

IT Services

Introduction to Active Research Data Management

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Who is Scientific IT Services?





□ A section of ETHZ IT Services

• Over 40 experts in various areas of scientific computing

□ With a background in different areas of science



Tell us a bit about yourselves

□ Your affiliation

□ Your research topic





Overview of today's workshop





Sample & protocol management



Data & Metadata





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Overview of active research data management



The data life cycle



Long term preservation:

Annotate, store, backup data at the end of a project or after publication



Open Science and Open Research Data



How can we share data in a FAIR way?

A few generic data repositories recommended by SNSF









Prepare to meet FAIR requirements when data are generated



Data and information generation during a research project



The "data spread": a common scenario in academic institutions















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The "data spread": a common scenario in academic institutions



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The "data spread": a common scenario in academic institutions



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How can we take care of the individual components and how can we bring things together?









Management of samples and protocols



Management of materials and samples

What?

- □ Biological samples
- □ Chemical samples
- □ Materials
- Devices
-
- How?

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ORACLE

FileMaker

Management of protocols

What?

- □ Step by step description of procedure
- Experimental/computational parameters (e.g. temperature, time, etc.)
- □ Machine used (experimental)
- □ OS, program, version, etc. (calculation)

How?





Laboratory Information Management System (LIMS)

□ LIMS are software for managing laboratory operations:

- **sample tracking** (*info about samples and about their storage*)
- sample data tracking (upload of data measured from samples, e.g. sequencing data, NMR, MS, etc.)
- **protocol management** (info about sample preparation/handling)

□ LIMS were first used in companies for tracking the growing number of samples.

□ LIMS were originally stand-alone solutions, which had to be integrated with other solutions such as ELNs. Nowadays **ELNs and LIMS are often combined** in one platform.





□ ETH ITS provides wiki services:



https://ethz.ch/services/en/it-services/catalogue/web-application-hosting/wiki.html



Size of Confluence Space/ git repository	Yearly price
<2 GB	free
<10 GB	300 CHF
<50 GB	1000 CHF

□ Some departments and/or institutes host their own wiki. Always contact your ISG for info.



Example of confluence wiki use in SIS

≡ === zürich Spaces - People Calend	lars Creat	e		Search	۹ 🛛 🕈 🕚
	☆	Dashboard / / ope	• – –	it な Save <u>f</u> or later	<u> </u>
🛱 Calendars		Created by Barillari Cate	rina (ID SIS), last modified less than a minu	ite ago	
PAGE TREE					
> administration		Location	Zurich, HG F33.1		
> customers		Time	09:00-13:00		
> How-To's		Program	1. introduction to openBIS		
> organisation			2. How to manage the lab invento	ry of materials and samp	bles
> outreach			3. How to manage lab protocols4. How to record experiments in t	he Electronic Lab Noteb	ook & upload data
 Personalized Health Data Services (PHdS) 			5. How to analyse data stored in c		
> processes	Ш	Participants			
> projects		Training material	https://gitlab.ethz.ch/sis-rdm-train	ing/openbis-training	
> services					
 SIS wiki organisation proposal 					
 trainings 					
✓ openBIS trainings		Like Be the first to	like this		No labels 🆠
• 2019.09.24					
• 2019.10.09		Write a comm	ient		
• 2020.01.23					
Organisational aspects of courses					
Space tools	«		Powered by Atlassian Confluence 6.15	5.9 · Report a bug · Atla	ssian News

Example of versioning in wiki

	/ 2020 History			← View Page	☆ Save <u>f</u> or later ····
Compa	re selected versions				
	Version	Published	Changed By	Comment	Actions
	CURRENT (v. 17)	Jun 11, 2020 16:33	Luetcke Henry (ID SIS)		
	v. 16	Jun 11, 2020 15:44	🜍 Plamada Andrei Valentin (ID SIS)		Restore
	v. 15	Jun 09, 2020 08:17	🜍 Plamada Andrei Valentin (ID SIS)		Restore
	v. 14	Jun 08, 2020 12:06	🜍 Plamada Andrei Valentin (ID SIS)		Restore
	v. 13	Jun 08, 2020 11:51	🜍 Plamada Andrei Valentin (ID SIS)		Restore
	v. 12	Jun 08, 2020 11:48	🜍 Plamada Andrei Valentin (ID SIS)		Restore
	v. 11	Jun 08, 2020 11:46	Plamada Andrei Valentin (ID SIS)		Restore
	v. 10	Jun 05, 2020 14:56	🜍 Plamada Andrei Valentin (ID SIS)		Restore
	v. 9	May 22, 2020 10:58	🜍 Plamada Andrei Valentin (ID SIS)	email update	Restore
	v. 8	May 22, 2020 10:58	Plamada Andrei Valentin (ID SIS)		Restore
	v. 7	May 22, 2020 10:46	🜍 Plamada Andrei Valentin (ID SIS)		Restore
	v. 6	May 18, 2020 14:29	🜍 Plamada Andrei Valentin (ID SIS)		Restore
	v. 5	May 18, 2020 14:28	Plamada Andrei Valentin (ID SIS)		Restore
	v. 4	May 15, 2020 14:29	🜍 Plamada Andrei Valentin (ID SIS)		Restore
	v. 3	Feb 14, 2020 14:34	🚱 Barillari Caterina (ID SIS)		Restore
	v. 2	Feb 14, 2020 14:34	🚱 Barillari Caterina (ID SIS)		Restore
	v. 1	Feb 14, 2020 14:32	🚱 Barillari Caterina (ID SIS)		Restore
Boturn to	Page Information				

Return to Page Information



Questions on Management of Samples and Protocols?







Management of Data & Metadata



Management of research data files

What?



Files / folders hierarchy

Review

Data management platform

openBIS



Processed - Processed

Results

File types and formats

□ File format: a **convention for encoding information** in a computer file

- □ Extensions typically *indicate* a specific file format
- □ Some file formats are preferable to others
- □ Stick to **non-proprietary** and **widely used** formats!
- Several general-purpose scientific data formats exist (e.g. HDF5, netCDF, FITS)

-	+
Binary	Text-based
Proprietary	Open
New kid on the block	Old as the hills
Compressed/encrypted	Uncompressed/unencrypted
Platform dependent	Interoperable
Complex	Simple



□ Goals of efficient file / folder organization:

- Easy to find something in the future (you, others)
- Easy to file something
- Save disk space (avoid multiple copies of files)
- Reusable components
- Avoid problems on different operating systems



Planning a good folder hierarchy

- Who? Individual, research group
- Where? Local disk, shared network drive
- Which operating system?
- What information are you going to search for?
- Avoid non-descriptive file and folder names (figure_02_summary_stats.png and not stats.png)
- Add descriptive text files to folders (→ Metadata)
- Document your hierarchy and file naming convention



Example hierarchy for a PhD project



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Example hierarchy for a research group





The project directory (for a computational project)

project	
- doc/	documentation for the study
 - data/ - raw_external/ - raw_internal/ - meta/	raw and primary data, essentially all input files, never edit!
- code/ - notebooks/	all code needed to go from input files to final results notebooks that document your day-to-day work
- intermediate/ - scratch/ - logs/	output files from different analysis steps, can be deleted temporary files that can be safely deleted or lost logs from the different analysis steps
- results/ - figures/ - tables/ - reports/	output from workflows and analyses
 - Snakefile - config.yml - environment.yml - Dockerfile	project workflow, carries out analysis contained in code/ configuration of the project workflow software dependencies list, used to create a project environment recipe to create a project container

Working in projects R Studio Sublime Text Visual Studio Code Visual Studio Code

Noble WS (2009) A Quick Guide to Organizing Computational Biology Projects. PLoS Comput Biol 5(7): e1000424



A project in ATOM

	Dockerfile — ~/Documents/project_template	
Project Remot	te × Dockerfile ×	
✓ ↓ project_template	1 FROM ubuntu:16.04-	
> Code	2 LABEL description = "Lightweight image with Conda, Jupyter Notebook and Snakemake"-	
> 🖬 data	3 ¬ 4 # Install Miniconda3 and prerequisites¬	
> 🖬 doc	5 RUN apt-get update &	
> intermediate	6apt-get install -yno-install-recommends bzip2 curl ca-certificates	
> 💼 logs	7 RUN curl https://repo.continuum.io/miniconda/Miniconda3-4.5.11-Linux-x86_64.sh -0 && \- 8 bash Miniconda3-4.5.11-Linux-x86_64.sh -bf -p /opt/miniconda3/ && \-	
> notebooks	9 ···· rm Miniconda3-4.5.11-Linux-x86_64.sh	
> in results	10 -	
> scratch	11 # Add Conda to PATH-	
,ftpconfig	12 ENV PATH="/opt/miniconda3/bin:\${PATH}" 13	
igitignore	14 # Use bash as shell~	
config.yml	15 SHELL ["/bin/bash", "-c"]¬	
Dockerfile		
	17 # Set up the Conda environment 18 COPY environment.yml.	
environment.yml	19 RUN conda env update – n root –f environment.yml && \∽	
I README.md	20 ····conda clean —all-	
Snakefile	21 -	
	22 # Install Jupyter Notebook and set default user to UID 1000- 23 RUN pip installno-cache-dir notebook==5.*	
	24 ENV NB_USER nbuser	
	25 ENV NB_UID 1000-	
	26 - 27 RUN adduserdisabled-passwordno-create-home \	
	28 ····	
	29	
		 日 ×
		• H •
	liv433l:project_template arasmus\$ pwd /Users/arasmus/Documents/projects/project_template	
	liv433l:project_template arasmus\$	
+ 🗔 🖂 🗙 Dockerfile 22:4	6	LF UTF-8 Dockerfile git+ 🎾 master 🗘 Fetch 🖹 1 file 🔰



□ Keep path names short (< 256 characters)

□ Recommendation for file names:

- Unique, reflect content (if possible)
- Use only ASCII characters
- Not include spaces
- Be aware of case sensitivity
- □ Bad examples:
 - data%20management%20plan.docx
 - sup figure 2.png
 - Iab meeting 19.10.2021.pptx

Good examples:

- Data_management_plan_SNF.docx
- sup_figure_02_summary_stats.png
- Iab_meeting_2021-10-19.pptx

- □ Use links / shortcuts to avoid duplications
- □ Use tags for orthogonal classifications
- □ Create template folders
- □ Some tools for automated file organization:
 - Mac: Hazel (<u>https://www.noodlesoft.com/</u>)
 - PC: DropIt (<u>http://www.dropitproject.com/</u>)





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Batch renaming of files

□ Windows

- Bulk Rename Utility (<u>www.bulkrenameutility.co.uk</u>)
- Advanced Renamer (<u>www.advancedrenamer.com</u>)
- Command prompt / PowerShell scripts

□ macOS

- Finder rename functionality
- Automator
- Command line / scripts

Linux

- Command line utility rename
- Métamorphose (<u>http://file-folder-ren.sourceforge.net/</u>)



ame	Rename Finder Items:	^	Date Modified	Size	Kind
a file_00001.tif			4 May 2018, 14:16	532 KB	TIFF image
a file_00002.tif	Replace Text O		4 May 2018, 14:21	17.3 MB	TIFF image
a file_00003.tif	Find: file_ Replace with: 2018-06-06_		4 May 2018, 14:24	17.3 MB	TIFF image
a file_00004.tif		_	4 May 2018, 14:25	5.3 MB	TIFF image
a file_00005.tif	Example: 2018-06-06_00001.tif Cancel Rename		4 May 2018, 14:27	3.4 MB	TIFF image
a file_00006.tif		_	4 May 2018, 14:28	3.4 MB	TIFF image
a file_00007.tif			4 May 2018, 14:29	3.4 MB	TIFF image
a file_00008.tif			4 May 2018, 14:29	3.4 MB	TIFF image
a file_00009.tif			4 May 2018, 14:29	3.4 MB	TIFF image
a file_00010.tif			4 May 2018, 14:29	3.4 MB	TIFF image
a file_00011.tif			4 May 2018, 14:29	3.4 MB	TIFF image
a file_00012.tif			4 May 2018, 14:30	3.4 MB	TIFF image
a file_00013.tif			4 May 2018, 14:30	3.4 MB	TIFF image
a file_00014.tif			4 May 2018, 14:30	3.4 MB	TIFF image
a file_00015.tif			4 May 2018, 14:30	3.4 MB	TIFF image
a file_00016.tif			4 May 2018, 14:31	3.4 MB	TIFF image
a file_00017.tif			4 May 2018, 14:31	3.4 MB	TIFF image
file_00018.tif			4 May 2018, 14:31	3.4 MB	TIFF image
a file_00019.tif			4 May 2018, 14:31	3.4 MB	TIFF image
file_00020.tif			4 May 2018, 14:32	3.4 MB	TIFF image
a file_00021.tif			4 May 2018, 14:32	3.4 MB	TIFF image
file_00022.tif			4 May 2018, 14:32	3.4 MB	TIFF image
file_00023.tif			4 May 2018, 14:32	3.4 MB	TIFF image
file_00024.tif			4 May 2018, 14:33	3.4 MB	TIFF image
file_00025.tif			4 May 2018, 14:33	3.4 MB	TIFF image
a file_00026.tif			4 May 2018, 14:33	3.4 MB	TIFF image
file_00027.tif			4 May 2018, 14:34	3.4 MB	TIFF image
file_00028.tif			4 May 2018, 14:34	3.4 MB	TIFF image
file_00029.tif			4 May 2018, 14:34	3.4 MB	TIFF image
a file_00030.tif			4 May 2018, 14:35	3.4 MB	TIFF image
a file_00031.tif			4 May 2018, 14:35	3.4 MB	TIFF image
a file_00032.tif			4 May 2018, 14:35	3.4 MB	TIFF image
a file_00033.tif			4 May 2018, 14:35	3.4 MB	TIFF image
a file 00034.tif			4 May 2018, 14:36	3.4 MB	TIFF image

File validation and compression

- □ Checksum algorithms are useful to verify data integrity
 - For datasets stored over long time periods
 - When transferring from one storage to another
 - Examples: cksum, md5sum, sha1sum
- Compression algorithms encode information in fewer bits than the original (bit-rate reduction)
 - Lossless vs. lossy compression
 - Lossy compression may lead to distortion / loss in quality but compression rates are typically much higher
 - Trade-off between processing time and disk space
 - Examples: zip, gzip, specific formats (TIFF, HDF5)
- □ Archiving combines many (small) files into a single (large) file
 - Nowadays mainly used together with compression
 - Required for long-term storage (LTS) and efficient data transfer
 - Examples: Tape Archive format (tar)



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Metadata

- □ Metadata is the *data about your data* (a.k.a. data model)
- □ Use of structured metadata **facilitates data organization** and searches
- □ (Machine-readable) Metadata is a key element of the FAIR data principles
- Existing metadata schemas are preferred (can be extended, if necessary)







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Metadata

Example for general research data: DataCite Metadata schema

Table 1: DataCite Mandatory Properties

ID	Property	Obligation
1	Identifier (with mandatory type sub-property)	м
2	Creator (with optional given name, family name, name identifier and affiliation sub-properties)	М
3	Title (with optional type sub-properties)	м
4	Publisher	м
5	PublicationYear	м
10	ResourceType (with mandatory general type description sub- property)	м

https://schema.datacite.org/

Table 2: DataCite Recommended and Optional Properties

ID	Property	Obligation
6	Subject (with scheme sub-property)	R
7	Contributor (with optional given name, family name, name identifier and affiliation sub-properties)	R
8	Date (with type sub-property)	R
9	Language	0
11	AlternateIdentifier (with type sub-property)	0
12	RelatedIdentifier (with type and relation type sub-properties)	R
13	Size	0
14	Format	0
15	Version	0
16	Rights	0
17	Description (with type sub-property)	R
18	GeoLocation (with point, box and polygon sub-properties)	R
19	FundingReference (with name, identifier, and award related sub- properties)	0

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Metadata



Example for discipline-specific data: **OME Metadata schema**

https://www.openmicroscopy.org/Schemas/



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ManufacturerSpec (extension base)


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https://idr.openmicroscopy.org/webclient/?show=project-1304

The Research Data Alliance (RDA) has created a community-maintained catalog of metadata standards: <u>https://rdamsc.bath.ac.uk/</u>

The catalog contains metadata standards that have been established in different research fields as well as relevant tools and use cases. Consider the following short descriptions of hypothetical research projects. Based on the description, try to identify one or several suitable standards from the metadata catalog.

Case 1: An online survey / questionnaire about attitudes towards climate change in different age groups. Documentation of the survey responses.



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□ Data Documentation Initiative (DDI), version 2 or 3

An international standard for describing surveys, questionnaires, statistical data files, and social sciences study-level information



Case 2: A study on the diversity and geographic distribution of butterflies in the Swiss Alps. Documentation of the recorded occurrences.

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□ Darwin Core (DwC)

Ecological Metadata Language (EML)

- Darwin Core is a standard to facilitate the sharing of information about biological diversity. DwC includes a glossary of terms, and documentation providing reference definitions, examples, and commentary. It is an extension of Dublin Core.
- EML defines a vocabulary and a syntax for documenting research data. It is in widespread use in the earth and environmental sciences. EML includes modules for describing the spatial, temporal, taxonomic, and thematic extent of data, for describing research methods and protocols, for describing the structure and content of data, and for precisely annotating data with semantic vocabularies.



Case 3: The crystal structure of a novel viral protein determined by X-Ray crystallography. Documentation of the protein structure.



Case 3: The crystal structure of a novel viral protein determined by X-Ray crystallography. Documentation of the protein structure.

Protein Data Bank Exchange Dictionary and the Macromolecular Crystallographic Information Framework (PDBx/mmCIF)





FAIRsharing.org provides an even more extensive resource of metadata standards, vocabularies, taxonomies etc.



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□ Types of metadata

- Descriptive (Title, author, identifier)
- Administrative (License)
- Technical (File size, checksums)
- Structural (Relation to other data)

□ Machine-readable metadata

- Annotation based on common standards
- Controlled vocabularies, taxonomies

Filters

Synonym query expansion 2 O On O Off Sources 🛛 **Special Collections** Full Text Availability Agricola (USDA/NAL) All BMJ 🛙 In Europe PMC 🛙 Chinese biological abstracts All manuscripts 2 Open Access 2 CiteXplore records EuroFIR @ Patents Europe PMC manuscripts 2 Preprint records PubMed/MEDLINE (NLM) Publication Type Language 🛛 ~ 0 0 Choose one Publication Type Choose one Language Choose one Language CC License 🛛 Afrikaans Albanian Choose one License Type 🗸 🛈 Arabic Armenian Article Sections Azeri Choose a section type Bosnian Bulgarian Catalan Data Links and Data Citations Chinese Czech Danish Choose one Link/Citation type Dutch English Esperanto External Links Estonian Finnish French ~ 0 Choose one External Links Provider Georgian

https://europepmc.org/advancesearch

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Machine-readable metadata

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- Controlled vocabularies, taxonomies
- Standardized metadata are the basis for ontologies (knowledge representations)

Basic Register of Thesauri, Ontologies & Classifications EMBL-EBI Ontology Lookup Service



Visualized term: blood (http://purl.obolibrary.org/obo/UBERON_0000178)



Types of metadata

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EMBL-EBI Ontology Lookup Service

□ How to apply metadata?

- File header (e.g. TIFF, netCDF)
- Sidecar files (e.g. XML, JSON)
- As columns in a database
- README text files
- Apply metadata early in your workflow (ideally during acquisition)

- □ System that allows **structured organization** of data
- Data is described by **metadata**
- □ Usually more FAIR-compliant than Files / Folders
- □ Searchable, scalable, flexible
- □ Allows user rights management
- □ Back up procedures are easily implemented

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Unsorted	Percival, Colin	Naive differences of executable code		26/08/11	complete spatial memory safety for C
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Annotations Databases	🔆 🔹 🖪 Murdoch, Steven J.; Dr	Chip and PIN is Broken	2010 2010 IEEE Symposium	26/12/10	View research catalog entry for this paper
Development Tools Information Retrieval / Se	🔆 🔹 🖺 Zhang, Zhenjie; Hadjie	Bed -Tree : An All-Purpose Index Structure for String Similarity Search Based on Edit Distance	2010 SIGMOD 2010	09/11/10	Proc. Title: ACM Sigplan Notices
Mendeley Presentations	🔆 🔹 🖪 Smirnov, Ilia	Overview of Stemming Algorithms	2008	04/11/10	Year: 2009 Pages:
Mendeley Research Misc Comp Sci	🕁 🔹 🖪 Dunning, Ted	Accurate Methods for the Statistics of Surprise and Coincidence	1993 Computational Linguistics	22/10/10	Abstract:
👖 mitalk	🔆 🔹 🖺 Kumar, Ravi; Raghava	Extracting large-scale knowledge bases from the web	1999 Proceedings of the 25th VLD	14/10/10	Tags:
Non-Comp Sci Programming Languages	☆ ● 🖻	Roots of the REST/SOAP Debate		12/10/10	
Reading Lists References / Manuals	🔆 🔹 🖻 Okazaki, Naoaki	Marginal Containers Covering Relevant Items (MACCORI)		02/05/10	Keywords: buffer overflows; c; spatial memory safety
Social Web Software Engineering	Gabrilovich, Evgeniy;	Wikipedia-based Semantic Interpretation for Natural Language Processing	2009 Journal of Artifical Intelli	24/02/10	City:
Software Libraries Task Tracker	🔆 🔹 🖺 Adobe System Incorpo	PDF Reference, version 1.7	2006	29/01/10	E dia ana
Create Folder	☆ •	Search Engine Book Slides		11/12/09	Editors:
ROUPS Document Metadata Extra	🔆 🔹 🛃 Smith, Ray	Hybrid Page Layout Analysis via Tab-Stop Detection	2009	23/09/09	Publisher:
DURA MAKIN' IT research papers	🔆 🔹 🖺 Haveliwala, Taher H	Topic-Sensitive PageRank	Context	19/05/09	URL:
MapReduce algorithms Mendeley	🔆 🔹 🖺 Pasula, Hanna; Marthi	Identity Uncertainty and Citation Matching		19/05/09	http://dl.acm.org/citation.cfm?id=1542504 Add URL
Mendeley Advisor Group Mendeley Book Club	🕁 🔹 🖺 He, Junfeng	On the Difficulty of Nearest Neighbor Search	2012	Jun 19	Catalog IDs
Mendeley Books MoSql Summer	🔆 🔹 🖺 Shute, Jeff; Oancea, Mi	Distributed RDBMS Supporting Google ' s Ad Business Today ' s Talk	2012	May 30	DOI:
Service & Cloud Architecture StyleWiz	🕁 🔹 🛐 Tallam, Sriraman; Cou	Safe ICF : Pointer Safe and Unwinding aware Identical Code Folding in the Gold Linker	2012	May 15	Files:

- □ System that allows **structured organization** of data
- Data is described by **metadata**
- □ Usually more FAIR-compliant than Files / Folders
- □ Searchable, scalable, flexible
- □ Allows user rights management
- □ Back up procedures are easily implemented
- **Examples**



Generic

ite





PostgreSQ

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Generic database workflow



Where is my data???

			DAT	AB	ASI			
Table 1		1	Table 2		Table 3			
Field 1	Field 2	Field 3	Field 1	Field 2	Field 3	Field 1	Field 2	Field 3
Value								
Value								
Value								
	Value							

Metadata + Data

- Structured data required
- DB-specific data (array DBs)
- No conventional file access

Metadata + Link to Data Files



Comparison: folder hierarchy vs. databases





	File / folder Hierarchy	Database System
Easy to use	Yes	Initial learning curve
Flexibility	High	Limited
Scalability (data volume)	Limited	Yes
Scalability (users)	Limited	Yes
Versioning included	No	Yes
Backup included	No	Yes

Data storage – Your options ...

External hard disks are cheap but unreliable and don't scale!





Data storage – Your options ...

- External hard disks are cheap but unreliable and don't scale! Polybox / SwitchDrive
- Network Attached Storage (NAS)
 - NAS offering from IT Services always check with your ISG first
- Cost Defined Storage (CDS)
 - For very large storage requirements (>100 TB)
- Long-term Storage (LTS)
 - Tape storage for data worthy of preservation ("Datenendlager")
 - Data should be compressed and sized between 10 200 GB
- Also consider backups (ideally follow 3-2-1 rule)
 - RAID is not a backup!

Details: https://ethz.ch/services/en/it-services/catalogue/storage.html

ETH news on cloud storage regulations: https://bit.ly/3BoQQD1



Array of

Disks





Questions on Management of Data Files?







Time for a break



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Electronic Laboratory Notebooks



Experimental description / notes

What to document?

Goals

Materials

- Methods
 - Experimental/computational procedure
 - Analysis procedures
- Results

Links to data

How?



Paper laboratory notebook



Electronic laboratory notebook (ELN)



Definition of ELN & requirements

An *electronic laboratory notebook* (also known as *electronic lab notebook* or *ELN*) is a software program or package designed to replace more traditional paper laboratory notebook. Laboratory notebooks in general are used by scientists and technicians to document, store, retrieve, and share fully electronic laboratory records in ways that meet all legal, regulatory, technical and scientific requirements.

Legal requirements

Electronic lab notebooks used for development or research in regulated industries, such as medical devices or pharmaceuticals, are expected to comply with the **21 CRF Part 11 FDA** regulations: <u>https://www.accessdata.fda.gov/scripts/cdrh/cfdocs/cfcfr/cfrsearch.cfm?cfrpart=11</u>

To our knowledge, in academia, there is no such requirement, but this can vary from one Institution to another.

Source: https://www.limswiki.org/index.php/Electronic_laboratory_notebook

ETHZ Regulations

□ ETHZ RDM guidelines came into action on 01.07.2022:

https://rechtssammlung.sp.ethz.ch/Dokumente/414.2en.pdf

Art. 5 Data collection and processing

¹ Digital data that are in the process of being collected or processed must be stored such that data can be restored in case of hardware problems or human error. Using storage systems centrally supplied by ETH fulfils this criterion. If such data are too big for being stored redundantly in the available infrastructure, researchers must be able to recreate them using existing code and documentation when required.

² Access rights to the storage system must be specified and regularly updated, e.g. upon the start of a new project. The scientific needs of all researchers working with the data must be considered by the access right system. Unauthorised access must be prevented by suitable technical and organisational measures, such as ETH Zurich's identity and access management system.

³ In order to ensure long-term accessibility and reusability, the use of well-documented, nonproprietary file formats is recommended.

⁴ The structure and the processing steps of all *Research Data* must be digitally documented in order to ensure adherence to the *FAIR principles*. Where documentation includes a lab journal, Electronic Laboratory Notebooks (ELN) are recommended.

ELNs vs. paper notebook

□ Advantages of ELNs over paper notebooks:

- 1. Sharing
- 2. Most ELNs have rights management
- 3. Most ELNs keep track of changes
- 4. Search functionality
- 5. Easier to link digital data
- 6. No issues with handwriting
- 7. Can be backed up

□ Disadvantages of ELNs over paper notebooks:

- 1. Require change in working mode
- 2. Some ELNs have a learning curve

Note-keeping applications



□ Most solutions are moving towards cloud-based services

□ Straight replacement of paper notebooks with some added values (e.g. sharing, searching)

□ Popular in academia due to ease of use

□ Do not provide a solution for data management

□ Do not comply with **21 CRF Part 11 FDA** regulations



ELNs with database back end



□ Structured ELNs compared to note-keeping applications

- Additional functionalities compared to note-keeping applications (e.g. workflow management, chemical structures drawing, etc)
- □ Can be discipline-specific or cross-disciplines
- □ Some systems offer an all-in-one solution for RDM

□ Many systems comply with **21 CRF Part 11 FDA** regulations

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Simplified illustration of a commonly used ELN architecture



Considerations for implementing electronic laboratory notebooks in an academic research environment. Nat Protoc 17, 179–189 (2022). https://doi.org/10.1038/s41596-021-00645-8

Which ELN to choose?

- The ELNs offer on the market is very large. Answering some of these questions might help you restricting the choice:
 - 1. Is it for personal use or group use?
 - 2. Can I/we use a cloud-based solution?
 - 3. Do I/we need specific features?
 - 4. What do I/we want to do with the ELN? (e.g. only write experimental descriptions, manage samples, manage data how big?, etc.)
 - 5. Commercial v. open-source
 - 6. Budget?
 - 7. Can I export my data?
 - How to pick an Electronic Laboratory Notebook: <u>https://www.nature.com/articles/d41586-018-05895-3</u>
 - Harvard University Comparison Grid: <u>https://datamanagement.hms.harvard.edu/electronic-lab-notebooks</u>

ELN guidelines for academic research labs

As part of the national DLCM project, ETH Zurich and EPFL prepared some ELN guidelines, available from: <u>https://www.dlcm.ch/services/dlcm-eln</u>

Stages of introduction of an ELN in an academic lab:

- 1. Initialization
- 2. Analysis of laboratory needs
- 3. Pilot phase
- 4. Production phase (*migration of existing databases or information; customization, integration with measuring instruments, integration with analysis pipelines and workflows*).



What is needed for a successful introduction of an ELN in an academic lab?

□ Based on our experience at ETHZ:

- 1. Commitment from the PI
- 2. Lead person in the lab who drives the process
- 3. RDM expert support

□ Examples of ELN implementation in academic institutions:

- Considerations for implementing electronic laboratory notebooks in an academic research environment. Nat Protoc 17, 179–189 (2022). <u>https://doi.org/10.1038/s41596-021-00645-8</u>
- Institutional ELN/LIMS deployment. EMBO Rep. 2020 Mar 4; 21(3): e49862. doi: <u>10.15252/embr.201949862</u>



Slow adoption of ELNs/LIMS in academia

The Barriers	Research lab	Diagnostic lab	
Limited budget	352		23
Time needed for implementation	235		21
Changes to existing working habits	266		25
Concerns about ELN being a system in the cloud	215		22
Contains features we do not need	130	1	7
Software in English only	76	I	10
No need for improvement	112	1	7

Source: Potential uses of ELNs in Academia survey (University of Southampton). J. Cheminform (2017) 9:31.

In our experience at ETHZ, the main reasons are:

- 1. Change in working habits needed.
- 2. Time needed for introduction in a lab.
- 3. Concerns about data retrieval when leaving the lab.



Questions on Electronic Lab Notebooks?







The ETH Scientific IT Services data management solution for research groups



openBIS info

Developed at **ETHZ** since 2007.

Used in **different quantitative scientific disciplines** by users inside the **ETH domain** and **beyond**.






openBIS: a complete solution towards FAIR data management





https://openbis.ch



Lab samples & materials

Inventory management

Lab equipment

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Barcode reader





Electronic Lab Notebook





Data management



Data archiving and unarchiving from LTS via openBIS (for ETHZ)

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Access to archived data (for ETHZ)

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ETH zürich

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Data publication: export to ETH Research Collection (for ETHZ)







Data publication: export to Zenodo

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RDM services @ ETHZ

□ ETH-wide services provided since 2018

ETH Research Data Hub (RDH)

ETH Departmental Data Hub (DDH) ETH Research Data Node (RDN)







For groups of a certain department/institute

- · Centrally managed
- Shared resource
- Department customization

For single ETH research groups

- Individually managed
- Dedicated resource
- Individual customization

ETH zürich

A national RDM service for the academic community

□ Service establishment funded by a swissunsiversities P5 project

□ Project: 2018-2020

□ Service start: 2021





https://openrdm.swiss/

What do the SIS's RDM services provide?



How do the SIS's RDM services help researchers?





Questions on openBIS and RDM services provided by SIS?





Code management

□ Code management is an integral part of active data management

We did not forget about it, it is a topic for next week's workshop on *Reproducible scientific computing and data analysis*



Take home messages



□ Data management should be an integral part of you work

- □ Try to establish standard procedures in the group, if not yet in place
- □ RDM requires **WORK** & **TIME**, but the time spent on this is an **investment** for the future!



Contact us for consultations / trainings on: data management, version control, reproducible computational workflows or data science support

sis.helpdesk@ethz.ch





Why is this all important for me?

Ok, time to start writing up my **PhD thesis**. Wow, 3 years of work. Let's begin..

to check the analysis I presented in this paper. Now, where are they?

I have a request from a reader

These results will make an excellent **publication**! Let me find all the data I need



My ex-PhD supervisor wants to know where my data are, so their new student can carry on my work

□ If you have well annotated, organized and backed up you data over time, all this will be easy!



Contacts

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https://twitter.com/ETH_SIS?lang=en



Any final questions on what we have seen today?



Feedback: <u>https://www.umfrageonline.ch/s/a13b937</u>



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