



Research Data Management proposal

Proposal title: *Laboratory Notebook and Database – Extensions* (Acronym: *LabNDB Ext*)

Project owner: Prof. Krüger (Head of the Institute), Prof. Holzapfel (Head of the Institute)

Additional team members and roles:

Jakob Harden, Institute of Technology and Testing of Construction Materials, University assistant, PhD student	Project manager, outreach, deployment, IT support
Selda Sherifova, Institute of Biomechanics, Postdoc	Team member, outreach, tutorials, testing
Mathias Eisner, Institute of Technology and Testing of Construction Materials, Student assistant	Team member, developer
Barbara Schmid, Institute of Technology and Testing of Construction Materials, Student assistant	Team member, developer
Philipp Knabl, Institute of Biomechanics, Student assistant	Team member, developer

*(Please add details of the staff who will undertake the activities, highlighting capabilities necessary and previous experience to undertake the project as attachment to the proposal. Please limit the information about each participant in the project to **500 characters**.)*

Detailed information on the staff and it's capabilities can be found in appendix 1.

Concept

*Describe the idea of the proposal (**max. 500 characters** including spaces)*

The main idea of LabNDB from the first RDM call remains in place: to collect, manage, store, analyse and reuse results from material testing processes in laboratories. This is mandatory to create a scientific body that supports transparency and reusability in the research and publication process. Beyond the already implemented basic functionalities, the need for further improvement points were identified in the first LabNDB development phase and will be handled in the extension phase.

Rationale

*What is the background to the proposal? (**max. 1000 characters** including spaces)*

The aim is to provide the researchers with an electronic lab notebook in the form of a database where management of experimental protocols and related data is done in connection with laboratory management. Products such as [SENAITE](#), [eLabNext](#), [ResearchSpace](#), [elabFTW](#), or [bookkit](#) only cover one or two of these aspects, and none of them offer a solution for FAIR RDM that is flexible enough: open for enhancements such as building a database that connects to other RDM services; easy for data re-use; and field-specific data classification. Even if a limited re-design may be allowed in the above-mentioned tools, their integration into the existing IT-environment (CyVerse, Repository, TUG-Online, etc.) would be complicated and/or very costly. Out of these tools, SENAITE is FOSS and can be adopted for the institutes' needs through a labour intense process. However, sustainability issues are foreseen as its framework has a limited developer community, therefore it can be obsolete in the future.

Objectives

*What goals do you plan to achieve? (**max. 1000 characters** including spaces)*

The main objective of the proposal is to improve the functionalities of LabNDB tool to prepare for product roll-out which can be adopted by different institutes of TUG at the very least. LabNDB is designed to aid not only ensuring FAIR data practices, but also laboratory management of, e.g., devices and materials. The main objective is divided into 8 sub-objectives each of which are additional LabNDB functionalities, namely: (O1) preview of rawdata for commonly used device file formats, (O2) booking calendar for test devices and workbenches, (O3) user authentication and authorization, (O4) SQL look-ups to TUG-Online inventory tables, (O5) end-user testing and documentation, (O6) code documentation, (O7) export to TUG repository and CyVerse, (O8) message board & notification.

RDM methodology and work programme

How do you intend to reach your objectives? What are the tasks in the project? What infrastructure or technology does the project require? Include a timeline and milestones/deliverables (max. 2000 characters including spaces)

The objectives are reached within 6 work packages (phases), see also the GANTT chart:

P1 - Project management: The kickoff takes place to plan for all the tasks to meet the objectives. The outcomes of this workshop and all other project plans are collected in the project handbook. Controlling meetings, the project owner meetings, managing deviations in the project plan, maintaining the communication inside the project team, the reporting to the controlling office and the reporting to the RDM team are also included in this phase.

P2 - Gathering information: The requirements for implementation of the new apps and functionalities, i.e., booking calendar, SQL look-ups, authentication, export to repository, alternative login options, and connecting the video tutorials with LLT and/or TUBE, are investigated and reviewed in a milestone meeting.

P3-P5 - Implementation Phase 1-3: It is planned to implement and improve the existing implementation the apps for: rawdata preview (O1), booking devices and sections (O2), user authentication - permissions - roles (O3), SQL look-ups for inventory - devices - rooms (O4), exporting data and metadata to the TUG repository and CyVerse (O7), message board & notification (O8). Development is distributed over 3 implementation phases, and is followed by the first end-user tests (O5).

P6 - Project closing and documentation: Code documentation (O6) as well as end-user documentation (O5), e.g., video tutorials, are prepared. Second run of end-user tests (O5) are performed, and the feedback is reviewed in the final milestone meeting.

Infrastructure/Technology: LabNDB is already deployed to a virtual machine on the institute's application server (Debian OS, apache2 reverse-proxy web-server, gunicorn WSGI enabled web-server, postgresSQL DBMS). There is no need for additional hardware. We continue the implementation using the Django web-framework. For graphical representations of the new features we plan to use nodejs and plotly-dash.

Impact, usage scenario and sustainability

What is the intended outcome of the project? How will the results be used (by your group or institute, and if applicable in other TU Graz faculties)? (max. 1000 characters including spaces)

The intended outcome is the LabNDB with improved functionalities. The solution is based on Django web-framework, which is used by millions of application and has a very large developer community. Therefore, sustainability issues are not expected on this aspect.



The web-based software will be used in daily research activities of both institutes involved in this proposal as well as FELMI, and there are already other institutes within and outside TUG which are interested in adoption. Further development and release conditions such as licensing must be discussed with other TUG units, especially if the tool is to be used outside the TUG as the demand shows.

Risk assessment

What risks are associated with the project? Do you have a plan to manage them? (max. 500 characters including spaces)

A working solution is already in place, all project team members who will work on app implementation now have the knowledge on developing a web application with the Django web-framework and the project team of LabNDB (developers and project management) stays the same. So we do not expect major difficulties regarding the implementation of the new features. The necessary IT infrastructure is already available and will also satisfy future requirements.

Requested budget

Please detail total costs of staff, travel, software and hardware. Are there any in-kind contributions in the projects? (max. 1000 characters including spaces)

Staff:

3 developers (M. Eisner, B. Schmid, P. Knabl) 8 months each, 10 hrs./week:

€ 21000,00 (estimation based on the real costs of the last project)

Other (hardware, software, travel):

not necessary/already available

In-kind:

S. Sherifova: 2 hrs./week for 12 months: € 4500,00 (73969,84/year based on 40 hrs./week)

J. Harden: 4 hrs./week for 12 months: € 6800,00 (55703,74/year based on 40 hrs./week)

€ 11300,00 (total in-kind)

Total project costs:

€ 32300,00

Appendix 1

Jakob Harden is a junior scientist at the Institute of Technology and Testing of Construction Materials with a focus on non-destructive testing. He started network administration during his studies; handled network, server and database administration for several companies; and is the IT-contact at the institute. Capabilities: software implementation in C, C++, Java, Python; server and database administration. During LabNDB development, he earned skills in web-based applications and project management.

Selda Sherifova is a postdoc at the Institute of Biomechanics focusing on experimental methods and data analysis. She is frequently involved in establishing new experimental protocols, where RDM can become even more challenging. She was the PO and PM for RDM biomECh vol 1, and was a collaborator in the first phase of the LabNDB project to enable digitalization of lab workflows in a FAIR manner. Thanks to this early collaboration, she is familiar with the structure and flow of LabNDB.

Mathias Eisner conducted experiments for his bachelor thesis at the Institute of Biomechanics, and currently is a master student in BME. He gained experience in database migrations and Python coding during his employment in AVL, which he transferred successfully to LabNDB development.

Barbara Schmid is a master student in BME with special focus on 'Biomedical Instrumentation and Sensors'. She gained experience in 'Continuous Integration' of software build- and test environments (mainly implementations in python) during her work in Infineon. She was the main responsible for the user-interface design of LabNDB.

Philipp Knabl conducted experiments for his bachelor thesis at the Institute of Biomechanics, and currently is a master student in BME. He was a team member of RDM biomECh, where he worked on design and analysis of the RDM survey, testing standardized documentation templates and development of apps for LabNDB. He has a strong interest in data management and Python, which he expanded significantly and applied within LabNDB development.