software
  - ▶ Setup Lab suitably
  - ▶ Identify Staffing for admin/infrastructure
  - ▶ Run a trial
  - ▶ Develop templates
  - ▶ Organise logistics /finances

# Conclusions

- ▶ This is a highly complex endeavour
- ▶ ALL of these considerations need to be taken into account – You need to ask the right questions
- ▶ You need to identify how to measure progress and success
- ▶ This requires dedicated time and people to make it happen
- ▶ PSDI are here to help!



# Relevant Talks

- ▶ Kanza, S. P. (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. P. (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. P. (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. P. (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. P., & 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. P. (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. P. (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. P. (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>
- ▶ Kanza, S. P. (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>



# Relevant Publications

- ▶ Kanza, S., Willoughby, C., Gibbins, N., Whitby, R., Frey, J.G., Erjavec, J., Zupančič, K., Hren, M. and Kovač, K., 2017. Electronic lab notebooks: can they replace paper?. *Journal of cheminformatics*, 9(1), p.31. <https://doi.org/10.1186/s13321-017-0221-3>
- ▶ Kanza, S., 2018. What influence would a cloud based semantic laboratory notebook have on the digitisation and management of scientific research? (Doctoral dissertation, University of Southampton). <https://eprints.soton.ac.uk/421045/>
- ▶ Kanza, S., Gibbins, N. and Frey, J.G., 2019. Too many tags spoil the metadata: investigating the knowledge management of scientific research with semantic web technologies. *Journal of cheminformatics*, 11(1), p.23. <https://doi.org/10.1186/s13321-019-0345-8>
- ▶ Knight, N.J., Kanza, S., Cruickshank, D., Brocklesby, W.S. and Frey, J.G., 2020. Talk2Lab: The Smart Lab of the Future. *IEEE Internet of Things Journal*, 7(9), pp.8631-8640. <https://doi.org/10.1109/JIOT.2020.2995323>
- ▶ Kanza, S., Willoughby, C., Bird, C.L. and Frey, J.G., 2021. eScience Infrastructures in Physical Chemistry. *Annual review of physical chemistry*, 73. <https://doi.org/10.1146/annurev-physchem-082120-041521>
- ▶ Kanza, S., 2021. Guidelines for Chemistry Labs Looking to Go Digital. *Digital Transformation of the Laboratory: A Practical Guide to the Connected Lab*, pp.191-197. <https://doi.org/10.1002/9783527825042.ch13>
- ▶ Kanza, S., 2021. Understanding and Defining the Academic Chemical Laboratory's Requirements: Approach and Scope of Digitalization Needed. *Digital Transformation of the Laboratory: A Practical Guide to the Connected Lab*, pp.179-189. <https://doi.org/10.1002/9783527825042.ch12>
- ▶ Kanza, S., 2021. Academic's Perspective on the Vision About the Technology Trends in the Next 5–10 Years. *Digital Transformation of the Laboratory: A Practical Guide to the Connected Lab*, pp.297-301. <https://doi.org/10.1002/9783527825042.ch22>
- ▶ Kanza, S. and Knight, N.J., 2022. Behind every great research project is great data management. *BMC Research Notes*, 15(1), pp.1-5. <https://doi.org/10.1186/s13104-022-05908-5>
- ▶ Kanza, S., Willoughby, C., Knight, N.J., Bird, C.L., Frey, J.G. and Coles, S.J., 2023. Digital research environments: a requirements analysis. *Digital Discovery*. <https://doi.org/10.1039/D2DD00121G>

viewpoint **ELN**



## Electronic Lab Notebooks:

One notebook to rule them all,  
a dream or a curse?

Dr Samantha Pearman-Kanza goes on a journey to  
the dark realm of ELN implementation

**I** often get asked, “What is your main tip for implementing an Electronic Lab Notebook (ELN)?” or “I want to implement an ELN, which one should I choose?” Or even “Why haven’t most universities implemented ELNs yet?”. We live in a digital age where we carry portable computers in our pockets, where we can remotely activate devices in our homes, and hoverboards even exist...kinda! So how on earth are we so technologically behind when it comes to recording our data in the laboratory? If you teleported someone from the past into most aspects of our present, they would be amazed by the overwhelming leaps and bounds that we have made, but if you did the same thing with a laboratory, it might be harder to gauge that level of progress.

So why aren’t universities falling over themselves to implement ELNs? Surely there is an ELN out there to “rule them all?”. Unfortunately, Sauron doesn’t deal in the ELN business, and as such, this is a much more complicated affair.

### Choice The hardest choices require the strongest will

There are over 80 active ELN vendors on the market. How on earth are you supposed to wade through those to figure out which one you want to use? Or even, which one(s) would even be appropriate for the research you want to undertake?

It takes time to implement and learn any new system, and that is frequently a commodity that researchers lack

### Diversity There is no ELN to rule them all!

The places where ELNs have been most successfully implemented are typically in industry. Now, some of this will obviously be because they have the money and more potential to persuade employees to use them, but the other much bigger reason is because often they are undertaking the same sort of work, which means if they can find an ELN that works for them, it can be implemented across the company. However, when we consider universities, they teach a range of sciences at an undergraduate level, which in itself would make it difficult to procure an ELN that would be useful for chemists, biologists, physicists, pharmacologists etc., just in terms of considering their teaching labs.

When you consider the wider picture of the vast range of PhD and postgraduate research that goes on at universities, it would be impossible to choose an ELN that would support all those different requirements, and you would either end up with something far too generic, or something that was too specific to one subject and didn’t cater for all the rest.

### Cost A burden to bear

Cost is ALWAYS going to be a huge barrier. The cost for licensing fees, additional infrastructure costs, e.g., computers in the lab, maintenance costs, and potential future development costs. These are a big commitment, and finances aren’t always available, and even if they are, the commitment to spend a large amount of money on implementing a new system is always going to be tricky, and let’s not even start on how difficult it could be to persuade a procurement department to agree to buy one...



# Got an idea to solve a data problem?

Speak to us!



You can reach the team through [psdi@soton.ac.uk](mailto:psdi@soton.ac.uk) and we will connect you





# Acknowledgements



**Thank you to everyone who has contributed to PSDI**

# PSDI & Personal Details - Questions

 [www.psd.ac.uk](http://www.psd.ac.uk)

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<https://www.jiscmail.ac.uk/PSDI>



[linktr.ee/samanthakanza](https://linktr.ee/samanthakanza)