

In this hands-on tutorial, we will demonstrate the use of electronic lab notebooks (ELN) in physics lab courses particularly from the lecturer's and supervisor's perspective. Together we will configure an ELN (here: eLabFTW) using open-source Python scripts that create user accounts and user groups automatically. Moreover, all experiments will be predefined such that students – in a real-world lab course – experience the ELN as a valuable tool for structured acquisition of all data and metadata at one place. We will further demonstrate (i) how tutors can efficiently access the written preparation of the students, (ii) how data is recorded in the ELN and accessed later in python-based data evaluation, and (iii) how data can be combined in order to allow for novel insights or experiments.

Let's get started ...

Exercise 1 ("Student" registration for the lab course and setup of the ELN)

Imagine you are a student who signs up for the lab course together with another student as a team of two.

Register your lab course team

- 1. Open the link <u>https://www.lap.physik.nat.fau.eu/fairmat-users-meeting-eln/</u> in a web browser.
- 2. Click on Registration form and fill in the form with first name, last name and email of you and your lab course partner. You may use fantasy names, but please enter valid email addresses to which you have access to, because you will receive an email for account activation later (password setting). The registration code is: fairmat24

Preparing the ELN for the lab course (plenum demonstration)

This step is a plenum demonstration; please stop here and listen before you continue with step 3.

Using a Python script (JupyterNotebook), we will set up (i) user accounts and student teams from the registration data, (ii) templates and settings, (iii) all lab course experiments in the ELN.

First login to ELN (hands-on)

- 3. Open the ELN in the web browser by following the link <u>https://training.elabftw.data.fau.de/</u>.
- Click on the link Forgot password?, enter your email address (one of the emails used for the team registration) and click Send reset link.
- 5. Open your mailbox (e.g. on your mobile, your laptop, web mail app) and click on the Reset password link in the email received from training.elabftw@discard.fau.de. Enter a new



password (length min. 12 characters) and save the new password. Remember the password!

- 6. On the lab computer, now log into the ELN (<u>https://training.elabftw.data.fau.de/</u>, enter your email and password).
- 7. When logged in, navigate to Experiments in the top menu. You will see the predefined experiments for the lab course. There are two categories of experiments:
 - a. Lab Course Day (green label): These entries are used for grouping the experiments of one lab course day for easy navigation. In addition, the report on the lab course day can be uploaded here; there is a to-do-step predefined that reminds this task.
 - b. Experiment (blue label): These entries are used for documentation and collection of all data and metadata related to one lab course experiment. The documentation includes (i) motivation, (ii) preparation (background), (iii) experiment description, (iv) results and observations, (v) evaluation notes, (vi) uploaded files (measurement data, figures, evaluation scripts), (vii) metadata and structured data.
- 8. Try out the navigation through experiments, e.g.
 - a. Use the filters (categories, tags) in the experiments overview.
 - Access experiments through the lab course day entry (with green label), section Linked experiments.

Exercise 2 (Written preparation to the lab course experiments)

Prepare yourself for the lab course experiments (student perspective)

Now, imagine being a student who prepares for the experiments of the forthcoming lab course day. In contrast to the traditional preparation (e.g. a written summary of experimental/theoretical background in one document), we prepare the experiments directly in each ELN entry (i) by identifying the motivation to the experiment, (ii) by answering questions from the experiment instructions and (iii) by describing the experiment. This comes with the benefit of having all experiment-related information at hand when actually doing the experiment in the lab.

- 1. Fill in the sections Motivation, Preparation, and Experiment description in the main text for the 3 experiments of this demo lab course according to the experiment instructions shown on the next page (gray box). In order to enter the edit mode, navigate to the respective experiment and click onto the pencil button. Note: At this point, you only have to complete the preparation tasks!
- Set the status of each experiment in the ELN to Preparation finished and check the to-do-step Preparation.



Experiment instructions (DemoLab, lab course day 1)

Experiment 1.1: I-V characteristics of a resistor

In this experiment, you will measure the currentvoltage (I-V) characteristics of a commercial resistor by sourcing voltages and reading the respective currents (see circuit diagram).



Preparation task

Fill the sections Motivation, Preparation

and Experiment Description in the respective ELN entry as follows:

- 1. What is the Motivation of this experiment (write down one sentence)?
- Answer the following question in the section Preparation: Which type of I-V characteristics do you expect?
- 3. Copy the circuit diagram from this page into the section Experiment description (the file can be found on https://www.lap.physik.nat.fau.eu/fairmat-users-meeting-eln).

Experiment

Measure the I-V characteristics of the given resistor for voltages from 0 V to 8 V.

Evaluation

Determine the resistance from the measured I-V characteristics. Update the ELN entry by storing the result to an eLabFTW extra field R (unit Ohm) in an extra fields section Results.

Experiment 1.2: FAIRmat

Preparation task

- 1. What is FAIRmat about? Write a one-sentence Motivation.
- 2. Find the FAIRmat logo in the internet and copy/paste it into the section Preparation.
- 3. Describe how you would draw the FAIRmat logo in the section Experiment description.

Experiment 1.3: Schrödinger's cat

Preparation tasks

- 1. What is the Motivation of having a cat?
- 2. Use the drawing tool in eLabFTW, draw a picture of Schrödinger's cat and insert it into the main text into the section Preparation (tip: use the option "Insert in text at cursor position" from the more-options-menu of the graphics file in the uploads section when in edit mode of the experiment).



Review the written preparation of the students (tutor/supervisor perspective)

This step is a plenum demonstration; please stop here and listen before you continue with exercise 3.

While it's beneficial for the students to have all written preparation organized in the respective ELN experiments, tutors/supervisors would like to see a compiled excerpt of the complete written preparation for each student team. We will demonstrate, how such excerpts can be generated using a Python script (plenum presentation).

Exercise 3 (Perform experiment 1.1 and document the results; student perspective)

Prepare the ELN entry

- In eLabFTW, navigate to Experiment 1.1: I-V characteristics of a resistor and enter the edit mode (pencil button).
- 2. Go to the main text and delete the default text between the heading "Results" and the table (if you want, you can enter observations from the experiment here).
- Change the column description of the table as follows.
 Column 1: V (V), column 2: I (mA).

Measure the I-V characteristic

- 4. Now, we are ready to perform the experiment and take measurement readings. The experiment is already prepared (DMM in DC current mode, power supply output activated). Use the turning wheel for adjusting the output voltage. Take readings for the following voltages: 0 V ... 8 V in steps of 1 V. Note all values in the table (using a decimal point for floats). Mind the units: note all voltage readings in volt, all current readings in mA.
- 5. Click Save.
- 6. Set the status to Experiment finished and check the to-do steps Experiment and Upload all data.

Exercise 4 (Evaluation of the measurement data; student perspective)

Create an API key

Modern application programming interfaces (API) use so-called API keys in order to authenticate the user.

- 1. In eLabFTW, navigate to the user menu in the top menu and go to User Panel.
- 2. Open the tab API Keys.
- 3. Enter a name for the API key and set the permissions to Read/Write.



- 4. Click on Generate an API key.
- 5. The API key will be shown. Make sure not to close the webpage, because for security reasons the API key is only displayed once.

Prepare the JupyterNotebook

- 6. Change to the browser tab with Jupyter and create a new notebook (with Python 3 kernel). Note: If you are working on your own computer, please make sure that you have JupyterNotebook and pyelabdata installed (see page 8 for details and required versions).
- 7. First, we will need to load some Python packages/modules. Enter:

```
import pyelabdata as eln
import numpy as np
import matplotlib.pyplot as plt
from scipy.stats import linregress
```

Execute the code box by pressing Shift-Enter on the keyboard (do so also after the following steps).

8. Now, let's define constants with the server URL of eLabFTW, your API key (copy-paste your API key from the eLabFTW webpage) and the experiment ID of experiment 1.1 (the ID is displayed in the experiment in edit mode):

```
URL = 'https://training.elabftw.data.fau.de/api/v2'
KEY = 'your-api-key'
EXPID = your-experiment-id
```

Access and visualize the data

9. In the next step, we will connect to the ELN and retrieve the data, which we have just

entered into the table of the experiment.

```
eln.connect(URL, KEY)
eln.open_experiment(EXPID)
data = eln.get_table_data()
print(data)
```

You should hopefully see your data.

10. Let's put the voltages and currents into separate variables (just for convenience).

```
V = data['V (V)']
I = data['I (mA)']
print(f'V = {V} V')
print(f'I = {I} mA')
```

11. Now, we will plot the data in a diagram with meaningful axis labels:

```
fig, ax = plt.subplots()
ax.scatter(V, I)
ax.set_xlabel('V (V)')
ax.set_ylabel('I (mA)')
```

You should see a nice diagram showing the I-V characteristics.



12. We want to attach this diagram to the experiment entry in the ELN.

eln.upload_image_from_figure(fig, 'iv_plot.png', 'comment')
Instead of "comment" you should enter a meaningful comment describing the diagram.

Evaluate the resistance from the I-V characteristics

13. In the next step, we will determine the resistance from the slope of the I-V characteristics.

```
fit = linregress(V, I)
print(fit)
R = 1 / fit.slope * 1000
print(f'R = {R} Ohm')
```

14. Now, let's store this important result in the ELN. In order to make it machine-readable, we

15. We also visualize the fit curve and the result for the resistance. For this, copy the 4 code lines from step 11 and add the following two lines:

ax.plot(V, fit.slope*V+fit.intercept, color='red')

- ax.text(4, 0.2, f'R = {R/1000:.1f} k\$\Omega\$', color='red')
- 16. Let's upload this figure to the ELN entry, too. Use the same command as in step 12, but change the filename to 'iv plot evaluated.png'.

Save the JupyterNotebook in the ELN

17. Finally, we save the JupyterNotebook to the ELN. In this way, all data are together: motivation and description of the experiment, raw data, figures, numerical results and the JupyterNotebook with the code that evaluated the data.

eln.upload_this_jupyternotebook('some comment')

Again, instead of "some comment" you should enter a meaningful comment describing the notebook.

18. In the ELN, set the status to Finished and check all remaining to-do steps of Experiment 1.1.



Exercise 5 (Comparison of all measurement results)

In this exercise, we demonstrate how easy it is to access and compare "interoperable" data (more precisely: data following an agreed standard). With just a few lines of code, it is possible to read all evaluated resistances from the previous exercise of all teams (and even across semesters). This enables

- new insights, e.g. monitoring of the performance of the lab course setups and identifying setups that show "outliers",
- novel lab course experiments based on a "big data" approach (e.g. spread of resistance values within the tolerance)

We will do this together ... or try it yourself with the following hints (note: in order to access the data of the other groups, they need to give you read permission to their experiment 1.1):

With eln.list_experiments (tags=['Exp_1.1']) you can get a list of IDs of all experiments, which have the tag Exp_1.1. Now, loop through these experiments and read the evaluated resistances from the extra field R using eln.get_extrafields('R', expid=i), where i corresponds to the respective experiment ID. When collecting all the resistance values of the experiments in a Python list (e.g. all_values), you can easily visualize the spread of resistances in a histogram using matplotlib's function ax.hist(all_values).

Have fun!



Remarks and further information

This hands-on training uses an as-installed training instance of eLabFTW (without SSO) hosted by FAU CDI (<u>https://www.cdi.fau.de</u>).

For the evaluation with Python, JupyterNotebook (version \geq 7.0) is required on the local computer (we use the Anaconda distribution). In addition, the package pyelabdata (version \geq 0.2.2) is used for accessing data stored in eLabFTW. pyelabdata can be installed via

pip install pyelabdata

(when using Anaconda, enter this command on the Anaconda Prompt).

Links:

- GitHub repository with ELN configuration scripts:
 https://github.com/FAU-PHYSIK-EP/labcourse_with_elabftw
- pyelabdata documentation on PyPI: <u>https://pypi.org/project/pyelabdata/</u>
- eLabFTW: <u>https://www.elabftw.net</u>
- Anaconda distribution: <u>https://www.anaconda.com/download</u>

Contact:

Dr. Michael Krieger, Lehrstuhl für Angewandte Physik, Department Physik, FAU Erlangen-Nürnberg, <u>michael.krieger@fau.de</u>, <u>www.lap.physik.fau.eu</u>

Data:

If you don't have real measurement data, you can use the following data:

V (V)	l (mA)
0	0
1	0.098
2	0.197
3	0.295
4	0.393
5	0.491
6	0.590
7	0.688
8	0.786