Enriching Scientific Research with Metadata: Electronic Lab Documentation Landscape at HZDR
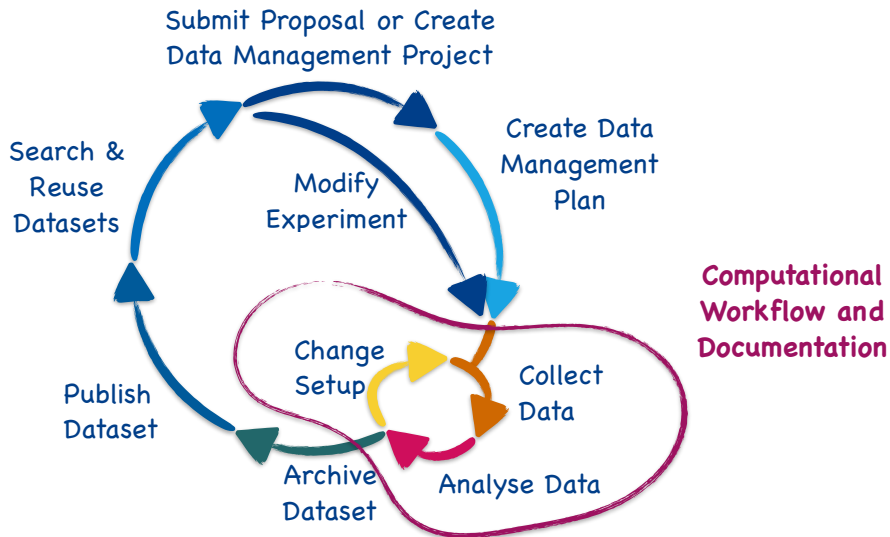
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Goal - Most complete description of the data set
Data life circle

Submit Proposal or Create Data Management Project

Create Data Management Plan

Modify Experiment

Search & Reuse Datasets

Computational Workflow and Documentation

Change Setup

Collect Data

Publish Dataset

Archive Dataset
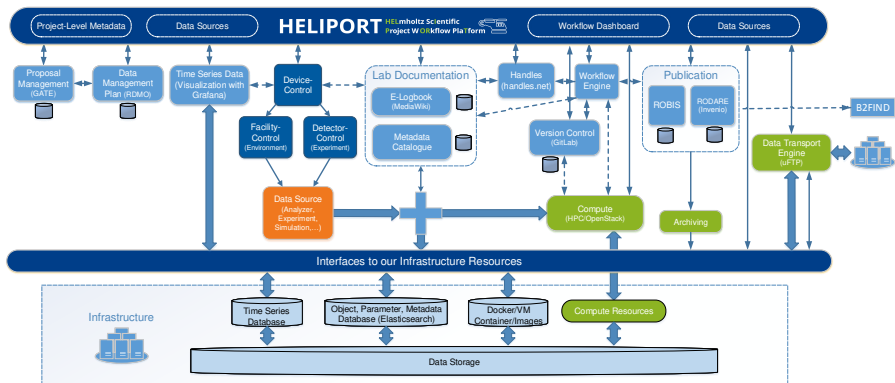
Analyse Data

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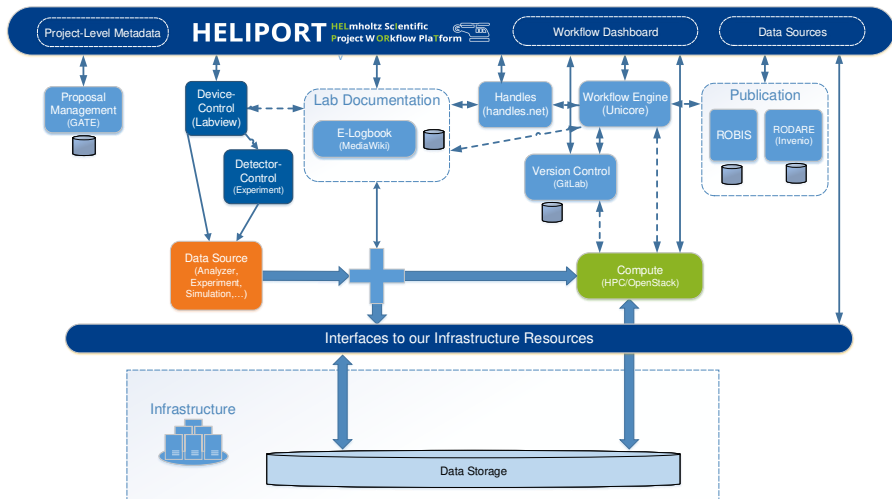# Mindmap for Components of Documentation

How to Initialise an Electronic Documentation

- Identify the essential elements (e.g. Sample, Measurement, data sets)
- Which properties describes each element?
- What are the relationships between the elements?
- How should the different elements be arranged in the documentation tool?
- Who has the right to edit what (rights management)?
- Which elements/properties are already in digital form and how can they be accessed?
- What are the IT resources and how can the electronic documentation be mapped to them?
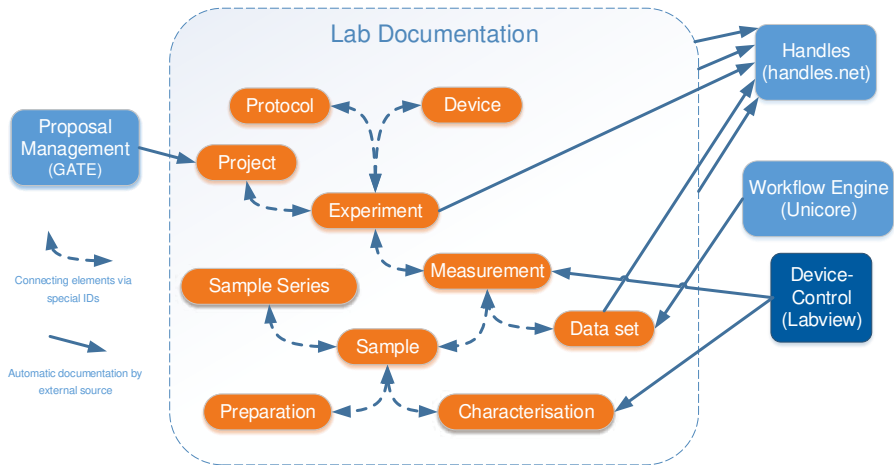
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Interaction Diagramm of a selected Experiment

Interaction Diagramm of a selected Experiment

Typical Documentation Structure

Lab Documentation

Proposal Management (GATE)

Protocol

Device

Project

Experiment

Sample Series

Measurement

Sample

Preparation

Characterisation

Data set

Handles (handles.net)

Workflow Engine (Unicore)

Device-Control (Labview)

Connecting elements via special IDs

Automatic documentation by external source

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Advantages of Electronic Documentation

- Gather information in individual ways from different sources by reusing already collected data
- Time savings by reusing gathered data through connecting existing elements to new elements
- Collaborative working from different places by multiple persons
- Advanced search for structured meta data, strongly depends on selected tool (data base type, API, etc.)
- Search within the program and from other programs
  - e.g. Within a jupyter notebook ask the API of the documentation tool for all datasets for device "xyz" measured with sample "abc" with parameter 1 = "1 unit" and parameter 2 > "2 unit" from last beamtime
- ...

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Why we used Mediawiki – which is not an ELN

- Mediawiki is not a typical ELN, but can be a central part for electronic documentation
- We have chosen it for the following reasons:
  - ✓ Open source
  - ✓ Was already in use by several groups
  - ✓ Highly adjustable pages including Template, Forms, flexible linkage ...
  - ✓ Large development community
  - ✓ rich on extensions: Draw.io, external data, ...
  - ✓ Extensive API, various import and export formats
  - ✓ Good integration into our existing IT landscape
  - ✓ Storing information in structured and unstructured ways possible
  - ✓ Advanced search options
  - ✗ Rights management needs work
  - ✗ Time consuming setup of an ELN for a group

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There is no perfect ELN

- Don't spend too much time trying too many tools!
- Most of the work is in talking to scientists about how they structure their work, so that it can have a structured documentation
- Even unstructured electronic notes (freetext wiki, HedgeDoc, GoogleDoc) are better than handwriting on paper...

Thank you for your attention

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Challenges of setting it up

- Define requirements to find the right electronic documentation tool
- How much man power is available in the IT department? The more complex and more configurable the tool, the exponential more support from IT department is needed.
- High initial overhead until advantages comes visible
    - Try to full fill small steps instead of all at once
- Different viewpoints/priorities and "language" between scientist and IT person
- Usage by the user only if they see an advantage (e.g. saving time) or if they have to.
- ...

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Resources

- ELN Showcase (public) `https://notes.desy.de/p/JwrpIb486`
- Multiple ELNs available (`https://zenodo.org/record/4723753`, `https://en.wikipedia.org/wiki/List_of_electronic_laboratory_notebook_software_packages`, etc.)
- Guides to find the right one (`https://www.forschungsdaten.org/index.php/ELN-Finder`,`https://repository.publisso.de/resource/frl:6415715`, etc.)

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