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Brave New Lab World – Electronic Lab Books Digitise Laboratory Documentation

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Abstract

At German universities and universities of applied sciences, a new way of working is currently opening up in the area of the structure and composition of laboratory work: Documentation by means of electronic laboratory notebooks (ELN). Researchers produce and use a colourful mixture of data such as graphic files, formulas, tables or microscopy files. At Heinrich Heine University Düsseldorf (HHU), advice and support for researchers in the field of research data management (RDM) is provided on a regular basis. In addition to assistance with applications, we also offer support using various RDM tools, including electronic lab books. Why it makes sense to use electronic lab books, how our path with them has progressed so far, and what are the current hurdles to be overcome are presented in this report.

1 Introduction

The Center for Information and Media Technology (ZIM) is part of the Research Data Management Competence Center (RDMCC) at HHU and has been providing researchers with the license-based ELN "Labfolder" in its own hosting variant for several years. In the course of the cooperation project "FoDaKo" (Knipprath, et al., 2020), funded by the German Federal Ministry of Education and Research (BMBF), a collaboration of the three North Rhine-Westphalian (NRW) universities Düsseldorf, Wuppertal and Siegen, we have been building an open source solution with "eLabFTW" at ZIM since 2018 after evaluating different software solutions.

From an infrastructural point of view, we have since then significantly promoted eLabFTW, as it fits better to the researchers' requirements. This is because Labfolder comes with licensing costs and is thus difficult to use meaningfully for short-term research projects with visiting scientists, not to mention cost-effective use in teaching, which we wanted to push just as much.

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On the campus of Heinrich Heine University, a new building with 70 % laboratory space for the life sciences was built in 2016 and has since been occupied. A good time to think about digitising the labs with the help of electronic lab books.

2 Requirements for an ELN

Both decisions for the software solutions were made on the basis of the researchers' wishes specifically for these ELNs. An important factor from the point of view of infrastructure was to arrive at a generic solution for the time being, with which as large a target group of researchers as possible can work well. Another important point was that no additional software is needed to use an ELN, but that the service can be offered completely web-based (see Figure 1: eLabFTW user interface in the web browser). After a simultaneous pilot phase of both lab books, it was decided to focus on the open source solution and only run eLabFTW, as it was more popular among researchers. Therefore, HHU discontinued the hosting variant of Labfolder at the beginning of 2022.

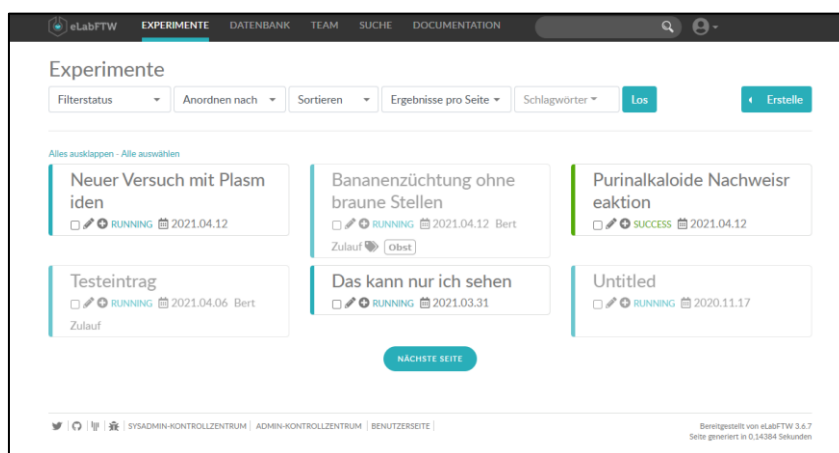


Figure 1: eLabFTW user interface in the web browser

Lab work should be able to be documented in a well-structured way. At the same time, researchers also want to be able to quickly file information in an unstructured area, especially during the active practice phase, so that they can document it neatly during follow-up work. The ELN Guide of the German National Library of Medicine (ZB-MED) (Adam & Lindstädt, Elektronische Laborbücher im Kontext von Forschungsdatenmanagement und guter wissenschaftlicher Praxis – ein Wegweiser für, 2020), as well as the newly published "ELN Finder" (Adam, et al., 2023), are very good guidelines for choosing a software solution.

Thus, the user side has different types of requirements for an ELN. In addition to technical requirements such as user-friendliness, the use of known file formats and the constant digital availability of data, there is also the desire for the possibility of completely withdrawing one's data from the ELN software and continuing to work elsewhere. In addition, there are specific professional requirements, which can differ greatly under certain circumstances. While the biologists and physicists are satisfied with the generic tool eLabFTW, the chemists have more specific requirements for an ELN. For example, they need a specific chemical formula editor so that the molar mass can be automatically transferred and so that a structure search is possible. In addition, although the measurement data can be uploaded

and downloaded, there is no direct opening in a suitable software. One of the regulatory requirements, especially for externally funded projects, is compliance with good scientific practice and good laboratory practice. This includes the secure storage of research data as well as ensuring their availability and retrievability.

2.1 Integration into the curriculum

Despite the steadily increasing use of the electronic lab book, there is often an internal barrier to use. The motivation of the employees is the essential point to be targeted here. We at ZIM are already in close contact with researchers to introduce the topic to students at an early stage and to present it attractively as part of the curriculum, in order to use the positive attitude of students towards digitization projects for the digitization of laboratory work.

With the aim of shaping a cultural change towards electronic lab books, as a pilot project in neurobiology, master students of the course "Cellular and molecular analysis of brain function" were introduced to the lab book software with the help of video tutorials in order to learn first steps in fluorometric imaging under lab conditions, i.e. how data should be generated and analyzed. Students can be more easily involved in research work, as entries can be easily shared via the ELN. In close cooperation with the teachers, the laboratory book can thus be optimized for teaching purposes. In this way, young scientists learn how to use electronic lab books at an early stage and will build on these new standards in their research.

In order to serve the different requirements of research and teaching, we have provided a separate instance of eLabFTW especially for teaching. Here it is important to the teachers that test data can also be deleted again and that students do not change important data of the research documentation during experimentation. Nevertheless, experiments can be transferred from the teaching system to the main instance via the export & import functionality.

By introducing ELN in teaching, we hope for a faster and broader adoption of electronic lab books, thus optimizing research work in the lab and advancing digitization there. We think that ELNs are a good opportunity to be introduced to research activities and procedures at an early stage in teaching and offer potential for independent learning in the laboratory.

3 On-site support and regional joint cooperation

The founding of a NRW-wide working group on the topic of ELB has helped us to identify the basic needs of researchers (Knipprath & Zulauf, ELB.nrw Startseite, 2019). The collaboration of the infrastructure institutions has allowed us to learn from each other: We received help with the implementation of a central authentication method, and help others with the use in teaching or when it comes to conceptual issues. Among other things, this working group discusses the technical implementation, as well as IT security concepts and interfaces to other research data infrastructure.

The networking of the various NRW institutions also provides a good overview, because in addition to eLabFTW, these institutions also use Labfolder, eLabJournal or RSpace as lab book solutions, among others (Kusch, Wiljes, & Knipprath, 2019). It has long since gone beyond NRW. Researchers from all over Germany became aware of our pioneering work and contacted us or the working group. Thus, the community grew to 100 members by now. Together, we have developed a guideline to help infrastructural institutions introduce electronic lab books. (Adam, et al., 2023)

At the same time, the collaborative project OER.DigiChem.nrw expanded the topic of electronic lab books in chemistry specifically with a focus on students. In this cooperation, the HHU Düsseldorf, the University of Wuppertal and the TH Köln University of Applied Science together create free educational materials (OER) for students and develop materials with which intentional learning can be better taken into account in the introductory phase of studies (Mertineit, et al., 2021). The tutorial videos on the use of eLabFTW (see Table 1: Title of the eLabFTW video tutorials) can be accessed via the ORCA.nrw portal, and are very suitable for designing or supplementing subject-specific learning spaces on the topic of electronic lab book within learning management systems.

No	Title	Length
1	First Steps - Login and User Page	3:56 min
2	First Steps - The Menu Bar	2:22 min
3	New Experiment - Create	2:05 min
4	Editing an Experiment - Editor and Co	3:15 min
5	Editing an Experiment - files and images	3:01 min
6	Editing an Experiment - keywords	2:32 min
7	Editing an Experiment - Molecule Editor and MOLFiles	2:23 min
8	Editing an Experiment - New fields with JSON	3:44 min
9	Editing an Experiment - Formulas with TeX Commands	3:22 min
10	Database Team and Templates - Create New Template	2:18 min
11	Database Team and Templates - Database Elements and Appointment Calendar	2:24 min
12	Experiments Finalise and Share - (Reading) Entitlement	2:27 min
13	Experiments Finalise and Share - Revisions and Timestamp	2:54 min
14	Experiments Finalise and Share - PDF and ZIP export	2:00 min

Table 1: Title of the eLabFTW video tutorials

3.1 General conditions at HHU

We got a better overview of the research scenarios at our own site by inviting different researchers from different disciplines, such as physics, biology and medicine, to talk about their requirements and to develop so-called use cases (Zulauf & Knipprath, 2019). Here we were able to create common frameworks afterwards, regarding the service eLabFTW. Currently, we meet monthly with power users to talk about problems and opportunities regarding the use of electronic lab books at HHU.

To establish the service, discussions have been held with the staff council, initial versions of procedure directories have been created, and data protection considerations have been thought about. One has to master the balancing act between the data protection rights of individuals and good scientific practice, i.e., weighing the possibility of deleting personal data against the obligation to retain and provide evidence. We solved this by requiring user consent when logging in via Shibboleth, where the data protection conditions are stored via a link, as well as via the point about laboratory documentation and retention period in the terms of use. Accordingly, regular sensitization of employees must be carried out so that the correct documentation of approved research data can be done. In addition, it is the responsibility of the team admins to regularly check whether the specified retention period of the stored data has been reached, and thus whether it can be deleted.

Immutability is ensured within eLabFTW by a timestamp facility. Here, researchers can record their work at that moment in an evidential manner. A digital possibility to store records of genetic engineering work according to the Genetic Engineering Records Ordinance (the so-called "Form-Z") electronically is currently being discussed and developed at our university. Researchers in genetic laboratories must keep track of every genetically modified organism in this spreadsheet, and must do

so for years (Justiz, 1990). The district government responsible for us does not specify the type of documentation - it can also be done explicitly in an electronic lab book. In order to implement this in a technically flawless manner, the PDF documents in question must be digitally signed with a user certificate so that this signature can be validated for years. Care must be taken here to ensure that the root certificate and a time stamp are included together with the signature (so-called long-term validation = LTV).

Currently, we are also collecting key figures in the context of the RDMCC in order to be able to support our researchers in a more targeted manner. In a project by our IT trainees, we developed a tool that, among other things, divides the users of eLabFTW into faculties and roles. The main user is the Faculty of Mathematics and Natural Sciences with 400 staff and 150 students, followed by the Faculty of Medicine with 230 staff and 50 students. In total, 88 teams have created 25,000 experiments.

3.2 Case studies

The RDMCC accompanies the Collaborative Research Center 1208 (CRC1208) very intensively with regard to research data management. The group has introduced the use of eLabFTW as mandatory and is currently developing, in close exchange with us, a way to extract data from the electronic lab book and store it in an archive. For research data we already offer an institutional repository based on the open source software DSpace at HHU. Now researchers of CRC1208 have programmed the tool LISTER - "Life Science Experiment Metadata Parser" (Musyaffa, Rapp, & Gohlke, 2023), which qualifies an export with additional metadata via the eLabFTW API and passes it as a JSON file to an interface of our separate archive based on DSpace. There, the metadata is both included in the DSpace metadata and stored as part of the data to be archived in the S3 object store or long-term storage. This approach ensures that the data can be used sustainably and robustly even without DSpace as a repository application. One goal is also to be able to search for experiments in the lab book archive very specifically, similar to the lab book platform. In addition, the lab book platform is relieved and the project supports good scientific practice.

Another application example can be found in the field of preclinical studies in medicine. There, eLabFTW is used as a central interface for the components of the quality management system and the digital storage of laboratory journals. Standard Operating Procedure (SOP) and a managed biobank for the safe long-term storage of biospecimens have been introduced (Hewera, et al., 2020).

The benefits already achieved can be illustrated very well using the example of neurobiology: Here, the chemical database within eLabFTW is maintained by everyone according to a fixed specification. Each of the 400 chemicals has its own entry in eLabFTW containing a table in which it can also be entered if this chemical needs to be reordered. The technical assistants thus have a shopping list directly at hand via a bookmark. In addition, the researchers can link the chemicals directly to their experiments and have the H- and P-phrases (hazards and safety instructions) quickly at a glance. The introduction of electronic lab books has also made it possible to establish a much more convenient way of working with a chemical database. In addition to chemicals, the working group also manages its optical elements, protocols and lists as well as preparation solutions via eLabFTW. Using eLabFTW resulted in a great time saving, because no or less repetitions have to be made, experiments and further data can be retrieved faster, and it is easier to follow up on old projects.

The feedback from the very different research groups is, on the one hand, an inspiration for other researchers and, on the other hand, offers us valuable input for the further development of the platform. The researchers are not only in constant exchange with the infrastructure staff and each other, but we also actively participate in the eLabFTW community and regularly consult with the main developer and

his company in order to continuously develop the open source software and adapt it to new circumstances.

4 Conclusion

The flexible and also license-free use of the open source lab book solution eLabFTW offers us broad possibilities for use, both in teaching with very many students and in more individual research use with requirements for adaptability for research teams and the realization of application interfaces. The question that remains open for us is whether it is still possible to continue a common monolithic platform approach, by understanding common requirements, with the existing dialogue within the user group, or whether a distributed strategy will become necessary. Other institutions divide by faculty, for example, but lose synergies in cross-cutting projects as a result. Bringing researchers together to form an eLabFTW user group has proven very valuable in arriving at common requirements, but also in picking up newcomers or sceptical users with concrete examples from other research groups.

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Bert Zulauf studied electrical engineering and process informatics at the University of Wuppertal (BUW) and management (MBA) at the Düsseldorf Business School of the Heinrich Heine University (HHU). After the consolidation of the University Computing Center and the Media Center, Bert Zulauf was responsible for the establishment of the then new E-Learning department at BUW as department head of the Center for Information and Media Processing from 2005. Since February 2015, he has headed the Research Data Infrastructure, Web Technologies and Application Support department at the Center for Information and Media Technology at HHU. Bert Zulauf led the BMBF project Research Data Management in Cooperation -FoDaKo of the Universities of Düsseldorf, Siegen and Wuppertal, and accompanied the student DINI competitions as a reviewer. He is co-initiator of the third-party funded projects ILIAS.nrw and OER.Digichem.nrw and was sub-project leader in the project "Lernwelt Hochschule" (Schwarz Stiftung). Bert Zulauf is involved in national and European committees, supports the Foundation for Innovation in Higher Education as a reviewer and is spokesperson for the DINI E-Learning working group.



Nina Knipprath has been working at the Centre for Information and Media Technology at Heinrich Heine University Düsseldorf as an administrator in the Research Data Infrastructure, Web Technologies and Application Support department since 2016, after completing her master's degree in computer science with a focus on bioinformatics with distinction. She worked on the project FoDaKo - Research Data in Cooperation, the joint project of the universities of Düsseldorf, Wuppertal and Siegen, which was about building and establishing a research data infrastructure at the respective universities. During the project, she not only built up an institutional research data repository, but also participated in the founding of a working group on the topic of electronic lab books in NRW. Subsequently, she is in the process of further establishing and expanding the university-wide research data competence centre with a focus on research data management tools, especially electronic lab books, as well as close cooperation with researchers at the site, for example with the Collaborative Research Centre Membrane Systems or the Cluster of Excellence CEPLAS.