

HELIPORT@HI-Jena

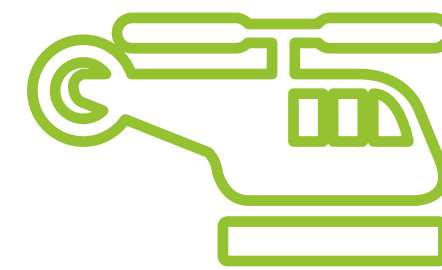
and related IT activities

Alexander Kessler¹, Joachim Hein², Malte Kaluza^{1,2}

¹ HI-Jena ² Institute of Optics and Quantum Electronics

HIJ semi-annual palaver 09.03.2022

- Cultural change and F.A.I.R. principles
- HIJ IT Infrastructure
- High Power Computing Partition in Draco Cluster
- HMC Project HELIPORT
- Our part inside HELIPORT
- Meta Data for Laser Systems and Experiments
- Collaboration for Meta Data Scheme
- HELIPORT and Digital Tweens
- Expected Benefit

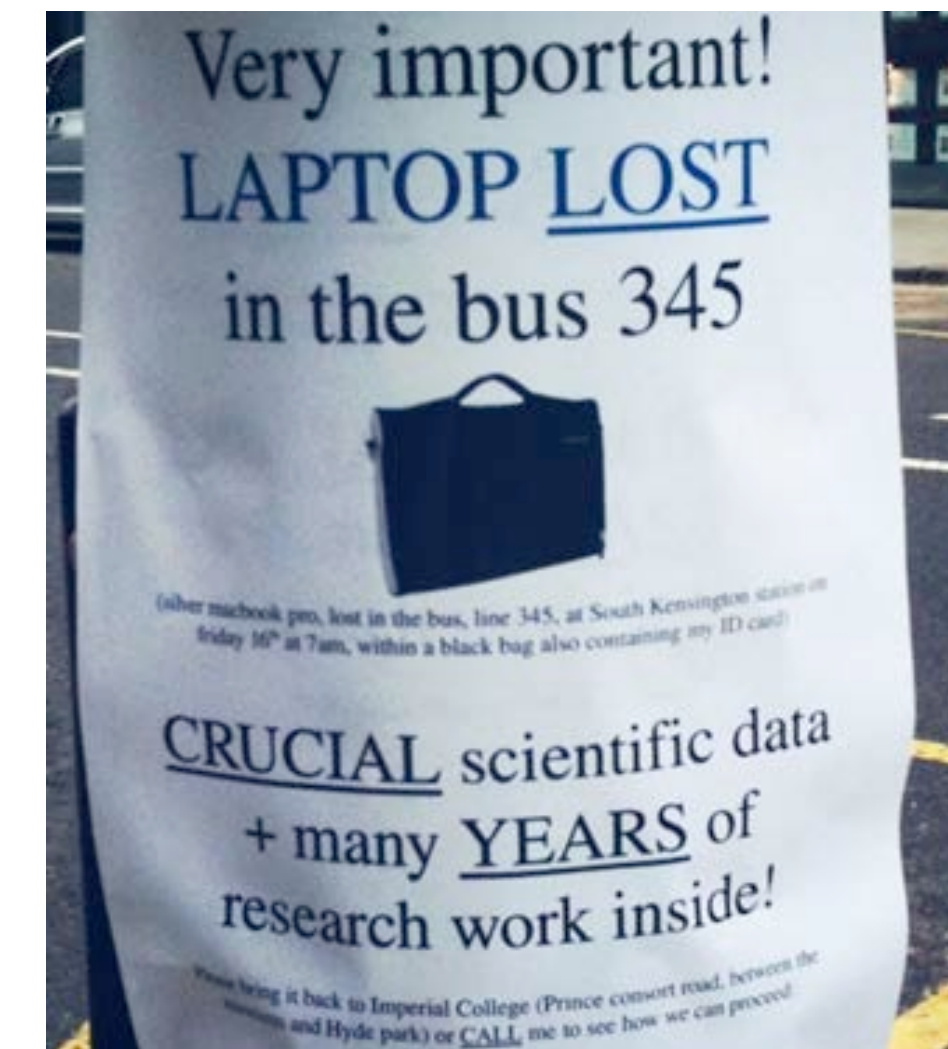
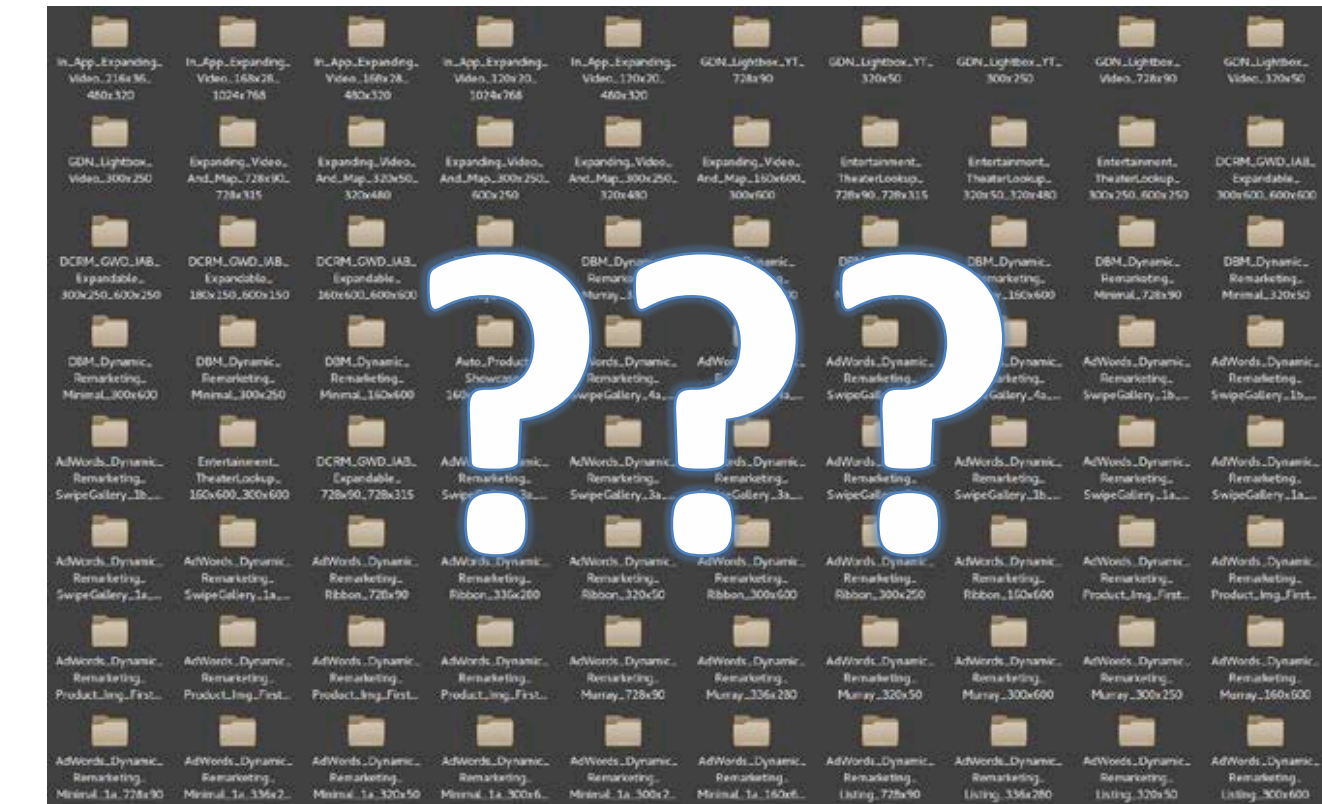


Cultural change and F.A.I.R. principles

- HIJ-IT meeting in February 2019. Consensus:
 1. We need a cultural change in handling of scientific data. Scientific data must comply with F.A.I.R. principles.
 2. supported by SW and HW infrastructure
- F.A.I.R. Principles:

[Wilkinson, M. D. et al. <https://doi.org/10.1038/sdata.2016.18>]

 1. Findable (POI¹, rich MD², registered in global Catalog)
 2. Accessible (via standardized com. Protocol)
 3. Interoperable (common Language for Knowledge Representation)
 4. Reusable (License, Provenance, Community Standards)



The F.A.I.R. Principles for HELIPOINT: <https://heliport.hzdr.de/principles/>

¹ Persistent Object Identifier; ² Meta Data

HPC Nodes and DMS and Storage Server

- 2020-2021: Project HDA founded by Thüringer Aufbaubank
(High Power Computer und Datenmanagement Architektur, Nr: 2019 FGI 0013)
 - Data management and storage server (phys. 320 TB -> ca. 500 TB with ZFS compression)
 - 516 GB RAM, 1x AMD EPYC 7302P 16 Cores, TrueNAS OpenZFS based
 - 4x hybrid CPU-GPU Nodes
 - CPU 2x AMD EPYC Rome 7702; 128 cores total; max. Freq. 3.35 GHz; 1 TB RAM
 - 4x NVIDIA Tesla V100 32GB RAM; Connected via 100 GB Infiniband
 - Some workstations for POLARIS, JETI, X-Ray and NLO groups
- In close collaboration with André Sternbeck:
 - Installation in HPC room @ Beutenberg
 - SW administration
 - Schooling and technical support



Thüringer Aufbaubank

Die Förderbank.

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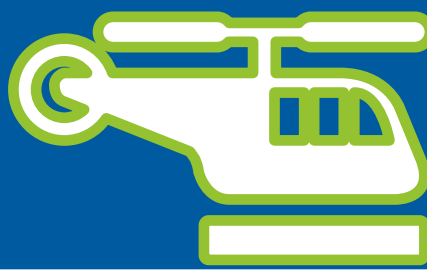
HPC Cluster

- HPC nodes became a partition of Draco cluster
<ssh <fsuid>@login1.draco.uni-jena.de>
- Your [fsuid](#) must be member of [hij-draco-users](#) group, contact me if you are interested
- HIJ has priority access
- Nodes are available also for other scientists
- Otherwise, HIJ can use other nodes, if better suitable
- Slides from hand on workshop:
<http://sternb.gitpages.tpi.uni-jena.de/hpc-101/>



Installed nodes in HPC Room at Beutenberg

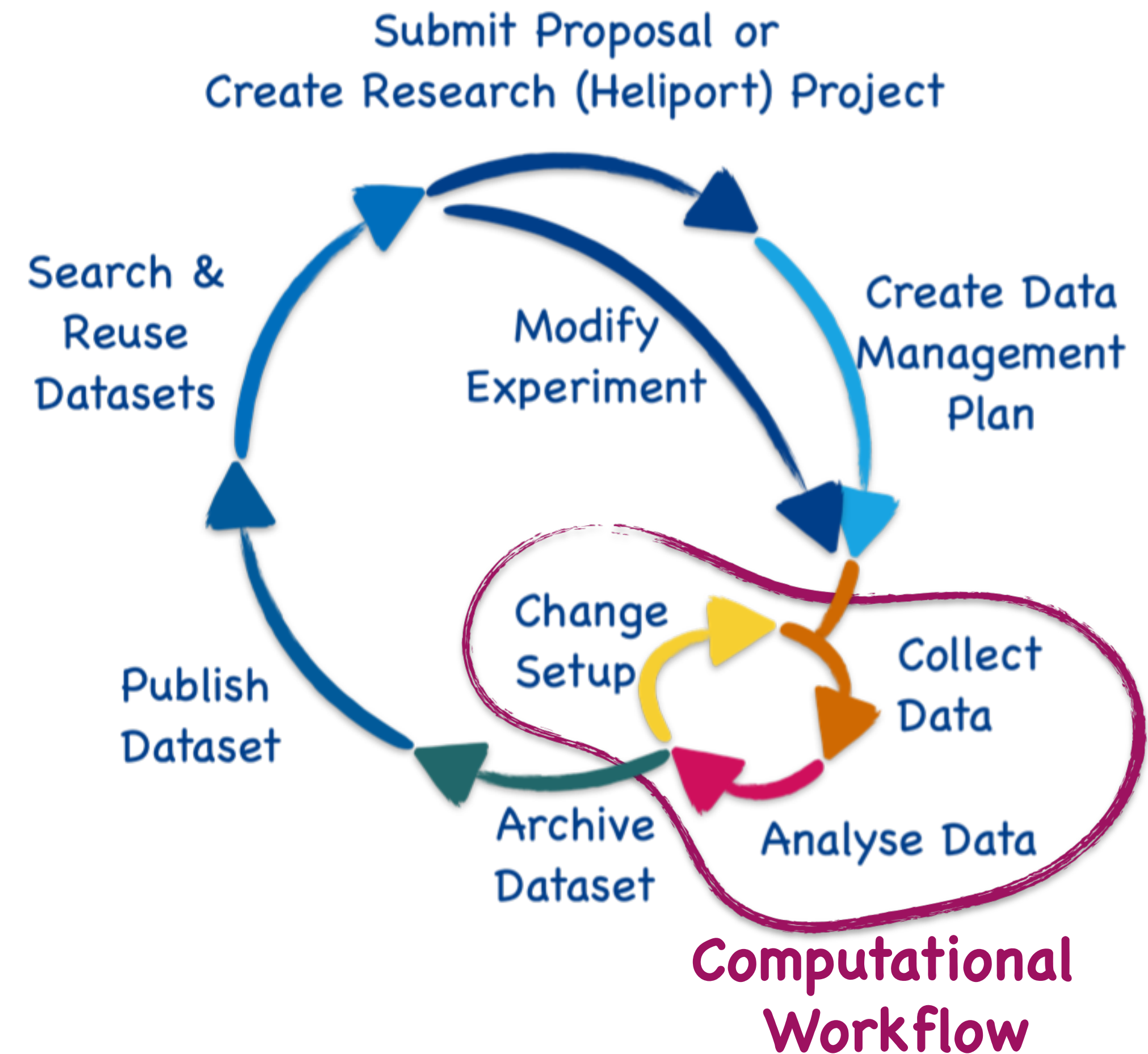
HELIPORT Project



HELMholtz Scientific Project WORkflow PlaTform

<https://heliport.hzdr.de/>

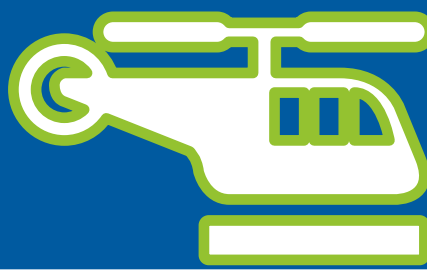
“HELIPORT aims at developing a platform which accommodates the complete life cycle of a scientific project and links all corresponding programs, systems and workflows to create a more F.A.I.R. and comprehensible project description”



Founded by:



www.hi-jena.de



- HZDR:
 - project management
 - core development
 - TELBE as use case
- HZ Jülich:
 - Unicore support
 - CWL workflows (Common Workflow Language)
- HI-Jena:
 - integration of POLARIS or JETI laser system and related experiments
 - Development of an experiment specific metadata schema



Oliver Knodel
Thomas Gruber
Mani Lokamani
Stefan E. Müller
David Pape



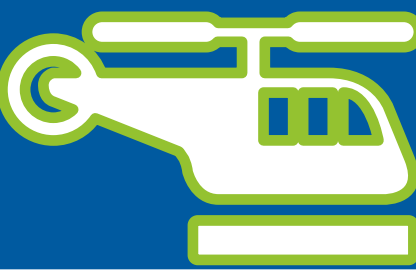
Bernd Schuller



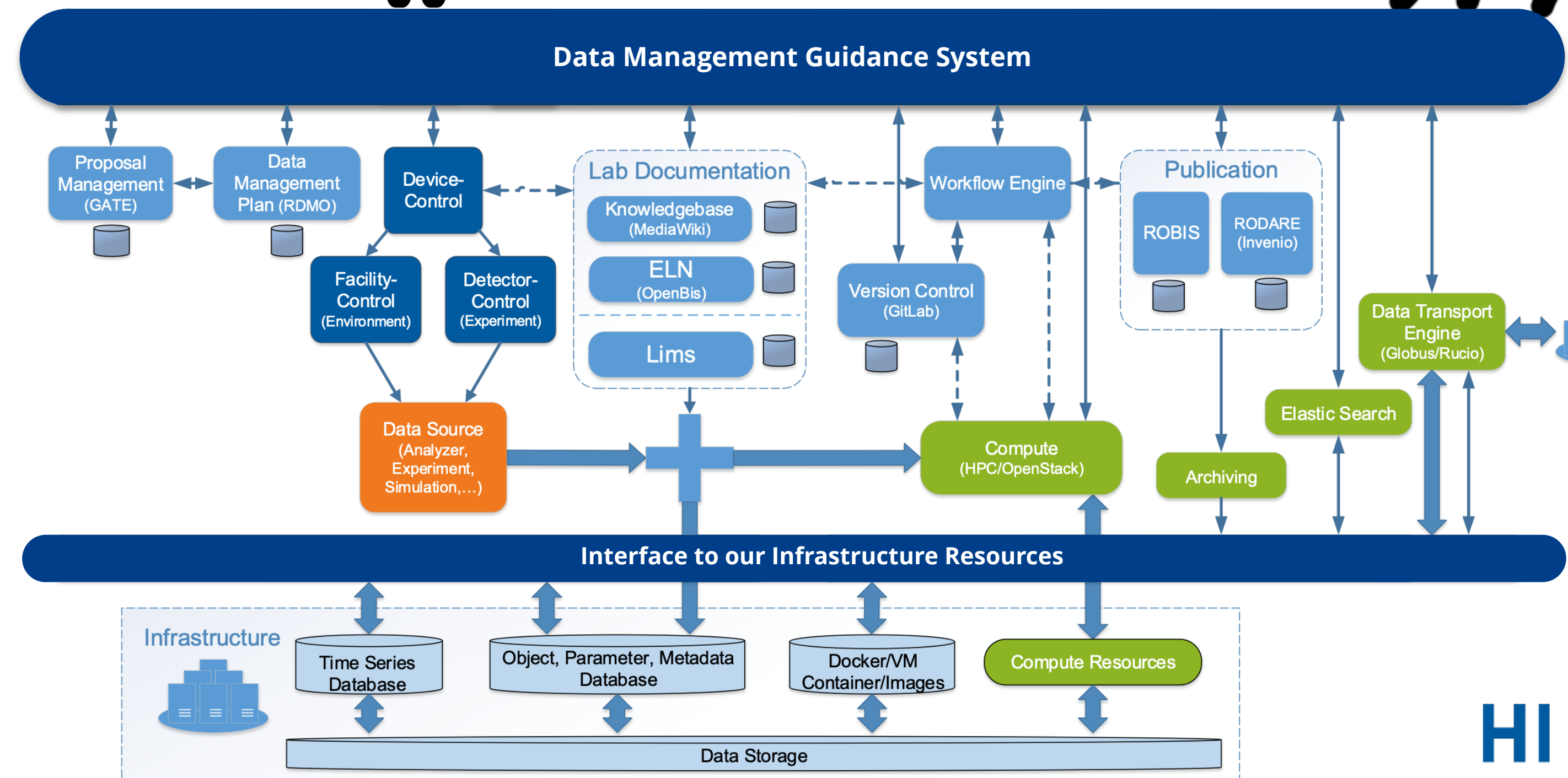
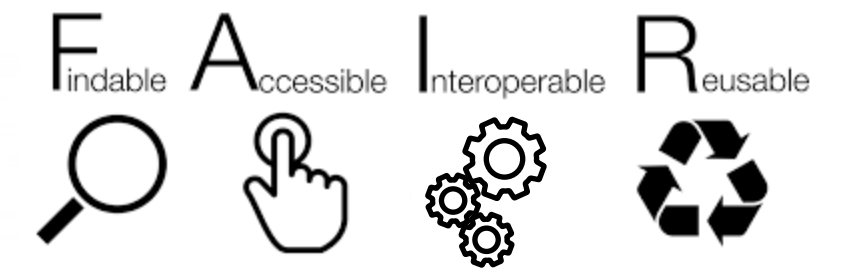
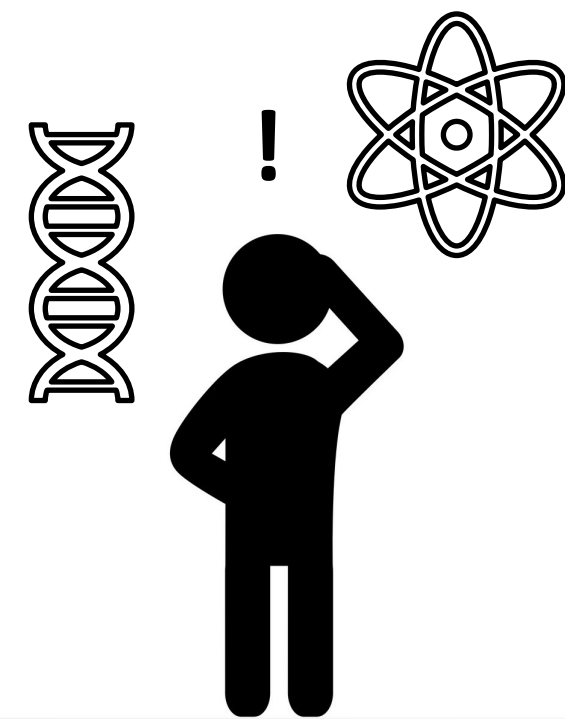
Alexander Kessler
Joachim Hein
Malte C. Kaluza
and:
???



HELIPORT, the Idea behind



- The HZDR IT infrastructure can support various experiments, but it is complex...
- Scientists often don't know which services are available and how to use them.
- An overarching system guiding scientists (and visitors) through the lifecycle of their research project (and our services) is inevitable.
- The concept of F.A.I.R. research becomes an important topic for scientists.



HELIPORT, the Idea behind

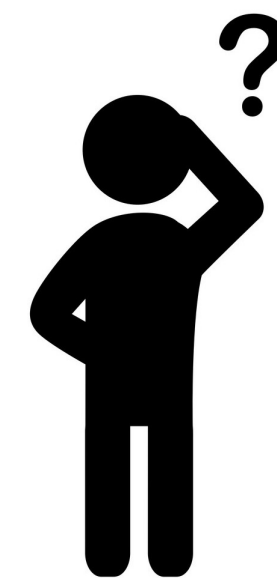


— Decision to use the guidance system to answer the most important questions of our scientists:



And how we can support them?!
What are the necessary steps towards a full comprehensible and FAIR research experiment ensuring data provenance?

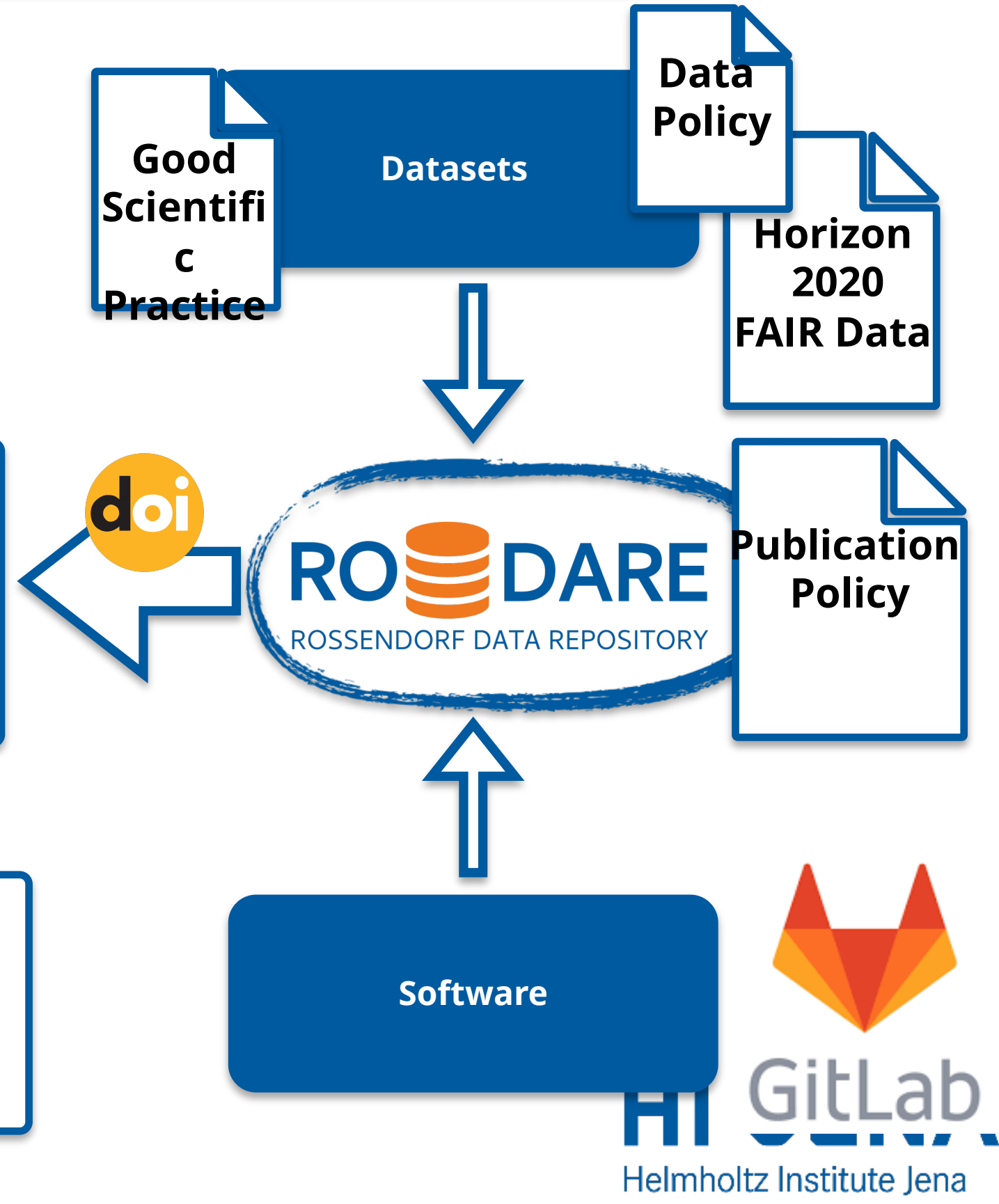
How can we automate recurring processes and keep track of status and data products?



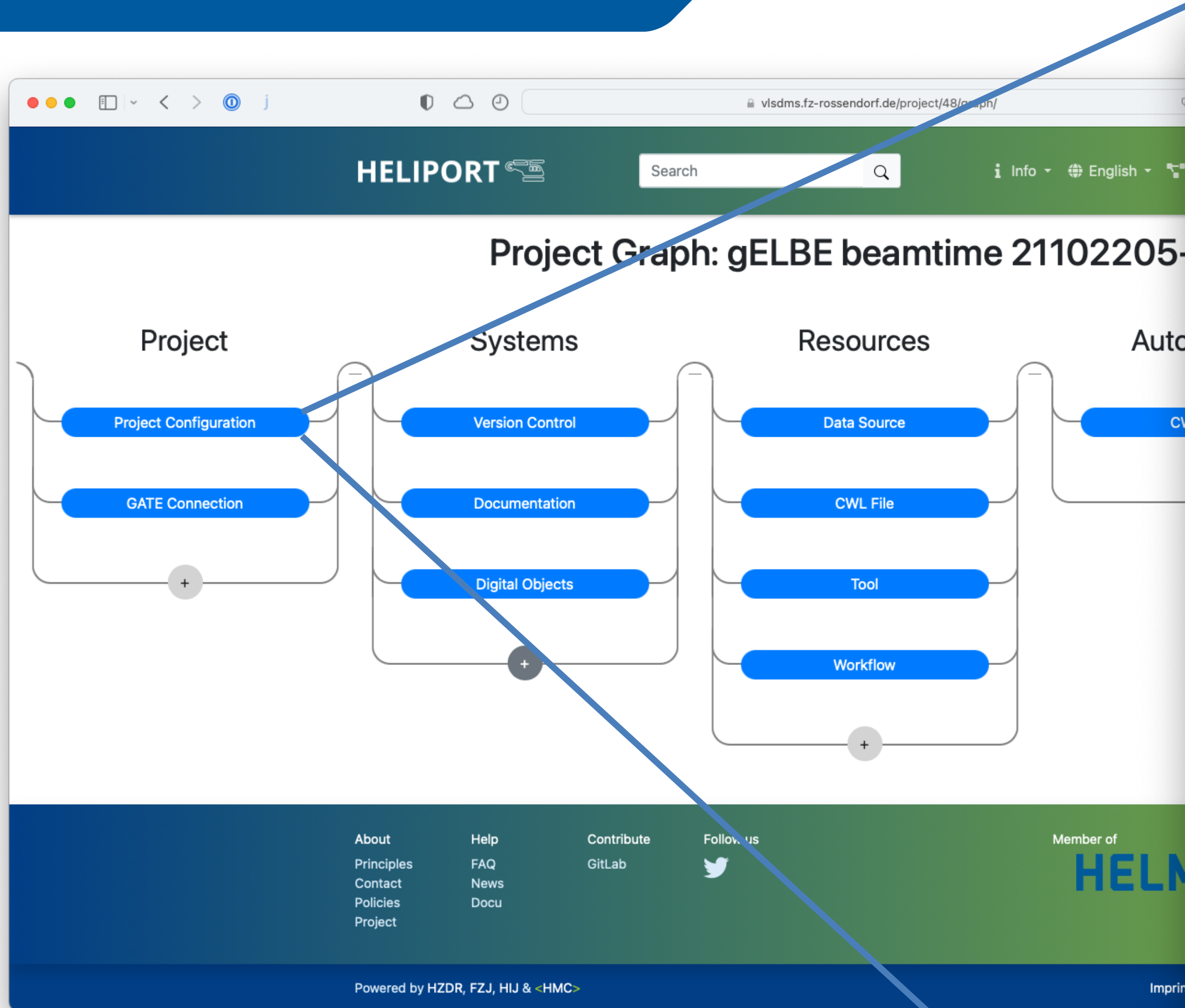
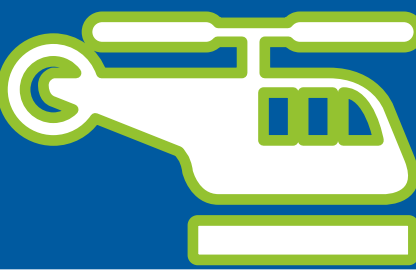
Which datasets or software can be published (and how)?

How can we bring new team members or external scientists into our project lifecycle and all associated tools?

Where are data, software and how can I gain access to both of them?



HELIPORT Web User Interface

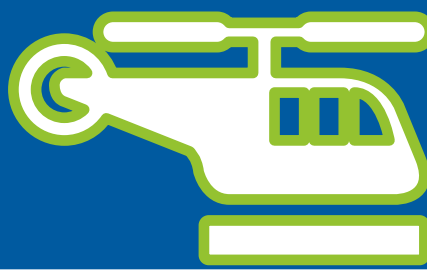


The screenshot shows the HELIPORT web interface for a specific project. The breadcrumb trail is 'Projects > gELBE beamtime 21102205-ST > Properties'. The main content area is titled 'Project Properties' and contains a table of key-value pairs for various project attributes.

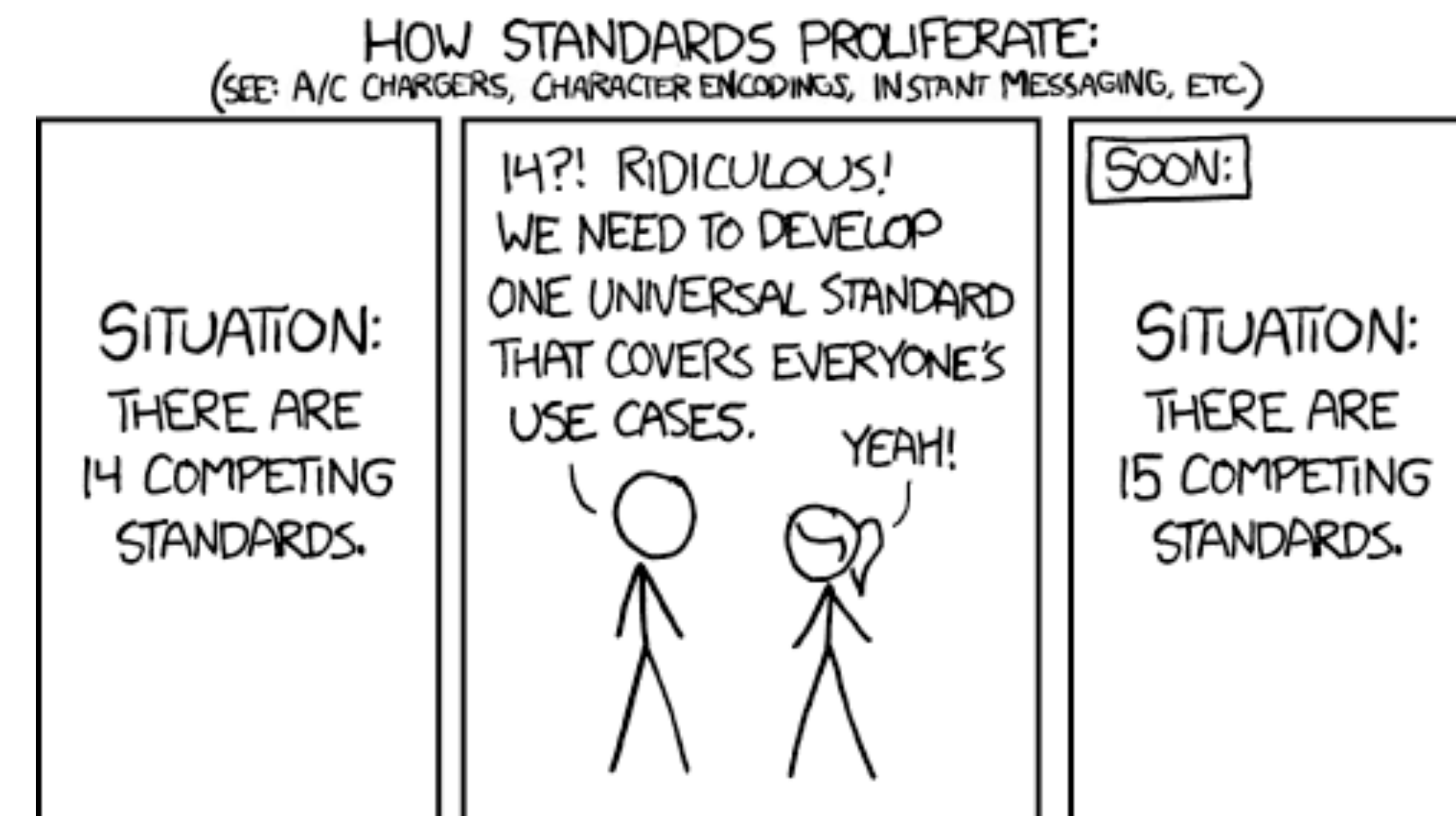
Property	Value
HZDR-ID	HZDR.FWCC.2021.762294
Handle	20.500.12865/HZDR.Projects.2021.FWCC.Project.48
Digital Object ID	2017
uuid	aaaffbb5-00d5-499d-acfb-f805647e9bf4
serialization url	https://vlsdms.fz-rossendorf.de/project/48/serialize/
Owner	Mueller, Dr. Stefan (FWCC) - 7394
Created	Aug. 20, 2021, 9:16 a.m.
Department	FWK
Title	gELBE beamtime 21102205-ST
Description	Tests of the detector system for the Stopping Target Monitor of the MU2E experiment in a high flux pulsed gamma beam (Resubmission of 20101909-ST due to COVID pandemic).

Below the table is an 'Edit' button. Underneath is a 'Members' section with a table:

Name
Ferrari, Dr. Anna (FWKH) - 5161

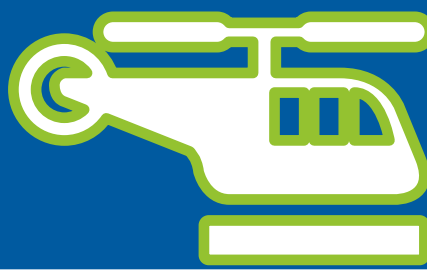


- Installation and Test of HELIPORT
- Installation of Services or Link to them
- Integration of POLARIS or JETI and Experiment in HELIPORT
- Definition of Meta Data Standard for High Intensity Lasers (HIL) and related experiments

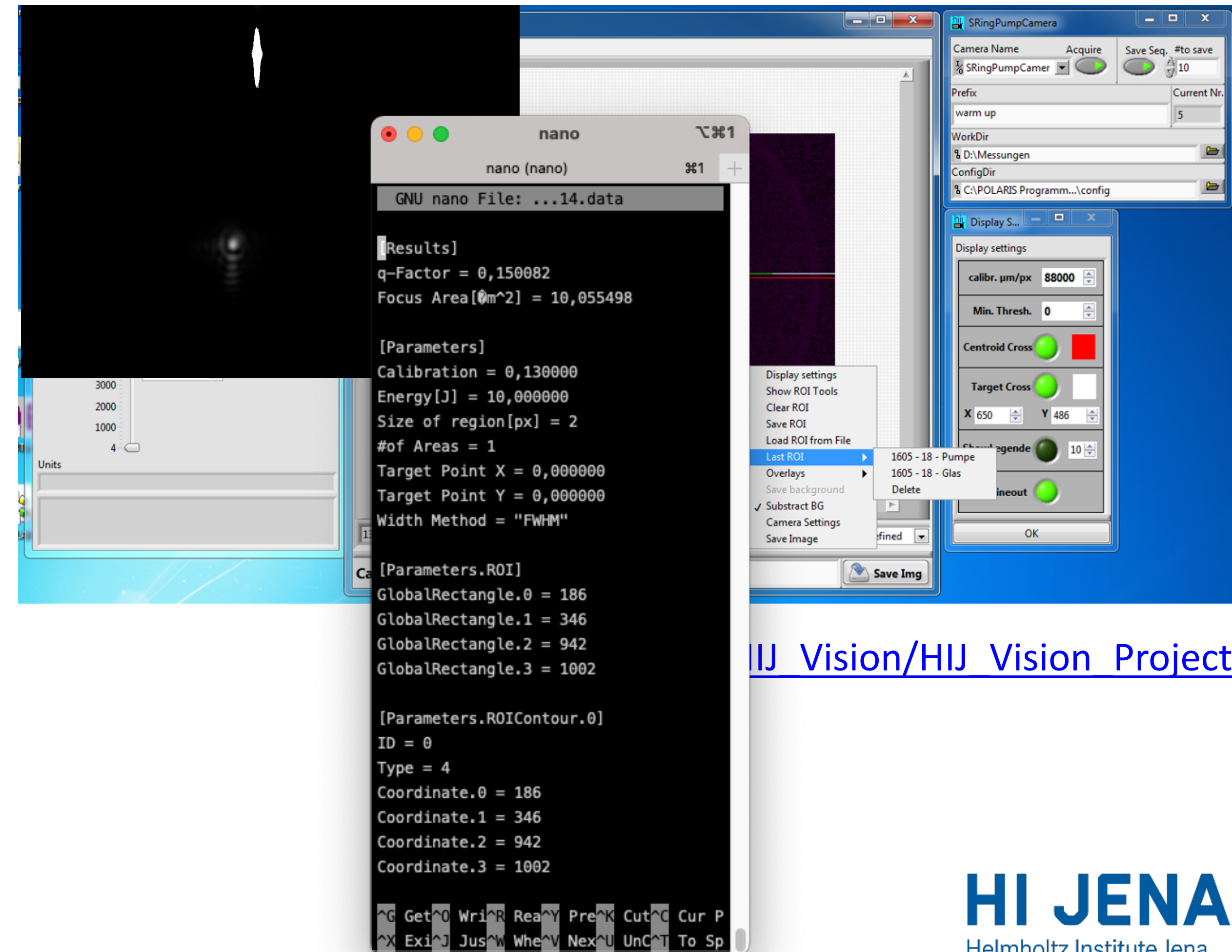


Source: <https://xkcd.com/927>

A very simple Meta Data Example



- HIJ-Vision Lib* saves in addition to the image the information, how the results were obtained.
- It contains settings like:
 - Camera (gain, exposure time, etc.)
 - Region Of Interest (ROI)
 - Calibration
 - Link to Background Image
 - and so on, everything that is important to reproduce results!

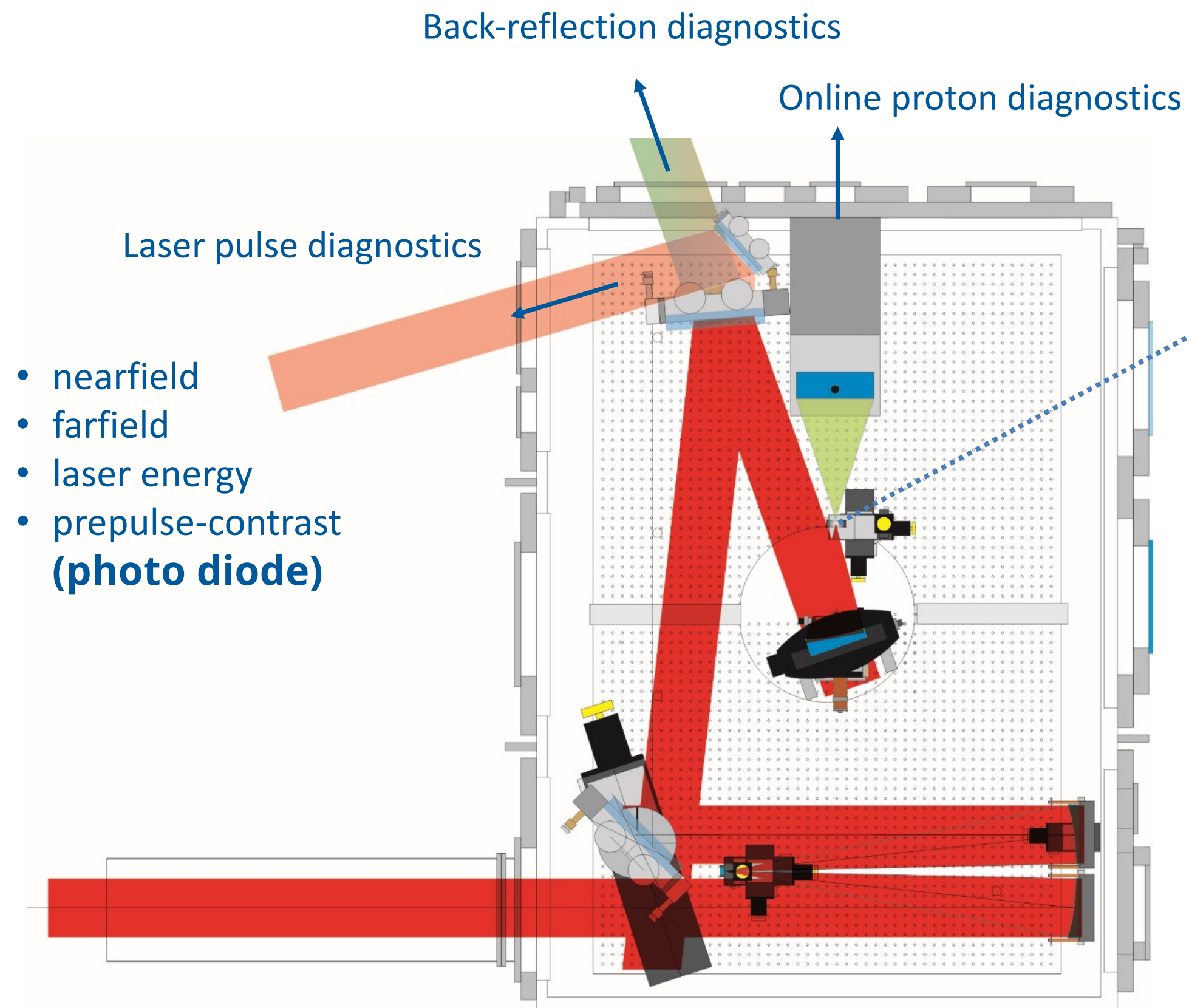


[HIJ Vision/HIJ Vision Project](#)

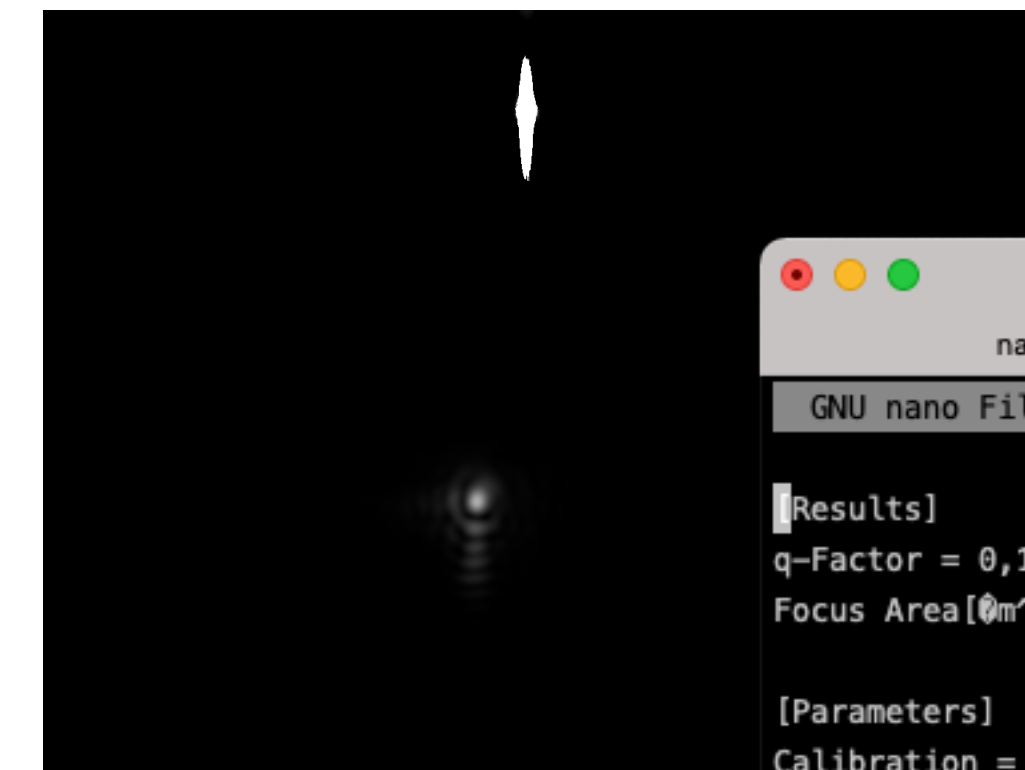
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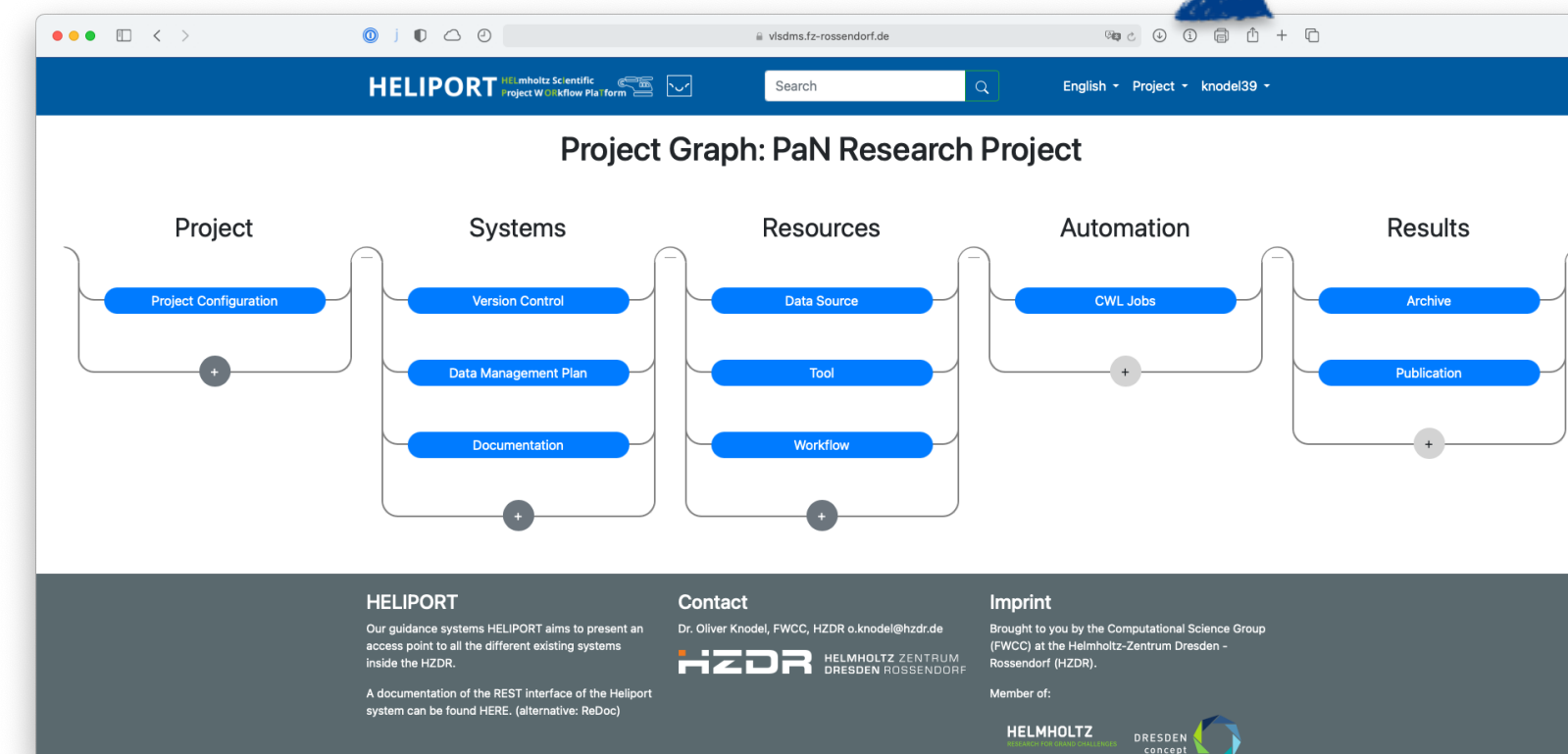
HIL typical experimental Setup



Malte C. Kaluza, Contrast Dependence of Laser-Driven Proton Acceleration, 18th Advanced Accelerators Concepts Workshop, Breckenridge, US, (2018)



In the HELIPORT project, our goal is to bring all together: images, settings, target metadata and everything else.



```

GNU nano File: ...14.data

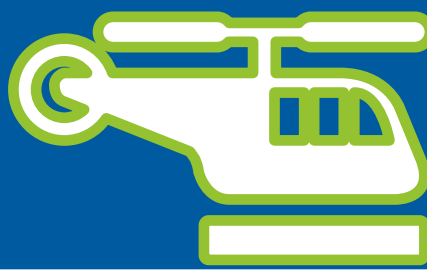
[Results]
q-Factor = 0,150082
Focus Area[0m^2] = 10,055498

[Parameters]
Calibration = 0,130000
Energy[J] = 10,000000
Size of region[px] = 2
#of Areas = 1
Target Point X = 0,000000
Target Point Y = 0,000000
Width Method = "FWHM"

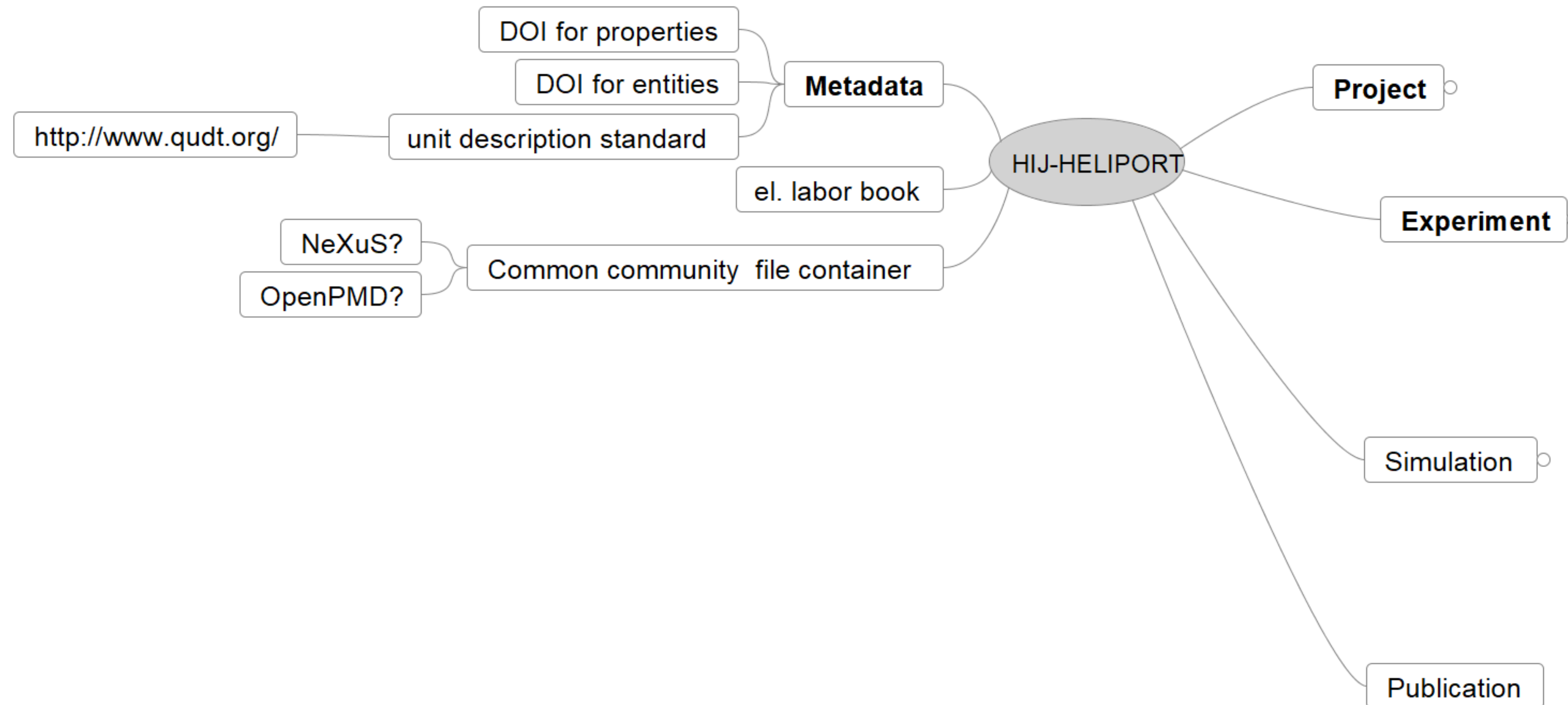
[Parameters.ROI]
GlobalRectangle.0 = 186
GlobalRectangle.1 = 346
GlobalRectangle.2 = 942
GlobalRectangle.3 = 1002

[Parameters.ROIContour.0]
ID = 0
Type = 4
Coordinate.0 = 186
Coordinate.1 = 346
Coordinate.2 = 942
Coordinate.3 = 1002
    
```

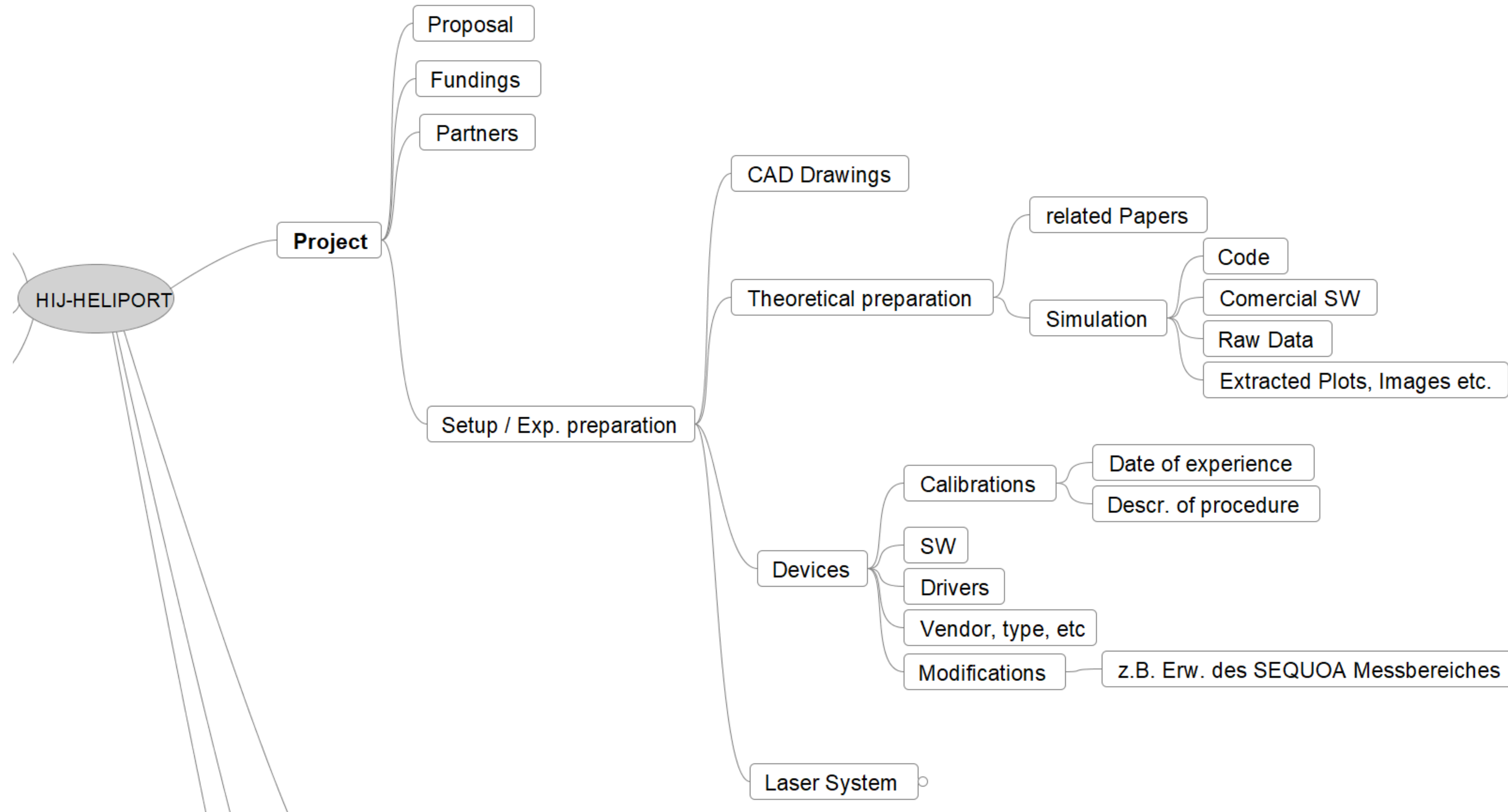
Topics to be described by Meta Data

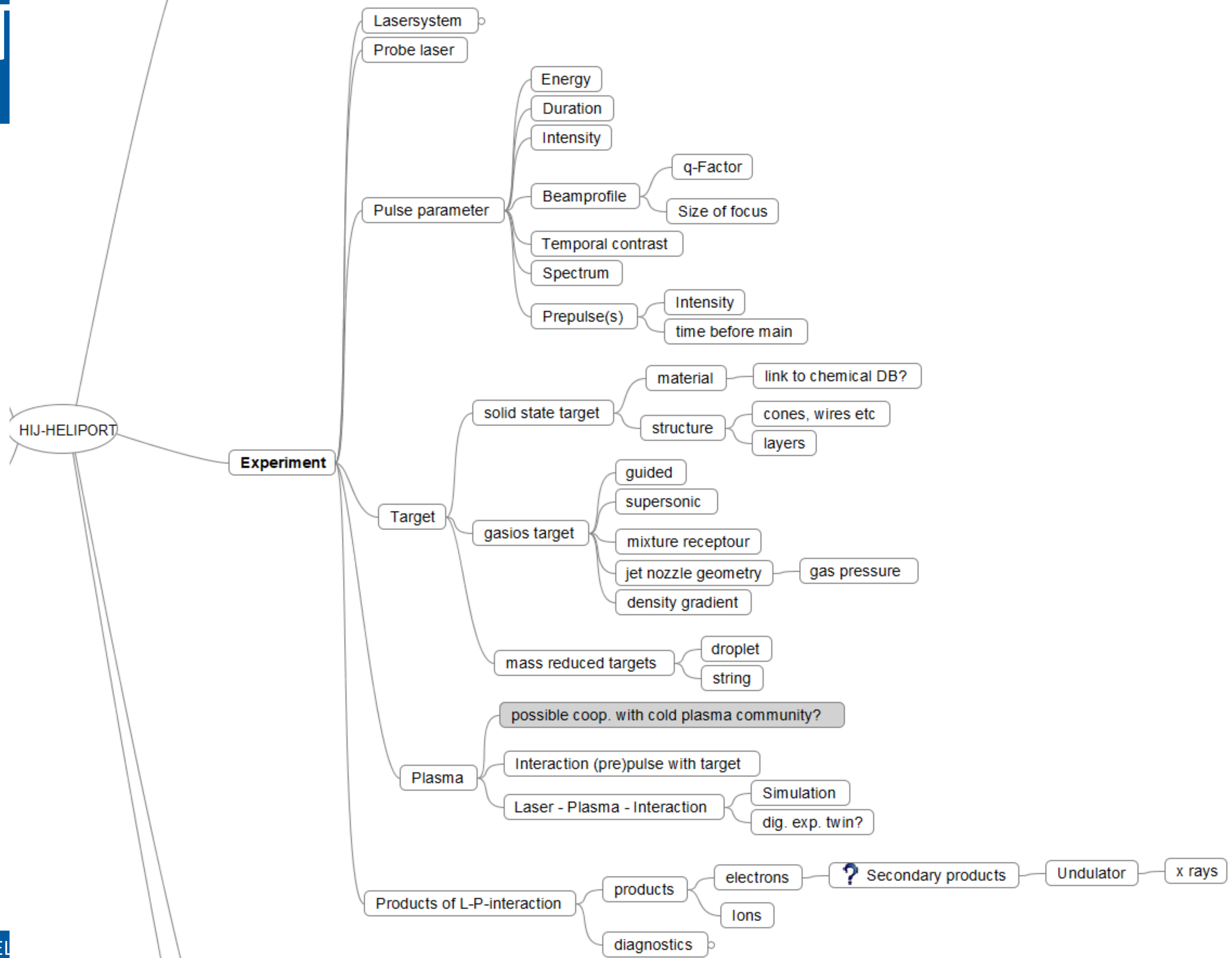
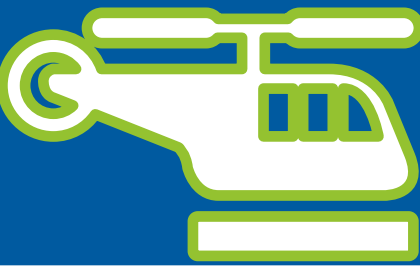


A mind map in order to get overview about topics to be described

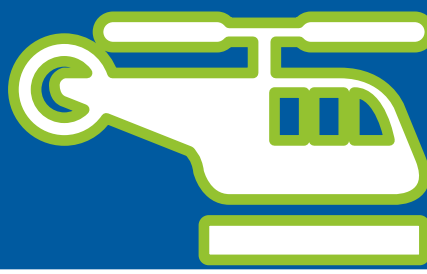


Topics to be described by Meta Data





Collaboration for MD Standard



- In all workshops the need for MD standard is expressed
 - Ideas exist in many facilities
 - here is a lack of cooperation
 - => lets bring different approaches together!
- <https://gitlab.hzdr.de/meta-laser/>
- Describe your work in wiki
 - Express wishes in Issues
 - Input is still limited...

GitLab Menu

Metadaten for HIL and experiments

Project ID: 4573

9 Commits 1 Branch 0 Tags 563 KB Files 563 KB Storage

The project will gather international efforts to define a metadata scheme for high experiments.

main metadaten-for-hil-and-experiments / +

Remove broken merge conflict marks
Huebl, Axel (FWKT) - 5135 authored 4 weeks ago

Upload File README Add LICENSE Add CHANGELOG Add C

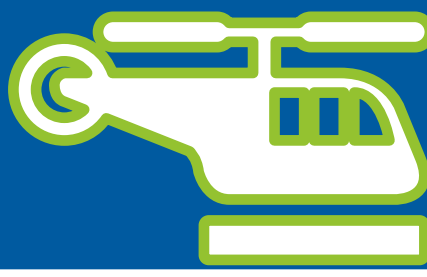
Set up CI/CD Configure Integrations

Name	Last commit
HIJ-HELIPORT.mm	Initial Commit: very first draft of ontolo

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Collaboration for MD Standard



Support from HMC

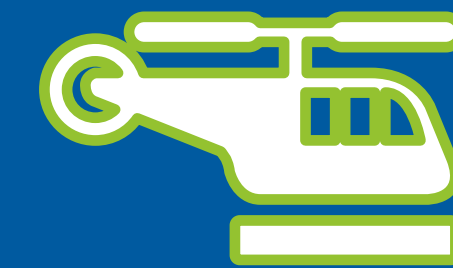
Oonagh Mannix (HZB), Witold Arndt (DLR)

- Mattermost channel* -> **Join us!**
- GitLab repository -> **Contribute!**
- Technical advice on defining MD dictionary and ontology
- Overview about existing MD Schemas

A screenshot of a Mattermost web interface. The browser address bar shows the URL: https://mattermost.hzdr.de/hmc-public/channels/metadata-in-the-laser-... The interface shows a channel named "Metadata in the laser community" with 31 members. A system message at 12:02 PM states that @Kessler, Dipl.-Phys. Alexander (EXTERN) - 145766 joined the channel. A message from Alexander Kessler at 1:36 PM discusses the need for a metadata standard for laser systems, mentioning the HELIPORT project and a workshop titled "better data for better science". The message includes a link to a presentation PDF. A second system message at 3:25 PM states that @Knodel, Dr. Oliver (FWCC) - 132739 joined the channel. The left sidebar shows the "HMC Public" group with various channels and direct messages.

* <https://mattermost.hzdr.de/hmc-public/channels/metadata-in-the-laser-community>

HELIPORT and Digital Tweens



ID	Name	Cluster Login	Directory on Cluster	Status
46	cat chain	hemera	~/heliport_jobs	✓
44	echo cat sleep	Choose a Login	~/heliport_jobs	✓
44	echo cat sleep	hemera	~/heliport_jobs	✓
51	one bad deed per week	Choose a Login	~/heliport_jobs	✗
51	one bad deed per week	hemera	~/heliport_jobs	✗
41	sleep 5 seconds	Choose a Login	~/heliport_jobs	⚠
41	sleep 5 seconds	hemera	~/heliport_jobs	⚠

Workflow Engine

Version Control

Compute (HPC, OpenStack)

UNICORE

- Analysis and Pre-/Postprocessing steps needs to be:
 - Documented and
 - Reproducible
- Capsuling every step in a workflow adapts the F.A.I.R. principles.



Edit a Scientific Workflow

Name: curl and cat stdout and stderr

Description:

Workflow Diagram:

```

    graph LR
      link((link)) --> curl((curl))
      curl --> cat1((cat_1))
      curl --> cat((cat))
    
```

Buttons: Save, Cancel, Fit to Screen, Delete Selection

ID	Name	Description
35	echo	

Buttons: Add

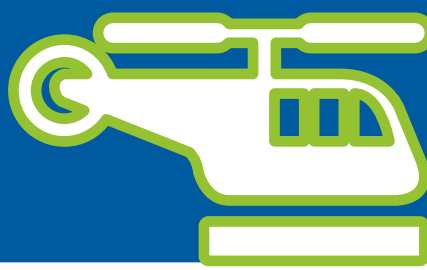


```

1 /*****
2 Copyright (c) 2019, KNOD
3 Author: u.knod@hzdr.de
4
5 *****/
6 #include "dmg_core.h"
7 #include "stdlib.h"
8 #include "unistd.h"
9 #include "math.h"
10
11 double let_leftrect(double from, double to, double n, double (*func)())
12 {
13     double h = (to - from) / n;
14     double sum = 0.0;
15     for (x = from; x <= (to - h); x += h)
16         sum += func(x);
17     return h * sum;
18 }
19
20 double let_rightrect(double from, double to, double n, double (*func)())
21 {
22     double h = (to - from) / n;
23     double sum = 0.0;
24     for (x = from; x <= (to - h); x += h)
25         sum += func(x + h);
26     return h * sum;
27 }
    
```



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For us:

- Tailored HELIPORT Instance and related Services
- Big step on the long road to F.A.I.R.
- Integration of existing nice HW into daily workflow, link between experiment and simulation

For Helmholtz Society and above:

- cooking recipe how to integrate HELIPORT into existing facilities

For HIL Community:

- common Meta Data Scheme

Our Main Problem is **the Staff ??? ...**

we need an FTE for this Project. The Position is since $\frac{3}{4}$ Year vacant...

Thank You for your Attention!

Special Thanks:

- to Nina Elkina for bringing us together
- to Oliver Knodel for taking us on board and for some slides used in this presentation