

FINAL REPORT

Project title	Laboratory Notebook & Database Extensions (LabNDB-Ext)
Project leader	M. Krüger, G. A. Holzapfel
Project team members	Jakob Harden (Project manager), Selda Sherifova, Mathias Eisner, Barbara Schmid, Philipp Knabl
Reporting period	01.10.2022 – 20.04.2023
Institute	Institut für Materialprüfung und Baustofftechnologie [2060] Institut für Biomechanik [7190]
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Please note: length approx. 4 – 5 pages

1 Goals and results

- Have the objectives defined in the proposal been achieved?
- Compare the objectives with the results achieved.
- Describe the “highlights” and problems that occurred in achieving the objectives.

Most of the objectives were achieved as proposed. Some of them were changed to better fitting to the overall project goals.

Table 1: Work packages

No.	Proposed objectives	Achieved results
1	Rawdata preview	A basis, that allows to preview rawdata from devices is implemented and tested. See also deviations in the work plan.
2	Booking devices and sections	Fully implemented and tested.
3	User authentication - permissions - roles	Security measures for the user authentication were fully implemented and tested. Role systems and roles were defined (management roles, QM-roles).
4	SQL look-ups for inventory - devices - rooms	Import of CSV-files from TUG-Online for devices and rooms is fully implemented and tested. See also deviations in the work plan.
5	End-user tests and documentation	A demo version is available and used by the end-users for testing purposes and for showcases. Workgroups were established to gather information regarding usability and requirements. Several workgroup meetings have taken place. The outcomes of the meetings are already incorporated and tested. See also deviations in the work plan.
6	Code documentation	Vast majority of the code is well documented.
7	Exporting data and metadata to the TUG repository and CyVerse	Prototype that allows for data and metadata export to the repository (invenioRDM) is implemented and tested.
8	Message board & notification	Fully implemented and tested.

There are some “highlights” in the development process worth to be mentioned.

The continued cooperation between the institutes IMBT/TVFA [2020] and BioMech [7190] is still the source of many good ideas and a fruitful development process. In addition to the planned cooperation, further cooperation with RDM biomECh vol 2. was established under the implementation of workflows.

In July 2022, we also began cooperation with the RDM marketplace project “LabLog 2.0” from FELMI-ZFE. The contributions from their project team members (A. Zankel, F. Rasras) represent a valuable source of feedback and return valuable information regarding the usability of our solution.

To our surprise, we could finish the implementation of the message board at a very early stage. Since the last report, it was extended and tested. This feature is one of the core tools of communication and process

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management.

Because of the change in the funded project costs, it was necessary to declare the connection to the repository as an optional component. We found out that communicating with the restAPI of the repository server is not very complicated and implemented a working prototype. This feature still has to be tested and is intended to support best practices in research data management in the future.

2 Work packages, milestones and current progress

2.1 Overview tables

- Explanatory notes:
Scheduled date: date according to the interim report.
Current date: date according to the plan valid at the time of reporting (completion of the project).

Table 1: Work packages

WP No.	Work package title	Stage of completion (in %)	Scheduled date		Current date	
			Start	End	Start	End
1	Project management	100	01.04.2022	15.04.2022	01.04.2022	22.04.2022
2	Concepts (gathering information)	100	15.04.2022	29.04.2022	23.04.2022	07.07.2022
3	Implementation phase I	100	29.04.2022	01.07.2022	08.07.2022	23.08.2022
4	Implementation phase II	100	01.07.2022	21.10.2022	24.08.2022	17.10.2022
5	Implementation phase III	100	21.10.2022	21.01.2023	18.10.2022	25.01.2023
6	Close-down (project closing, documentation)	100	21.01.2023	31.03.2023	26.01.2023	20.04.2023

Table 2: Milestones

Milestone No.	Milestone Title	Scheduled date	Current date	Milestone achieved on
0	Project start	01.04.2022	01.04.2022	01.04.2022
1	Project kickoff workshop	---	22.04.2022	22.04.2022
2	Concepts end (gathering information end)	29.04.2022	15.06.2022	07.07.2022
3	Implementation I	01.07.2022	23.08.2022	23.08.2022
4	Implementation II	07.10.2022	19.10.2022	19.10.2022
5	Implementation III	13.01.2023	25.01.2022	25.01.2023
6	Project end	31.03.2023	20.04.2023	20.04.2023

2.2 Description of the work carried out during the reporting period

- Describe the work carried out during the reporting period based on the work packages.
- Describe any deviations in the work plan.
 - The description should also include changes in the methodology.
- Describe any changes and/or adjustments in the work plan and their effects on the completion of the project.

Work carried out

- WP 1: Project kickoff workshop, project planning, basis for the project handbook

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- WP 1: Project handbook that contains all information about the project (including: general information, objective and performance planning, task scheduling and cost planning, project context relationship tools, project organization and culture design, project proposal, flipchart protocol of the project kickoff workshop)
- WP 1: Initialization of topic-related workgroups (used to integrate end-users into the development process)
- WP 1: Developer workshop (gather information for further development, feature definitions, data-structure design, user-interface design)
- WP 1: Project presentation, RDM marketplace kickoff meeting
- WP 1: Project presentation, RDM marketplace barcamp
- WP 1: Project presentation, Institute meeting at IMBT/TVFA
- WP 2: Workgroup meetings, meeting protocols
- WP 2: Adaptation of deployment scripts and deployment documentation
- WP 2: Feature implementation, message-board and notifications
- WP 2: Feature implementation, CSV-import from TUG-Online for test devices and laboratory rooms
- WP 3: Feature implementation, redesign of code used to integrate manually collected measurement data into the process workflows (data structure and user-interface)
- WP 2, 3: Feature implementation, booking calendar (test device and workbench booking)
- WP 3, 4: Feature implementation, lab process workflows for BioMech, FELMI-ZFE and IMBT/TVFA
- WP 2, 3, 4, 5: Several deployments of test releases on the project test server
- WP 4: Interview with Marketplace as a basis of an article for the TU Graz innovation report
- WP 4: Workgroup meetings, meeting protocols
- WP 4: Feature implementation, device settings and device calibration
- WP 5: Feature implementation, pdf-export framework, pdf-export of materials, samples and process workflows
- WP 5: Project presentation, RDM marketplace barcamp
- WP 6: Feature tests, project closing workshop and project end report

Work, not defined in the workpackages:

- A Meeting with the data security committee and the workers' council (BRWiss) has taken place. The purpose of the meetings was to evaluate requirements regarding data security and measures against profiling of employees. The outcomes of the meetings were incorporated into an implementation guideline (GitLAB issue) and the first draft of the data security plan (see next point).
- A first draft of a data security plan is available (including data security concepts and general security measures). The required information regarding security issues and security measures were acquired from the information security guideline (ZID). David Camhy from the Institute of Urban Water Management (SWW) also shared his experience from one of his former projects.
- Numerous discussions were held with the project owner of "LabLog 2.0" (FELMI-ZFE) to establish and deepen the cooperation. As an outcome of these talks, several laboratory process workflows were implemented by the project team and tested by the end-users of FELMI-ZFE. For the test phase, we also established and shared an additional test instance of LabNDB on the test server.
- Feature implementation, export of data and metadata to the repository of TU-Graz (invenioRDM, restAPI). A prototype was implemented and the main functions were tested using the test instance of the repository of TU Graz.
- Implementation of a framework used to export PDF files for processes, materials and samples but also for other tables of the database. That framework, based on a Django-library and the PDF-LaTeX compiler, is fully implemented and tested.

Deviations in the work plan:

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A minor deviation in the project was the renaming of the project phases “Gathering information” to “Concepts” and “Project closing” to “Close-down”. However, the content has not changed.

There are three major deviations in the work plan. Those deviations are related to the objectives “rawdata preview” (1), “end-user tests and documentation” (4), and “SQL look-ups for inventory - devices - rooms” (5).

Deviation 1, rawdata preview: In several meetings and discussions, it turned out that the preview of device data is very time consuming and can be achieved only for some file formats (the Messphysik format and simple CSV-files). Additionally, the file formats are related to devices where one device can produce different file formats. Therefore, we decided to implement the software infrastructure to handle devices and their respective file formats and a small set of file parsers. We implemented a prototype to test the graphical representations for the often used Messphysik file format. That helped us to find out what issues we must solve in the future development.

Since this objective is closely related to the implementation of test workflows (laboratory tests) we decided to implement the workflows in the course of this objective instead. Therefore, we implemented at least one laboratory workflow that is often used from each institute involved in this project (IMBT/TVFA, BioMech, FELMI-ZFE). Despite the different requirements of the three institutes, all of the workflows matched the existing architecture of the solution quite well. From now on, it is clear that LabNDB can be a good solution for all kinds of laboratories.

Deviation 2, end-user tests and documentation: At the beginning of this project, we found that it would be a good idea to integrate the end users not only for testing purposes but also into the design of the solution. We established five workgroups (WG Authorization & Permissions, WG Materials & Samples, WG Processes & Tests, WG data export and WG Laboratory facilities). Each workgroup works on a specific topic. Workgroups consist of project team members and stakeholders (administrative staff, scientific staff, laboratory staff) of three different institutes on three faculties. The organization and management of the tasks performed in the workgroups were based on “agile project management”.

Therefore, we designed the workflow for the workgroups as follows:

- Evaluation (project team members present the current solution, acquire feedback, gather information and requirements)
- Implementation (adapt solution, implement required features, perform developer tests, deploy solution)
- Testing (end-users are allowed to try out the solution and are encouraged to submit feedback to the developers)

This iterative process was repeated two times over the course of the project.

In the beginning, it was planned to provide the end-user documentation separately from the software. The outcome of several discussions was, that it would be much more useful to include the entire documentation in the solution.

The advantages are:

- the documentation is available where it is needed
- it is easier to maintain and update the documentation in the course of further development
- documentation updates are deployed side-by-side with new or updated features
- web-based documentation supports features not available in file-based documentation (videos, animations, ...)

Deviation 3, SQL look-ups for inventory - devices - rooms: The initial plan was to update inventory, device and room information from the database of TUG-Online directly using SQL lookups. It turned out that the data could be obtained as tables in CSV format only. Therefore, we implemented a feature to update the database using CSV files from TUG-Online. That feature automatically updates existing ones and adds new items.

Changes in the work plan

The initial phase of the project took longer than expected. First we had to ask all stakeholders and to define and establish all workgroups. Second we had to introduce all workgroup participants into the workflow. This deviation has since been compensated during the project. The closing phase of the project also took us longer than expected because the implementation of some laboratory workflows were complicated and took longer. Therefore, the project end date shifted from 31.03.2023 to 20.04.2023.

3 Project team, cooperation and sustainability

- Have there been major changes in the project team?
- If some work is done together with other projects (RDM Marketplace or other): describe the cooperation between the projects.
- Are the current results visible at your research group/institute/faculty? Describe your dissemination activities?
- What are the specific plans to sustain the achieved results?

Changes in the project team: P. Knabl was a project team member and developer in the former project “LabNDB”. Since he finished his studies abroad in July, he joined the project team again.

Cooperations: As mentioned, cooperation with the RDM Marketplace pilot project “LabLOG 2.0” (FELMI-ZFE) is established. Several meetings with the project team of “LabLOG 2.0” took place. We implemented a small set of laboratory processes for FELMI-ZFE and shared an instance of LabNDB for testing purposes. Later, the end users of FELMI-ZFE tested the procedures and shared feedback with the project team. In general, the cooperation was very beneficial for both projects. FELMI-ZFE also stated a high level of interest to join the future development of LabNDB.

Additionally, team members of RDM biomECh vol.2 contributed to the testing workflow implementation as a case study within that project.

Visible results: We continuously deploy a test version of our solution on our test server. That allows all members of the workgroups to test the solution and become familiar with the look and feel of the user interface and the workflows. As mentioned, we also deployed a separate test instance for “LabLOG 2.0” of FELMI-ZFE. These test versions are accessible within the network of TU Graz. That enables interested persons of TU Graz, to create a demo account and test the solution by themselves.

Sustainability: The plan is to continue development in the upcoming years on our institutes. We are also reaching out to new collaborators and customers at different universities to evaluate their needs and to investigate how we can collaborate on further development. One of the next steps is to submit a project proposal to acquire additional funding for the implementation of the outcomes of this project in the laboratories of IMBT/TVFA, BioMech and FELMI-ZFE, and we are currently investigating suitable funding opportunities. The proposal will include activities regarding staff training, end-user documentation, transformation of existing working processes, change-management and the implementation of required features. We also plan to keep end-users (customers) integrated in the development process. We consider this as an important contribution to sustainable RDM practices.

4 Project costs

- Provide a brief overview of the current project costs.
- Are there any deviations from the cost plan?

Table 3: Project costs

Funded	Spent
€ 15,000.00	€ 15,000.00

The costs are related to the fee of the three developers (M. Eisner, B. Schmid, P. Knabl) employed for that project. Other contributions are institute in-kind and therefore not part of the costs shown above. Up to this date, no money was spent on hard- or software.

There are no deviations from the cost plan concerning the project funding.

Here, it is to mention that the in-kind performance of J. Harden and S. Sherifova is in the range of approx. 400 working hours (approx. € 14,000.00). Additional costs, for hiring our developers, that go beyond the project funding were paid by IMBT/TVFA (approx. € 3,800.00).