Supplementary Information:

Draft on Specifications for Electronic Laboratory Notebooks (ELN) in the Photon and Neutron Community

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Discussion of (some) existing ELNs

This section gives an overview on Electronic Lab Notebooks (ELNs), that are of interest for usage at large-scale research facilities and could be of interest for use cases that have related needs for the experimental documentation, e.g. integration of automatic input from machines, parallel editing and scalability.

Each of the following sections gives a concise overview of the concept and highlights the capabilities of a specific ELN.

Snip

Snip introduces a novel approach in the field of ELNs, catering to the nuanced demands of contemporary scientific research. It's designed to bridge the gap between diverse digital data and manual input, offering a user-friendly platform for researchers. Central to its functionality is the ability to merge digital snippets from various sources with hand-written annotations and sketches, creating a coherent and versatile documentation. This method enhances both the usability and interpretability of scientific records, encouraging collaboration and ease of understanding. By balancing technological integration with the simplicity of manual contributions, snip presents itself as a practical and adaptable tool in the landscape of scientific data documentation.

In its core design, snip stands out as a user-centric ELN, ingeniously tailored to meet the dynamic needs of modern research. It fosters global collaboration through real-time updates, allowing researchers from around the world to engage in fluid discussions and share insights instantaneously. Snip's versatility is further exhibited in its ability to ingest formalized snippets from experiments and analyses, integrating diverse data sources into a two-dimensional document. A hallmark of its innovative nature is the ad-hoc, free-form annotation capability via pen entry, enabling researchers to craft a creative collage that intertwines the empirical state of experiments with insightful opinions and interpretations. Additionally, snip incorporates a robust user management system, complete with a permissions structure, ensuring secure and efficient control over lab book access and edits.

As experimental research continues to advance at a rapid pace, propelled by technological breakthroughs and interdisciplinary collaborations, there arises a compelling need for innovation in the realm of documentation and data management. The intricate and diverse nature of modern scientific data – encompassing everything from intricate genomic sequences to extensive environmental data sets – calls for a documentation approach that transcends traditional boundaries. The limitations of paper-based methods become increasingly apparent in the face of such complexity, where they fall short in managing, integrating, and making sense of the multifaceted data generated. Today's research landscape, characterized by its dynamic and voluminous data production, demands a shift towards more sophisticated, digital solutions. These solutions must not only accommodate the sheer volume and variety of data but also enhance accessibility, analysis, and collaboration, thereby aligning with the evolving requirements of contemporary scientific inquiry.

The collaborative nature of contemporary science adds complexity to documentation, with projects often spanning multiple disciplines and locations. This necessitates tools that support both local measurement recording and remote collaboration. Essential now are technologies that enable online access and simultaneous data interaction by multiple users. Such advancements are crucial in the research community, not only for streamlining data management and teamwork but also for opening avenues to new research methods and discoveries.

Unlike the template-based systems that focus on rigid protocols and recipes, snip embraces a more dynamic and user-driven methodology. This approach is designed to cater to a wide range of scientific disciplines where experimentation is not always linear or predictable. In snip, users are not confined to predefined templates; instead, they have the creative freedom to document their research in a way that best suits their unique processes and findings. This flexibility allows for the documentation of non-standard experiments, ad-hoc observations, and innovative procedures that might not fit into the conventional template mold. Snip's design philosophy recognizes the diverse and often unpredictable nature of scientific research, offering a platform that adapts to the user's needs, encouraging creativity and personalized organization in the documentation process.

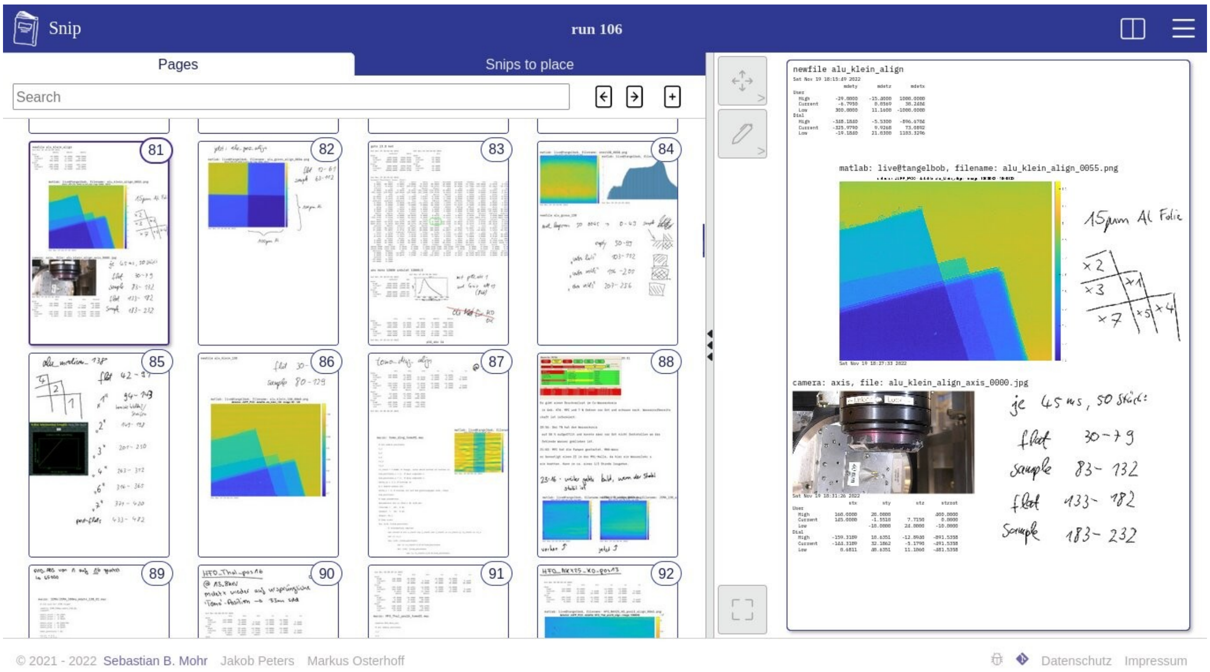

Figure snip1: On the left, overview of multiple pages in snip. On the right a single page is shown, this page shows handwritten notes and typed text, as well as imported pictures and a drawing.

Further enhancing snip's versatility in handling non-traditional experimental workflows is its unique feature of creating manually crafted, creative collages of experimental states, see figure snip1. These collages allow researchers to visually compile and juxtapose various aspects of their experiments – from raw data and images to handwritten insights – into a cohesive, yet flexible, narrative. This method is particularly effective in documenting ad-hoc experiments that do not follow predefined paths but evolve iteratively. By enabling researchers to assemble and reassemble these data snippets in a way that best represents their current understanding and hypotheses, snip not only aids in capturing the complexity of these experiments but also in visualizing the progression and shifts in research directions. This creative freedom in documentation goes beyond mere record-keeping; it becomes an integral part of the experimental journey, encouraging a deeper engagement with the research process and fostering a more comprehensive understanding of the outcomes.

Resources:

- Citation snip-Whitepaper: https://resolver.sub.uni-goettingen.de/purl?gro-2/142223
- Contact: Markus Osterhoff <mosterh1@gwdg.de>
- Repository: https://gitlab.gwdg.de/irp/snip/
- Production version: https://snip.roentgen.physik.uni-goettingen.de/

MLZ ELN (based on TUM Workbench)

Workbench is currently under development to be used as ELN solution at the Heinz Maier-Leibnitz Zentrum (MLZ), the national center for research with neutrons, located in Garching near Munich (www.mlz-garching.de). The aim is to seamlessly integrate the ELN into the existing, local instrument and software infrastructure, facilitating user access control, direct input from the instrument control system as well as an intuitive user interface. During the testing of existing software products for their compliance with the FAIR data criteria and the specific workflow at the MLZ, it became apparent that none of the available open source solutions meets all the critical requirements.

The MLZ ELN is based on the universal research data and project management platform *TUM Workbench* (https://www.ub.tum.de/workbench). This platform, is/was developed at the Technical University of Munich (TUM), and facilitates data management by enabling collaboration and semi-automatic documentation. Within DAPHNE4NFDI, we took the ELN part of *TUM Workbench* and currently develop it to meet the requirements discussed in the main part of this paper <https://doi.org/10.1080/08940886.2024.2432265> (see Table 1). The ELN has only been a small part of the TUM Workbench software package. Thus, it was rather basic and needs a lot of development work including improvements on the front- and backend structure.

The MLZ ELN is being developed to serve users on a wide range of neutron instruments offered at the MLZ. In a first step, the ELN is to the instrument control system NICOS (https://www.nicos-controls.org/), and it also obtains information from the **G**arc**h**ing **O**nline **S**ystem **T**ool (GhOST), the user office software managing proposal submission and the review and beam time allocation (system?) at MLZ. Workbench, connected to this system, allows automatic recording of information, which greatly facilitates the maintenance of the logbook. Even more important is the ability to automatically record instrument readings, experiment parameters, and a brief overview of measurement. Almost all instruments at MLZ are controlled by the Networked Instrument COntrol System (NICOS) (www.nicos-controls.org). NICOS allows automatic transfer of information to the MLZ ELN. This avoids possible errors in manually capturing experimental parameters and saves time. In the development of the MLZ ELN, much attention is paid to parallel editing capabilities for collaborative work and defining clear authentication and authorization procedures for which we develop a convenient and flexible role model.

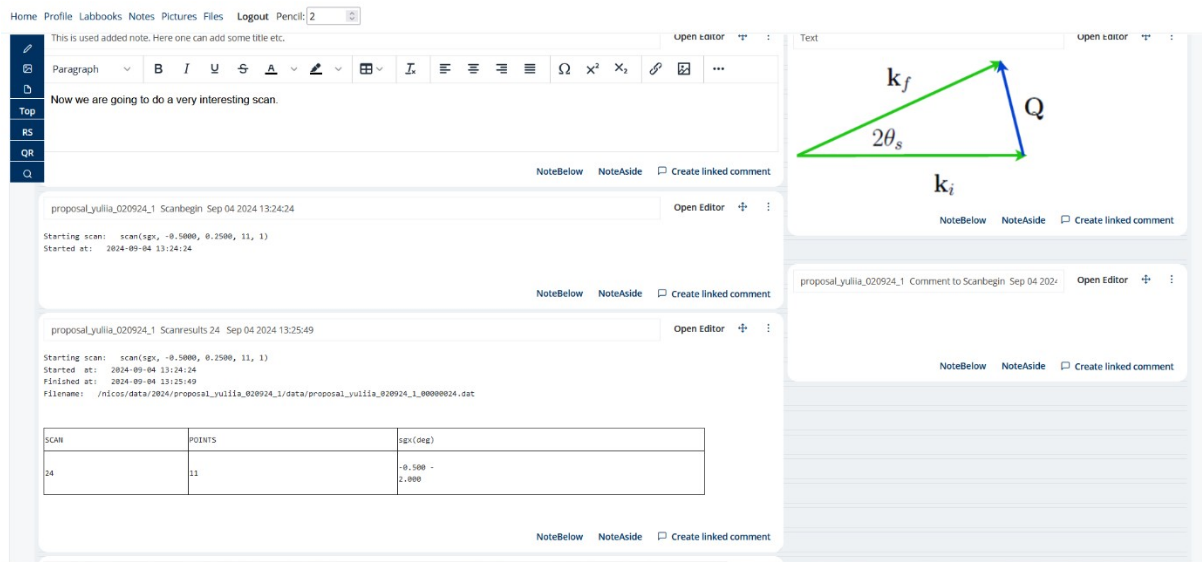

Figure bench1. Snapshot of the MLZ ELN with some typical features. Notes (marked as white boxes on grey background) can contain general text, figures, tables, etc. Comments to notes can be added.

MLZ ELN software will create an electronic logbook for each experimental beam time. The ELN entries, see figure bench1, are organized in 'Notes' which contain either instrument and scan information provided by the instrument control system or user annotations and entries, e.g. remarks on experiment conduction or preliminary analysis. Access rights and read/write and delete permissions for notes are organized via role models, details are still under discussion. For instance, it is discussed whether automatically created notes (e.g. by NICOS) should be editable by the user including even the possibility to delete such automatic messages for the sake of a more human-readable concise ELN. The backend being developed will allow us to adjust the role model depending on the decision made. Track changes, history and versioning are also included.

While the MLZ ELN based on TUM Workbench is still under active development, many of its elements have already been implemented and are being tested. Below is an overview of the main features:

- Data Input (Manual)
    - Input from multiple sources: Data entry into the ELN is possible from multiple sources via different interfaces. In addition to standard input from a desktop computer, it is possible to enter data from a mobile device, as well as import images from built-in cameras. Convenient features include the ability to create sketches or schematic drawings, as well as the ability to connect a portable tablet for drawing.
    - Parallel Input: A critical feature for larger user groups eventually including scientist participating remotely all around the world is the ability for parallel input by several users. Write locks and live-reload capabilities exclude that entries from one user/source are overwritten by others.
    - The application interface is simple and convenient: It is intuitive to create a new note or add a comment to an existing one, create a thumbnail, or import a screenshot or images. A text editor offers basic features known from other office applications.
- Data Ingestion from Instrument
    - MLZ uses a network based control system NICOSto operate neutron instruments. NICOS has an integrated service to post messages or graphically rendered results to the ELN. This greatly facilitates the documentation of the experiment by users and at the same time eliminates possible errors in manually entering measurement parameters.
- Data Management
    - Security, user access and ownership is controlled by a role model to prevail manipulation and enable cooperation in real time.
    - Users can collaborate on notes related to instrument data. Write-locks with live-reload for all users prevent mutual overwriting.
    - Track changes, restore versions.
    - Backup.
- ELN Access / Data Access
    - The ELN is accessible from anywhere, at any time, and from any device via the world wide web.
    - The MLZ ELN provides an SSO interface for Keycloak. Data can be accessed in an easy and reliable way.
    - Data can be annotated, tagged, and searched by full text.
    - Data can be exported to common formats, e.g., pdf, json, ELNFileFormat

myLog

In 2023, European XFEL GmbH (EuXFEL) replaced its previous ELN system, based on the PSI ELOG (https://elog.psi.ch/elog/) by a new integrated ELN instance called myLog (https://mylog.connect.xfel.eu) based on Zulip, a commercial team chat software solution (https://zulip.com/). The decision for this was motivated by the good experience that some EuXFEL groups had with Zulip for team communication: in particular its structure consisting of streams and topics, as well as the powerful text integration options, e.g. Media embedding, direct LaTeX support, programming code syntax highlighting, and programmable bots for automatic notifications.

On top, self-hosted Zulip instances became services with versatile integration to other service components of a facility, thanks to a REST API and with client libraries. Thanks to these requirements the myLog instance at EuXFEL is integrated with the metadata catalogue myMdC, the control system Karabo and the DAMNIT service for data analysis as shown in figure mylog1:

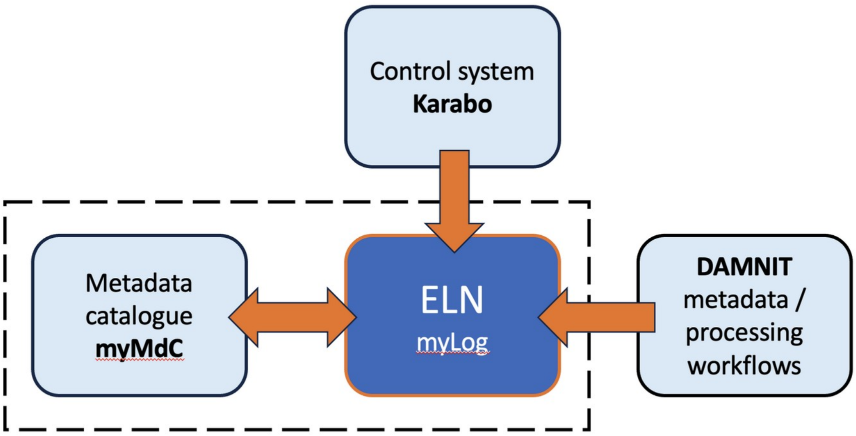

Figure mylog1: myLog is tightly integrated with the EuXFEL metadata catalogue and shares the actual ELN instance display, with editing capabilities from both interfaces. Other services, Karabo and DAMNIT, can export content like graphs and tables to a myLog instance.

The myLog service is made up of separate per-proposal ELN instances, which are streams in Zulip. The management of ELN instance members and visibility scope is realized through myMdC, such that experiment team members of a proposal become assigned to the ELN stream with full edit permissions. The view on the ELN content is mirrored and synchronized between myMdC and myLog.

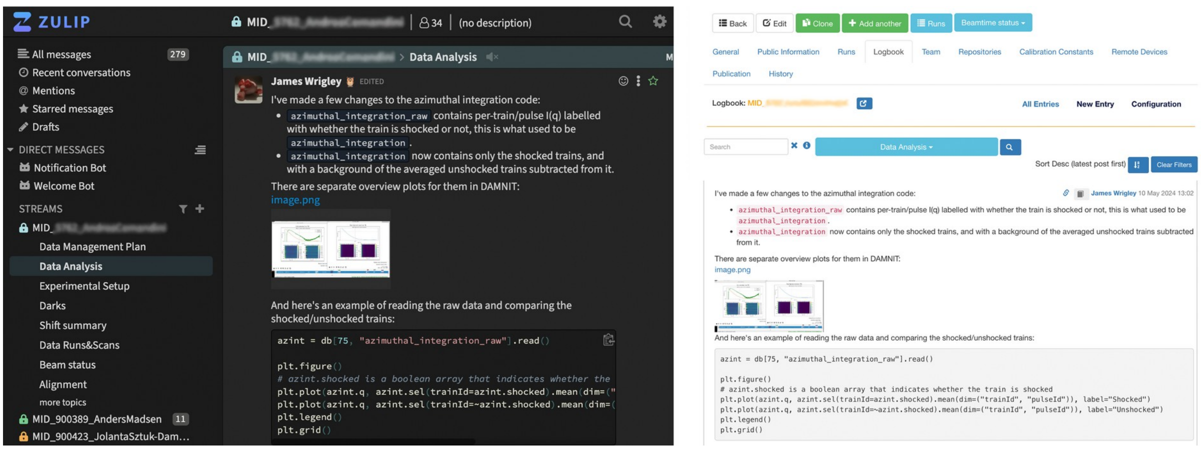

Figure mylog2: The same ELN entry as seen from the myLog interface (left) and from the logbook section of the metadata catalogue (right).

The myLog ELN is linked from the logbook view of myMdC (right panel in figure mylog2, link next to the Logbook name). All EuXFEL data support staff has read access to the myMdC logbook view, but not to the myLog view (left) unless explicitly added to the experiment team of a proposal.

While each proposal gets its own Zulip stream in the ELN system that can be seen as a logbook instance of its own, logical aspects/groups of the work to be logged get assigned to topics within the logbook (e.g. sample preparation, beam setup, data analysis etc.). In order to facilitate experiment and data analysis documentation workflows, both the control system and the DAMNIT tool can feed content into the myLog topics.

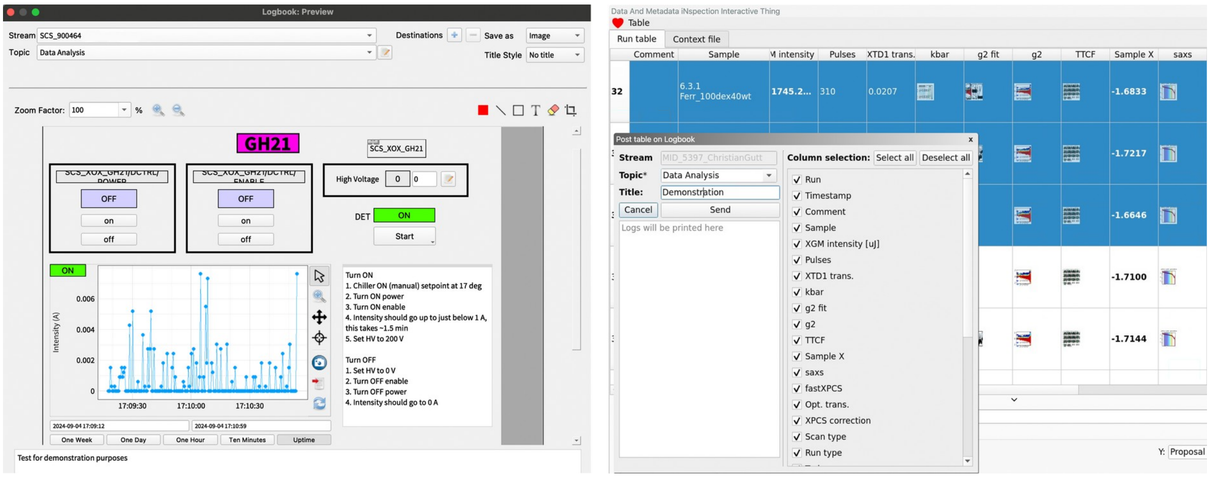

Figure mylog3: Examples of exporting content to myLog: a scene from the control system Karabo (left) and an overview table from the DAMNIT tool (right).

Information like graphs from quasi-real-time monitoring can be exported from scenes of the Karabo GUI (left panel of figure mylog3) and thus document “online” data analysis or other experimental parameters. In the near-online domain the DAMNIT software, which is also organized in per-proposal instances, collects metadata as soon as available from recorded data “runs” i.e. data files. DAMNIT can also manage data analysis workflows employing other software and collecting results from such processing steps. The tabular DAMNIT information – organized in runs per line and (meta)data variables of interest per column – can be selectively exported to myLog streams as well (right-hand panel figure mylog3).

Meanwhile myLog has been adopted by all EuXFEL instruments and their users. The integration features are being further developed in order to enhance user experience. The EuXFEL data department envisages myLog also as an important component for the implementation of Data Management Plans (DMPs). Communication through dedicated DMP topics in the proposal logbooks supported the planning of data management during selected experiments in a DMP pilot phase, spring 2024.

eLabFTW

A free and open source electronic laboratory notebook build for web browsers, developed by Nicolas Carpi[1]. It comes with an integrated authentication mechanism and a dedicated authorization scheme, organizing access rights to experiment’s by grouping users in groups and teams. Input to the ELN can come from the user via a web editor or ingested through an API. The content of elabFTW has a native support for versioning, that may be controlled from the web frontend. Additional to the ELN, it comes with a database (aka inventory management system) to store additional information, e.g. on samples, instruments and the option to link to these from within the notebook. Multi resource input, e.g. from

[1] https://www.elabftw.net/

multiple users, is partly supported in elabFTW. More specifically, multiple agents (one at a time) may add information to the same notebook.

What would usually be called a *(laboratory) notebook* is denoted *experiments* in the context of elabFTW. See figure elab1 for an overview of multiple experiments documented in this instance. Each experiment has its own right management where a group, team or individual may be granted read and/or write access. Additionally, a status, e.g. *running* or *success*, and a rating of the conducted experiment may be given.

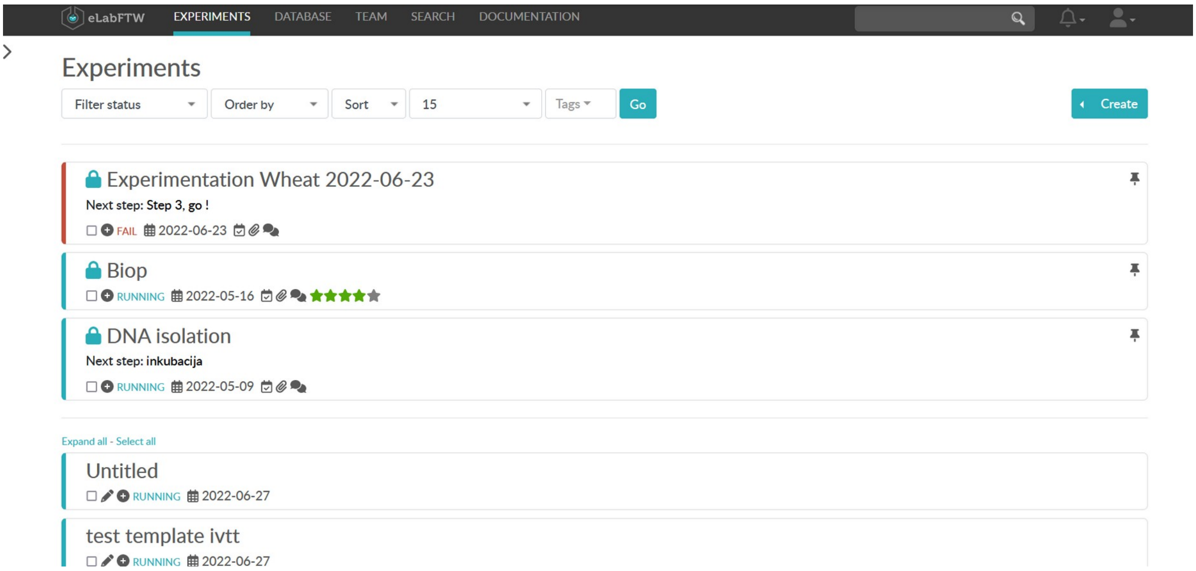

Figure elab1: Dashboard of existing experiments in elabFTW. Other menu headings are database, team, search, documentation and profile management.

From the list of available experiments an existing one may be chosen or a new one created. A detailed view of the experiment is shown, see figure elab2. A typical experiment in elabFTW has a detailed description of the experimental steps in flow text, including tables, images and further objects. Additionally, related metadata and data may be attached to the experiment. To prove original work, e.g. for patents or scientific discoveries, a time stamp option is included, producing trusted stamps following the RFC 3161 protocol (https://www.rfc-editor.org/rfc/rfc3161). An experiment may be locked and prohibit further modification after completion.

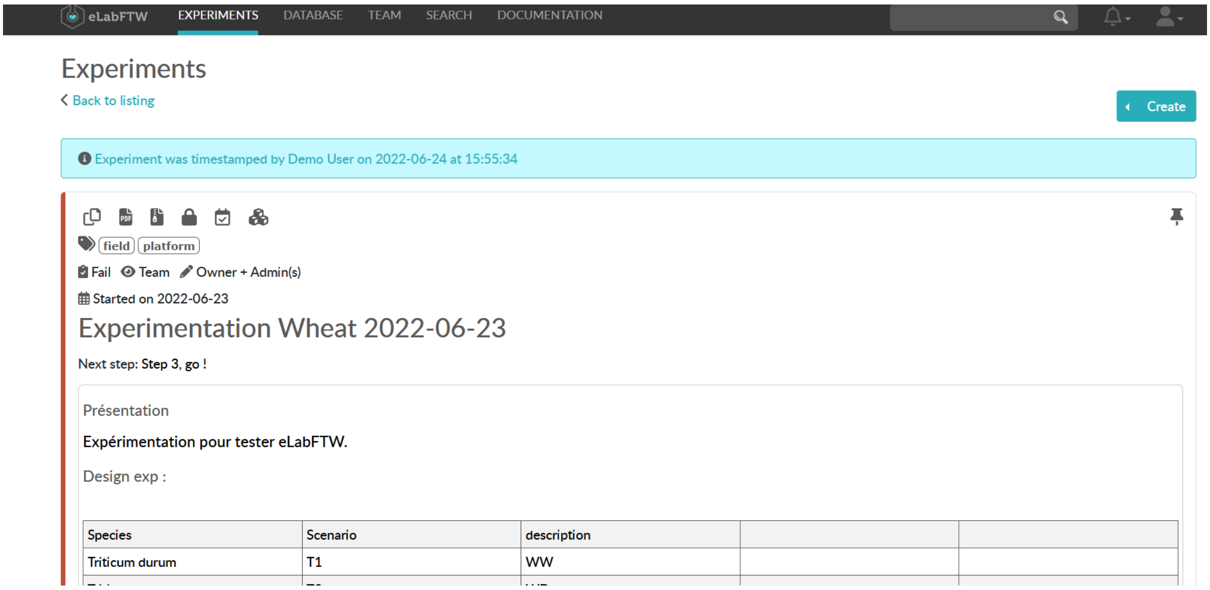

Figure elab2: Overview of an experiment. Each experiment is its own logbook instance, with free form text field, authorization management and additional metadata and data.

In summary, elabFTW is a well established, widely used and stable ELN solution that is well suited for individuals or groups that don't rely on live editing or multi agent inputs.

Resources:
website: www.elabftw.net

github: www.github.com/elabftw/

LablMotion, based on Chemotion

LablMotion is an open source software, which is based on the established Software Chemotion-ELN and is currently developed at KIT. The focus of this generic extension is to include typical workflows in heterogeneous catalysis containing catalyst synthesis, catalytic activity/stability measurements, modification of setups/devices, and *in situ/operando* material characterization. Therefore, LablMotion is separated into a number of functional areas, covering 1) research plan, 2) materials (including standard characterization), 3) catalyst synthesis, 4) setups/devices and 5) advanced characterization and catalyst activity testing. Moreover, a link to the Adacta-Software and SciCat can be established.

1. Area 1 – research plan

The aim of the research plan, see figure motion1, is to freely plan or document a set of experiments of all kinds, e.g. a beamtime. It can be freely designed with a combination of tables, text fields and interactive links to materials, syntheses, reactions and characterizations. Also images as well as other types of materials can be added as attachments. References can be linked in the respective field.

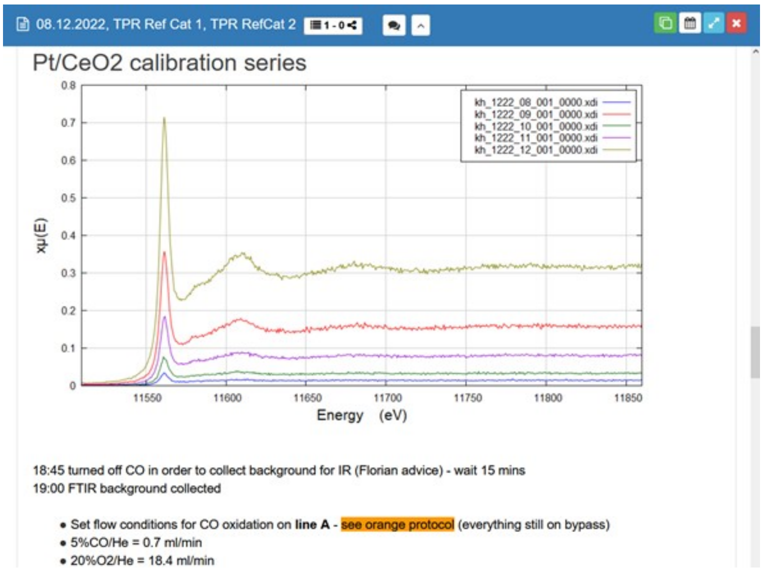

Figure motion1: The research plan feature in the LabIMotion ELN used for the documentation of a beamtime.

2. Are 2 – materials

As the name states, the materials hub defines all materials. Here, the identifier, potential external labels, (chemical) structure and additional information on the substance are brought together. Standard characterization can be directly linked to the respective material as well as references to literature or specific results.

3. In the synthesis tab, details on the sample preparation can be found, such as precursors, temperature, reactor, etc. Besides the standard attachments (analyses and references), in LabIMotion, also complete workflows may be stored and serve as template for consecutive entries, as seen in figure motion2.

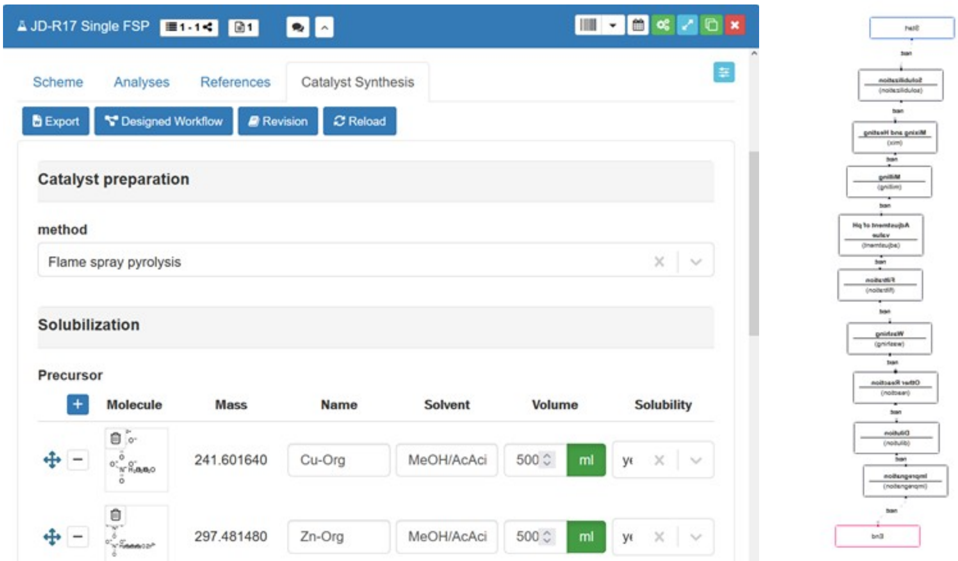

Figure motion2: Details (left) and workflow (right) for the catalyst synthesis in LabIMotion.

4. Devices and setups are documented in the respective fields, shown in figure motion3. An import/export feature to Adacta is currently being developed with the aim to monitor possible changes in the configuration and modifications of the devices. Setups for e.g. beamtimes can easily be virtually configured by dragging and dropping single components to the respective fields.

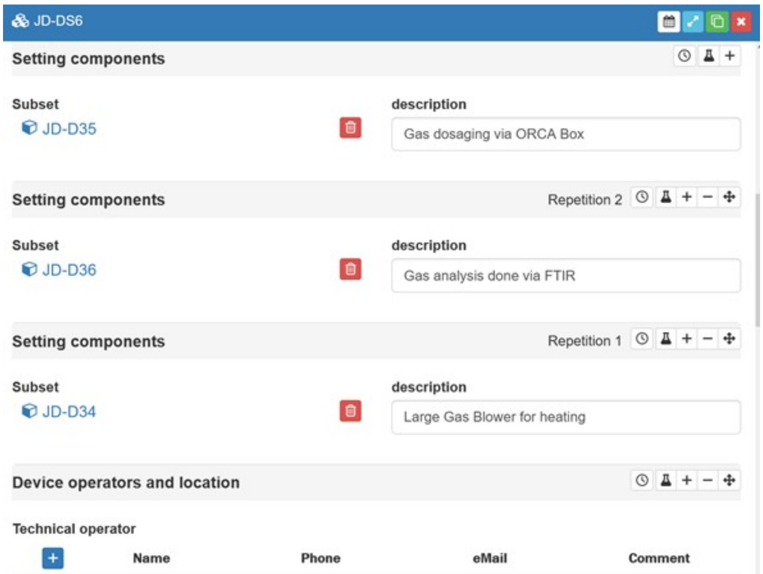

Figure motion3: Overview over the device/setup tab.

5. Lastly, catalytic and advanced characterizations can be described in detail in the Testing tab, see figure motion4. Here, an overview over the applied conditions (gases, temperature, devices, etc.) can be added. Currently, all types of raw data can be linked. In future, a first evaluation of different kind of data will be possible within the ELN. Also here, workflows can be freely established and used as templates.

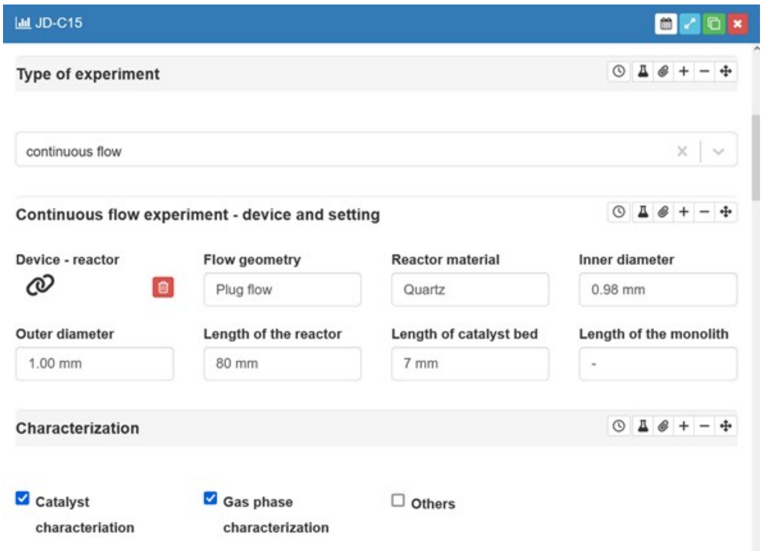

Figure motion4: Overview over the catalytic and advanced characterizations tab.

All Features:

· Data Input

- User friendly Interfaces, User guidance *via* templates and workflows
- Browser based data input, therefore no limitations regarding input sources

· Data Ingestion from Instrument

- Multiple possibilities available, analogous to the Chemotion application https://doi.org/10.1016/j.acax.2019.100007

·Data Management

- User authentication via database authentication or SSO via external services (Shibboleth, ORCID, GitHub, NFDI AAI)
- Collection can be shared between users.
- Hierarchical user groups can be used to curate data
- Backup

· ELN Access / Data Access

- Information from the ELN can be exported as .json files
- As browser based application, it can be accessed from anywhere
- Full Text Search
- Data Annotation, Tagging

LabIMotion is currently still under constant development. The stable version running 24/7 is expected to be deployed in summer 2024. Further adaption and features will be added over the next years.

Resources:
https://chemotion.net/docs/labimotion

OpenBIS

OpenBIS is an Open Biology Information System (open-source software framework) created to support comprehensive data management for various experiment types and research areas. It enables the tracking, annotation, and sharing of data across distributed biological research projects. This system is applicable to fields such as Phenomics, Transcriptomics, Genomics, Proteomics, and Metabolomics. Additionally, it offers specialized features for specific needs, such as High-Content Screening (HCS)/Imaging and Next Generation Sequencing. OpenBIS, developed at ETH Zurich in Switzerland since 2007, is a server-client based application designed for effective data management. This system ensures accessibility through a user-friendly interface, facilitating the principles of FAIR (Findable, Accessible, Interoperable, and Reusable) data management . OpenBIS comprehensively covers all aspects of managing research data, including an electronic lab notebook, a digital catalog for (meta) data, and tools for sample and protocol management. OpenBIS effectively handles various experimental methods, making it an ideal solution for collaborative work in research laboratories. FAU Erlangen-Nürnberg actively promotes OpenBIS for research data management (RDM). OpenBIS is a viable alternative ELN for managing photon and neutron (PaN) data. OpenBIS can handle any type of biological data, contextualize it within experiments, and enrich it with metadata (Figure openbis1).

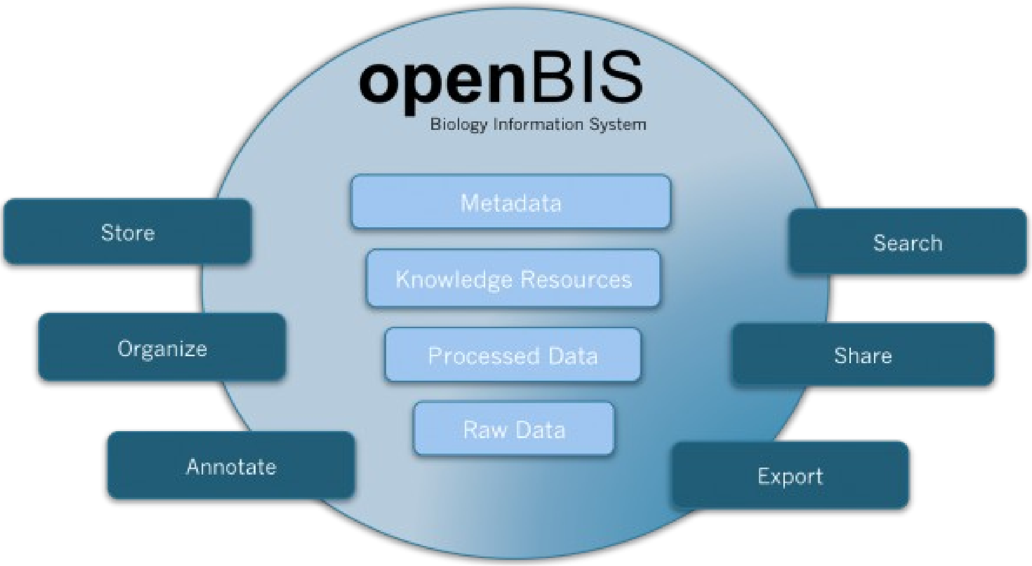

Figure openbis1: Illustrating openBIS, a software framework designed to organize and annotate (meta)data from biological experiments. It offers query and display functionalities, integrates data into pipelines, and facilitates sharing with other researchers.

The openBIS platform offers three main functionalities:

1. Inventory management for laboratory samples, materials, protocols, and equipment.

2. A laboratory notebook for documenting lab experiments.

3. Data management for storing all data related to lab experiments, including raw, processed, and analyzed data, as well as scripts and Jupyter notebooks.

Users can choose to utilize all functionalities or only selected ones. In the most general use-case, the **Inventory** is shared by all lab members, providing access to information about available lab materials and commonly used protocols (Step 8: Decision on an ELN.). Additionally, each lab member has a personal folder in the **Lab notebook** to organize their projects and experiments. This folder can be shared with other lab members or collaborators who have access to openBIS. Experimental steps documented in the lab notebook can be linked to protocols and samples stored in the inventory, as well as to other experimental steps. **Data** of any kind can be attached to the corresponding experimental step in various ways, depending on its size. Data can also be exported to data repositories such as Zenodo or the ETH Research Collection (ETH internal function). This setup allows for a comprehensive overview of workflows and information, from initial data generation to data analysis and publication. OpenBIS originated within the life sciences field, with the initial use cases at FAU also being in life sciences. A demo installation is available at [OpenBIS Demo] (https://openbis.ch/index.php/demo/#demo). Figure openbis2 shows OpenBIS data set collection.

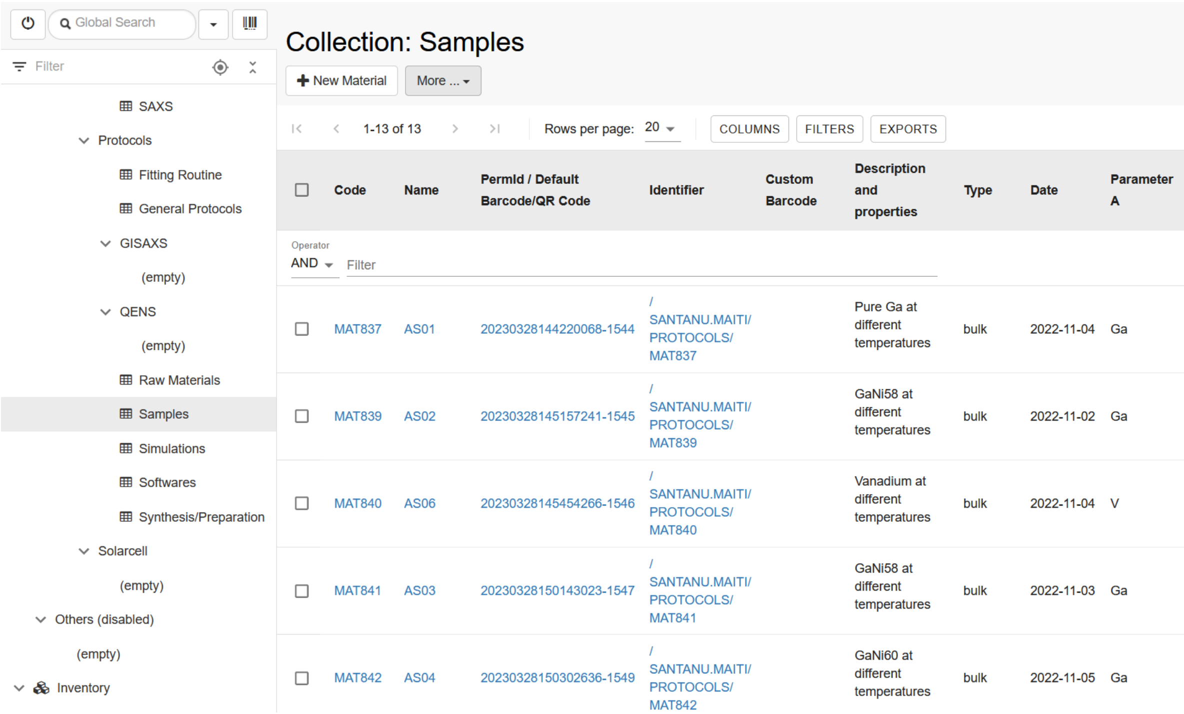

Figure openbis2: Data set collection: Different datasets generated from the original sequencing data can be collected.

There is an upcoming use case involving the integration with OpenBIS. In the context of DAPHNE4NFDI, it is important to consider that catalogs within DAPHNE4NFDI are evolving towards comprehensive RDM solutions. For instance, SciCat offers extensive capabilities for custom data and attachment uploads, and it integrates seamlessly with tools such as Jupyter and ELN/SciChat.

Combined Functionality Table for discussed ELNs

Title	**snip**	**elabFTW**	**MLZ workbench**	**myLog**	**LablMotion**	**OpenBIS**
Application Programming Interface		**y**	**y**	**y**	**y**	**y**
Intuitive User Interface		**y**	**y**	**y**	**y**	**y**
Reliability		**y**	**y**	**y**	**y**	**y**
Open Source		**y**	**y**	**y (Zulip GUI)**	**y**	**y**
Documentation		**y**	**Not complete**	**under construction**	**y**	**y**
Content Export		**y**	**y**	**n (no bulk export)**	**y**	**y**

Title	snip	elabFTW	MLZ workbench	myLog	LablMotion	OpenBIS
Parallel Editing		n	y	n	n	n
Authentication		y	y	y	y	y
Authorization		y	y	y	y	y
Searchable		y	y	y	y	y
Scalable		y	y	y	y	y
Image Import		y	y	y	y	y
Server Deployment		y	y	y	y	y
Free-form Input		y	y	y	y	y
Recovery Option		y	y	n (but history exists)	y	y
Auto Save		n	y	y	n	n
Federated Identity Management		n	y	n	y	y
Links/Tags		y	y	y/n	y	y
Software Image		y	y	y (Zulip pkg)	y	y
Local Deployment		y	y	n	y	y
Camera Input		n	y	n (only via control system scheme export)	y	y
Notes		y	y	y	y	y
Schematic Input		y	y (only for instrum ents)	y	y	!
Entry Highlighting		y	n	y (in terms of tagging people)	n	n
Cross Platform		y	y	y	y	y
Voice Input		n	Upload as mp3 file	n (not directly)	n (file upload possible)	n

Title	snip	elabFTW	MLZ workbench	myLog	LabIMotion	OpenBIS
Summary Tables		**n**	**y**	**y (via DAMNIT)**	**y**	**y**
Experimental Management		**y**	**n**	**y (if using DAMNIT-imported tables)**	**n**	**y**
Sketches		**n**	**y**	**n**	**y**	**y**
Data Import		**y**	**y**	**y**	**y**	**y**
Integration of Software		**n**	**n**	**y**	**y**	**n**

Exemplary workflow for ELN Evaluation to a specific use-case

An example of the proposed workflow to evaluate an ELN for a specific use-case is outlined here for a total of three made-up ELNs. The use case for this example is a **personal documentation tool** for a PhD candidate, i.e. measurements in a laboratory, documentation of data analysis, experimental design and discussion notes.

Proposed workflow from this white paper:

1. Identify eligible ELN's
2. Identify features and define importance
3. Decide for a cut-off criterion on P_n (e.g. 0.7)
4. Test and evaluate ELN functionalities
5. Calculate P_n's
6. Check cut-off criterion
7. Further test and discuss on ELN's passing the criterion
8. Decide for an ELN or refine work flow and repeat (if necessary)

Example:

Please note that the following workflow is an example, consisting of made up names, ratings, parameters, factors and limits for the ELNs. It has to be adapted for real use cases.

Step 1: Three different ELNs were found to be eligablet: *SciencePRO*, *flowtext* and *SketchMe*.

Step 2: Define a list of specifications and their respective importance, necessary for a personal ELN. (See table below for a comprehensive list of possible specifications for this made-up use case.)

Title	Description	Imp
Intuitive User Interface	Interface designed for human interaction, enabling a intuitive and productive user experience with a professional programmed and designed GUI	5

Title	Description	Imp
Reliability	Enabling legally binding documentation of research by introducing a record of changes, e.g. version control or audit trail.	5
Content Export	Content of the ELN is store able and accessible, in a free and wide spread data format, e.g. as pdf or html.	5
Searchable	Humans and machines are able to search for information, e.g. by full text search, filtering for keywords or indexes.	5
Image Import	Import of wide spreed image file formats into the ELN, from the cloud structure or the file system.	5
Free-form Input	Basic type of input capable of containing any kind of information represented by characters and numbers, further, elements to organize and style these e.g. tables, lists, headings, fonts and colors.	5
Recovery Option	Reliable mechanism to store the content of an ELN and restore it in the case of data loss.	5
Documentation	Source of information, documenting the status, capabilities and functionality of an ELN, e.g. utilized as a source of training for new users.	4
Sketches	Drawing of illustrations, e.g. sample structures or technical setups.	3
Schematic Input	Enabling the creation of predefined methods for repetitive and unified inputs, e.g. templates for users or instruments.	3
Auto Save	Mechanism to automatically store and synchronize the input.	3
Links/Tags	Possibility to create links and tags in the ELN, to easily mark specific positions and retrieve the respective information.	2
Experimental Management	Functionality of an ELN that enables and enhances the planning, preparation and progress tracking of experiments, e.g. by to-do lists or connection to a sample database.	2
Data Import	Import of raw and derived data into the ELN, e.g. inclusion of a collected data set as a table.	2
Integration of Software	Possibility to include and execute software code inside the ELN, e.g. by inclusion of ipython notebook features.	1
Voice Input	Inclusion of recorded voice files or voice to text transcripts in the ELN e.g. for preparation in wet labs.	1

Step 3: Deciding for a cut-off criterion on the FOM of 0.75.

Step 4: The functionalities are ranked on a scale from 1 to 10 (satisfaction parameter) for all eligible ELNs. Necessary functionalities with a importance of 5 need a satisfaction of at least 7 to be marked as satisfying for usage.

Title	ELN1: flowtext	ELN2: SciencePRO	ELN3: SketchMe
Intuitive User Interface	7	10	8
Reliability	7	9	8
Content Export	8	9	8

Title	ELN1: flowtext	ELN2: SciencePRO	ELN3: SketchMe
Searchable	8	10	10
Image Import	7	7	7
Free-form Input	9	10	7
Recovery Option	5	8	8
Documentation	6	7	9
Sketches	1	5	10
Schematic Input	1	8	5
Auto Save	5	8	8
Links/Tags	1	6	1
Experimental Management	1	8	1
Data Import	1	9	6
Integration of Software	7	6	1
Voice Input	5	1	1

Step 5: Calculation of the FOM P_n.

$$P_n = \frac{\prod_{necessary\, F_i} \begin{cases} F_i\, satisfied : 1 \\ else : 0 \end{cases} * 1}{\sum I_i} \frac{\sum_{i=1}^{n} I_i * S_i}{S_{max}}$$

The Formula calculates a number P_n taking all desired specifications F into account. Every single specification F_i is identified by an index i and accompanied by its importance parameter I_i. Additionally, a satisfaction parameter S_i is introduced, ranking the actual usability and maturity of the respective specification on a range from 1 to S_{max}.

The maximum satisfaction parameter S_{max} is 10 and the sum of the importance factors is 56.

Title	Imp.	ELN1: "*flowtext*"	ELN2: "*SciencePRO*"	ELN3: "*SketchMe*"
Intuitive User Interface	5	7	10	9
Reliability	5	7	9	8
Content Export	5	8	9	8

Title	**Imp.**	**ELN1: “*flowtext*”**	**ELN2: “*SciencePRO*”**	**ELN3: “*SketchMe*”**
Searchable	5	8	10	10
Image Import	5	7	7	7
Free-form Input	5	9	10	7
Recovery Option	5	5	8	8
Documentation	4	6	7	9
Sketches	3	1	5	10
Schematic Input	3	1	8	5
Auto Save	3	5	8	8
Links/Tags	2	1	6	1
Experimental Management	2	1	8	1
Data Import	2	1	9	6
Integration of Software	1	7	6	1
Voice Input	1	5	1	1
FOM	/	**0**	**0.82**	**0.73**

Step 6: ELN1 “flowtext” gets a score of 0, due to the fact that the necessary functionality “Recovery Option” does not satisfy the limit of at least 7. Only ELN2 “SciencePRO” passes the cut-off criterion of 0.75 on the FOM.

Step 7: ELN3 “SketchMe” does score slightly below the cut-off, but had some unique features. Thus also this ELN is included in the discussion process.

Step 8: Decision on an ELN.

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