HI JENA
Helmholtz Institute Jena

HELIPORT@HI-Jena

and related IT activities

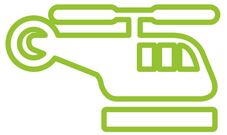
Alexander Kessler[1], Joachim Hein[2], Malte Kaluza[1,2]

[1] HI-Jena [2] Institute of Optics and Quantum Electronics

HIJ semi-annual palaver 09.03.2022

Outline

- 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

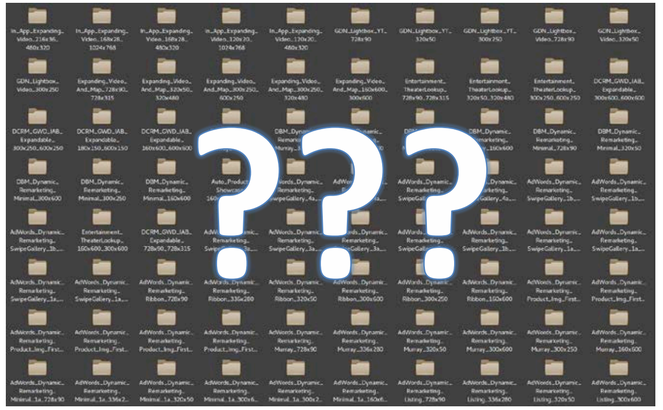


HI JENA
Helmholtz Institute Jena

www.hi-jena.de

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 (POI[1], rich MD[2], 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 HELIPORT: https://heliport.hzdr.de/principles/

[1] Persistent Object Identifier; [2] Meta Data

HI JENA
Helmholtz Institute Jena
www.hi-jena.de

HPC Nodes and DMS and Storage Server

- 2020-2021: Project HDA founded by Thühringer Aufbaubank

  (**H**igh Power Computer und **D**atenmanagement **A**rchitektur, 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 colaboration with André Sternbeck:
  – Installation in HPC room @ Beutenberg
  – SW administration
  – Schooling and technical support

Thüringer Aufbaubank
Die Förderbank.

HI JENA
Helmholtz Institute Jena

www.hi-jena.de

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

HI JENA
Helmholtz Institute Jena

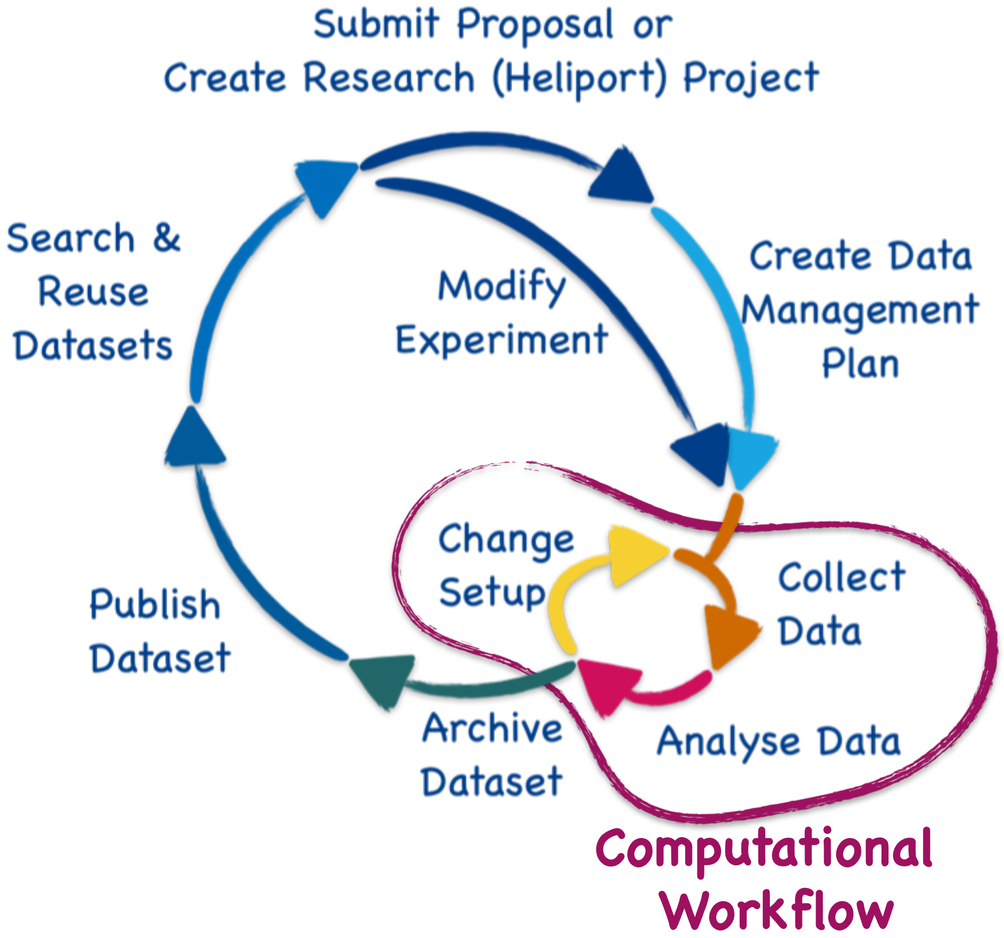
www.hi-jena.de

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:

HMC HELMHOLTZ METADATA COLLABORATION

HI JENA Helmholtz Institute Jena

www.hi-jena.de

HELIPORT Participants and Roles

- 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

HZDR
HELMHOLTZ ZENTRUM DRESDEN ROSSENDORF

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

JÜLICH FORSCHUNGSZENTRUM

Bernd Schuller

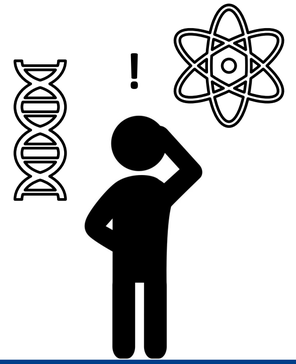
HI JENA
Helmholtz Institute Jena

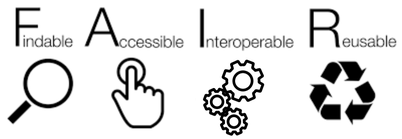
Alexander Kessler
Joachim Hein
Malte C. Kaluza
and:
???

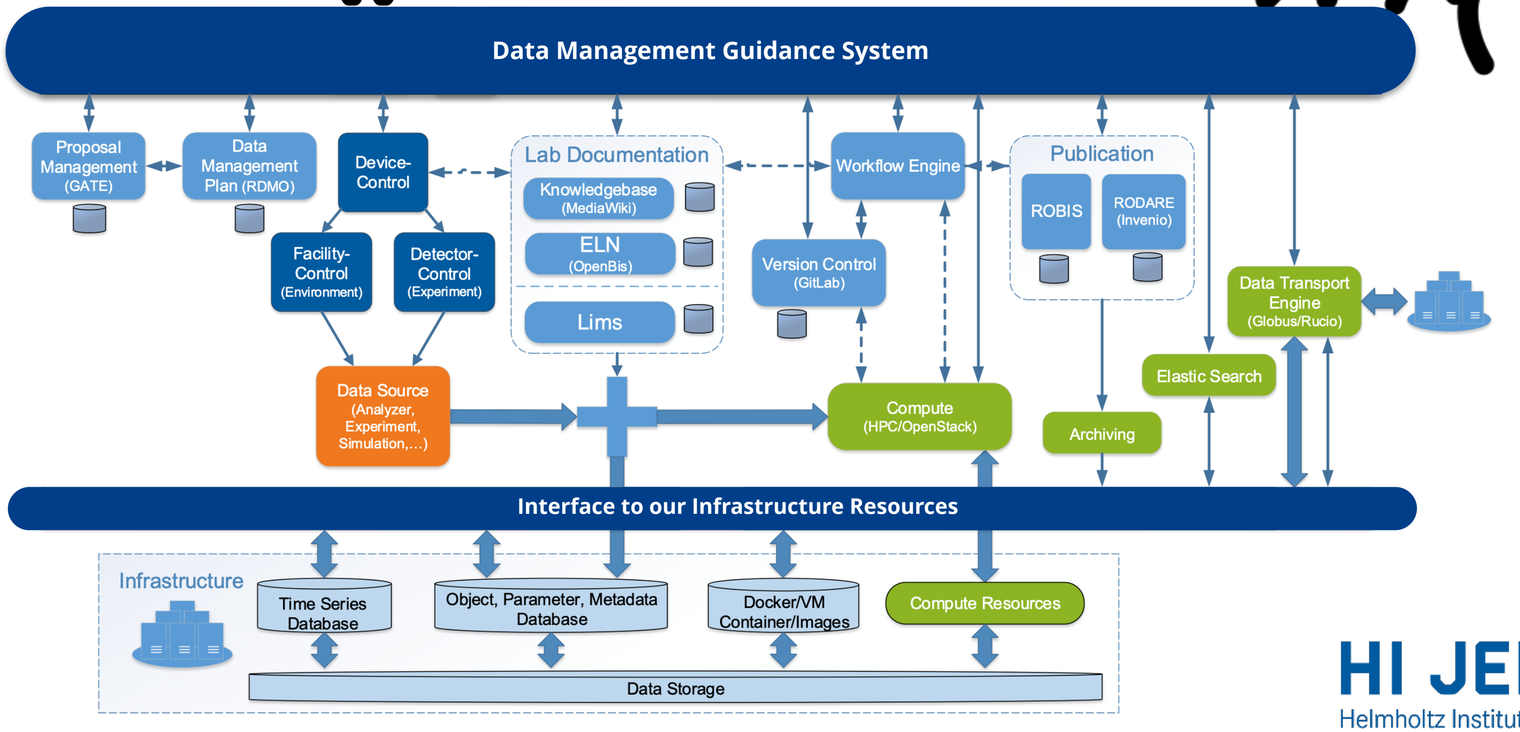
HI JENA
Helmholtz Institute Jena

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.







HI JENA
Helmholtz Institute Jena

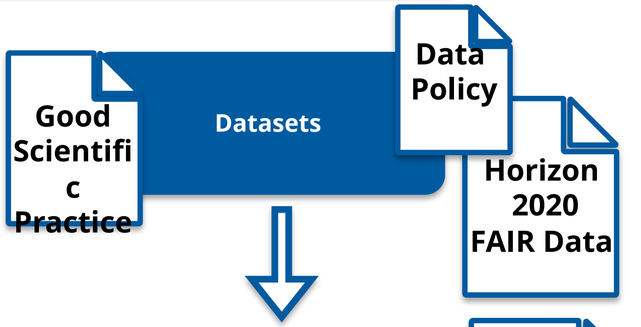
www.hi-jena.de

HELIPORT, the Idea behind

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

What are the necessary steps towards a full comprehensible and FAIR research experiment ensuring data provenance?

And how we can support them?!



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

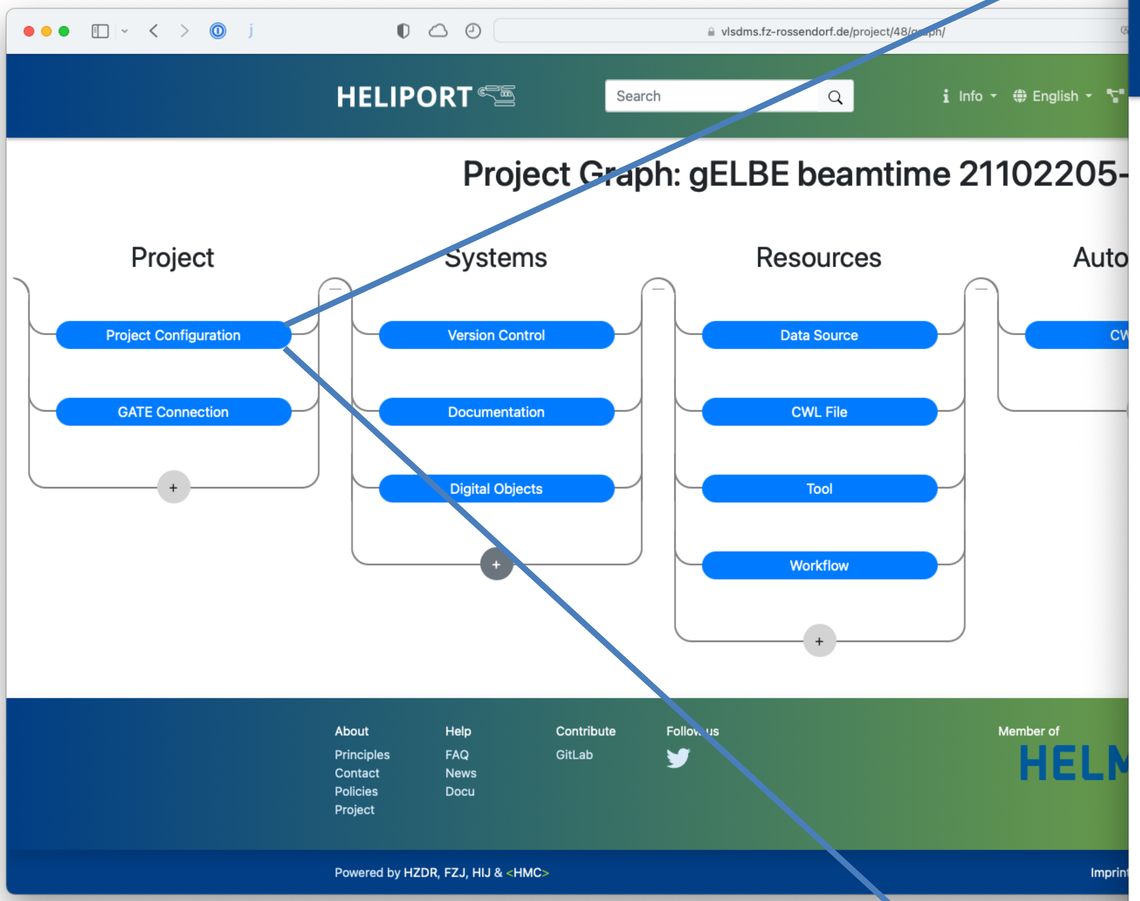
Which datasets or software can be published (and how)?

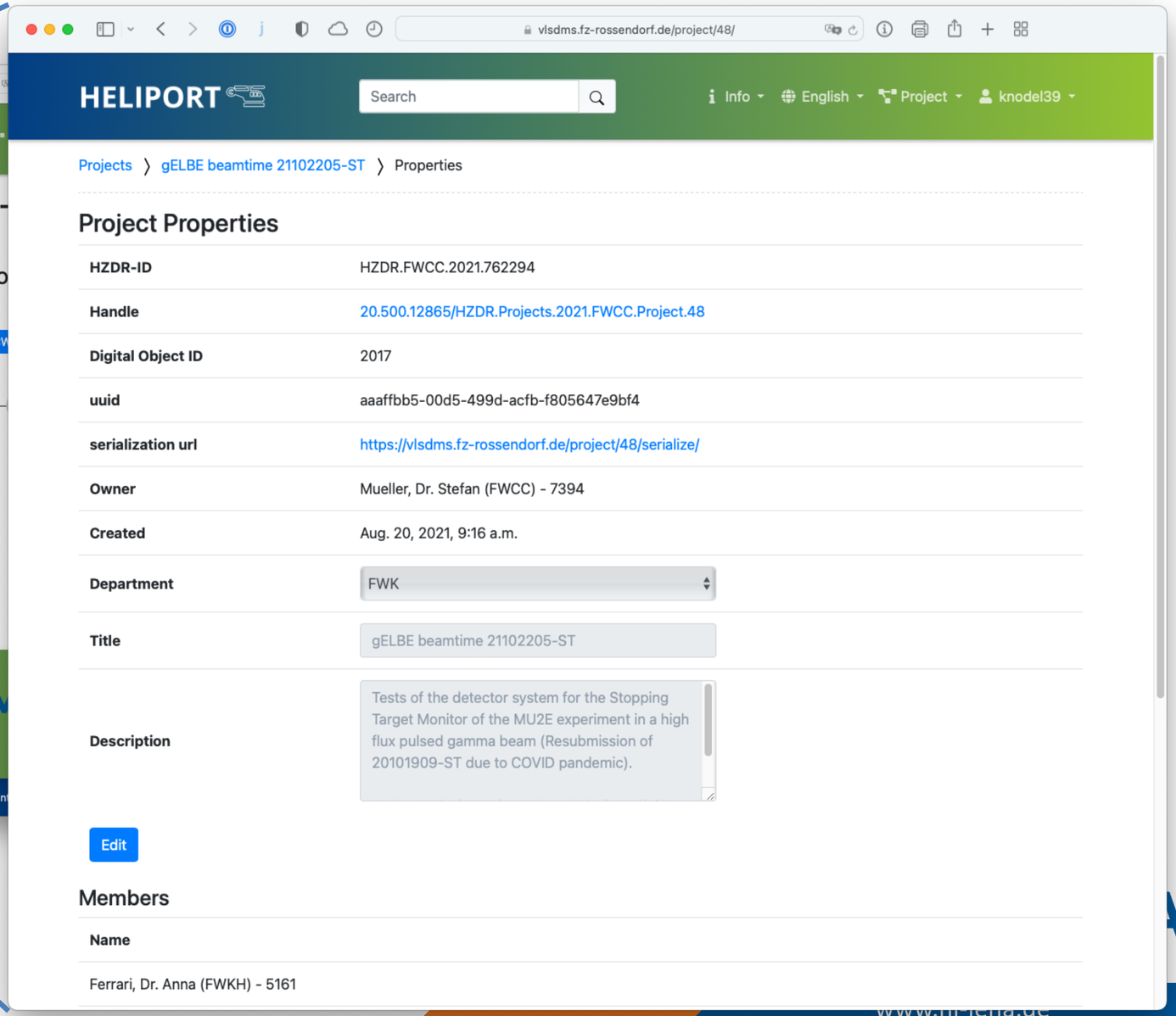
How can we bring new team members or external scientists into our project lifecycle and all associated tools?

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

Helmholtz Institute Jena

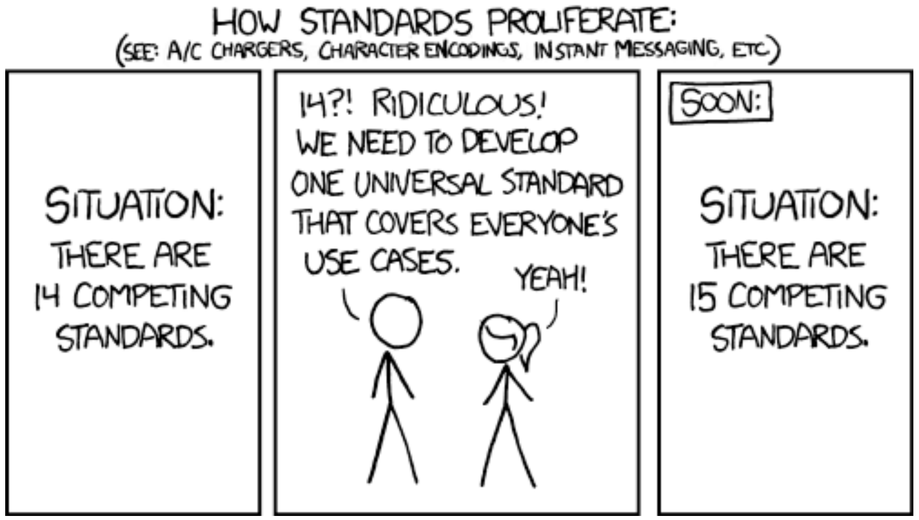
HELIPORT Web User Interface





HELIPORT: our Part

- 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

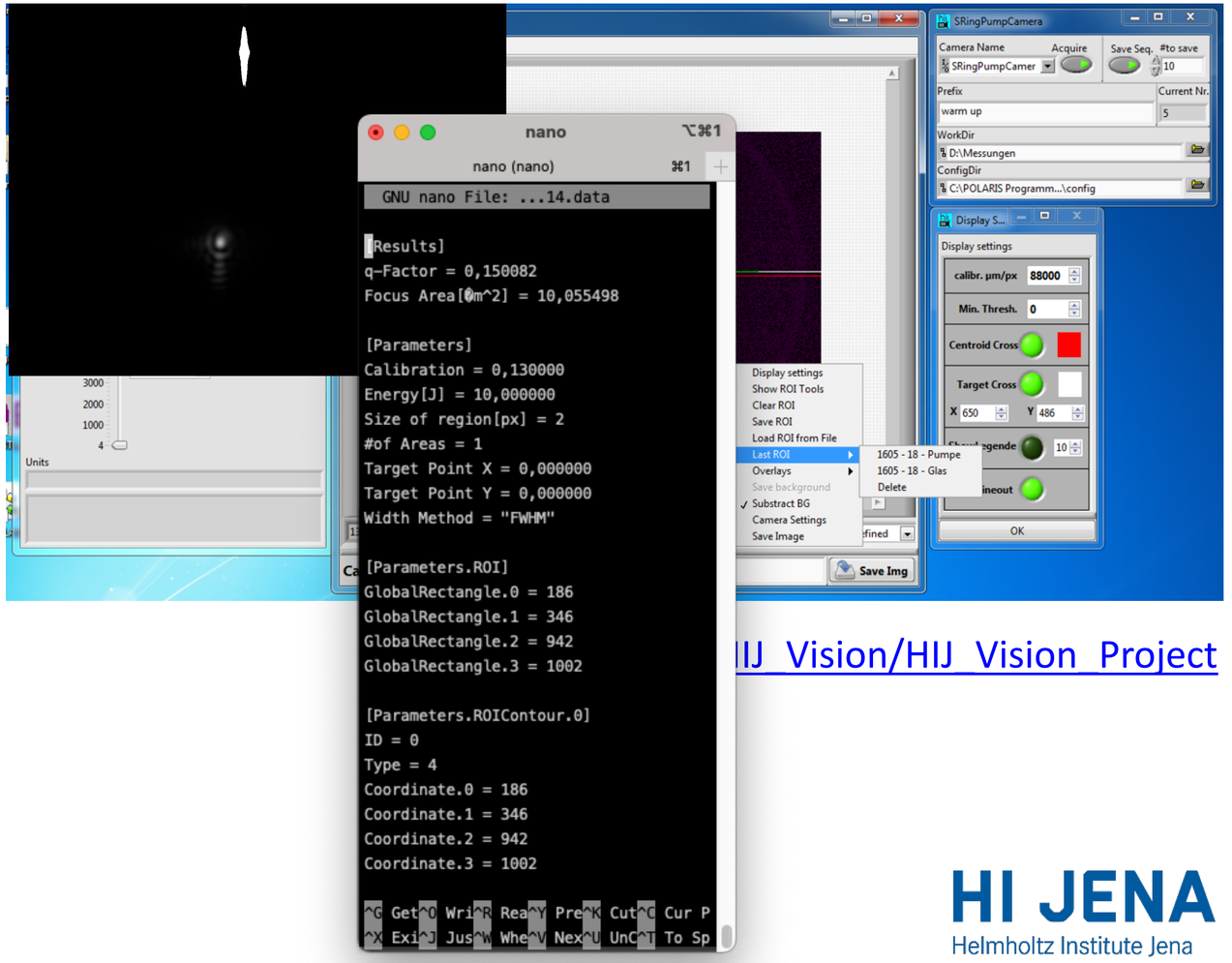


Source: https://xkcd.com/927

HI JENA
Helmholtz Institute Jena
www.hi-jena.de

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!

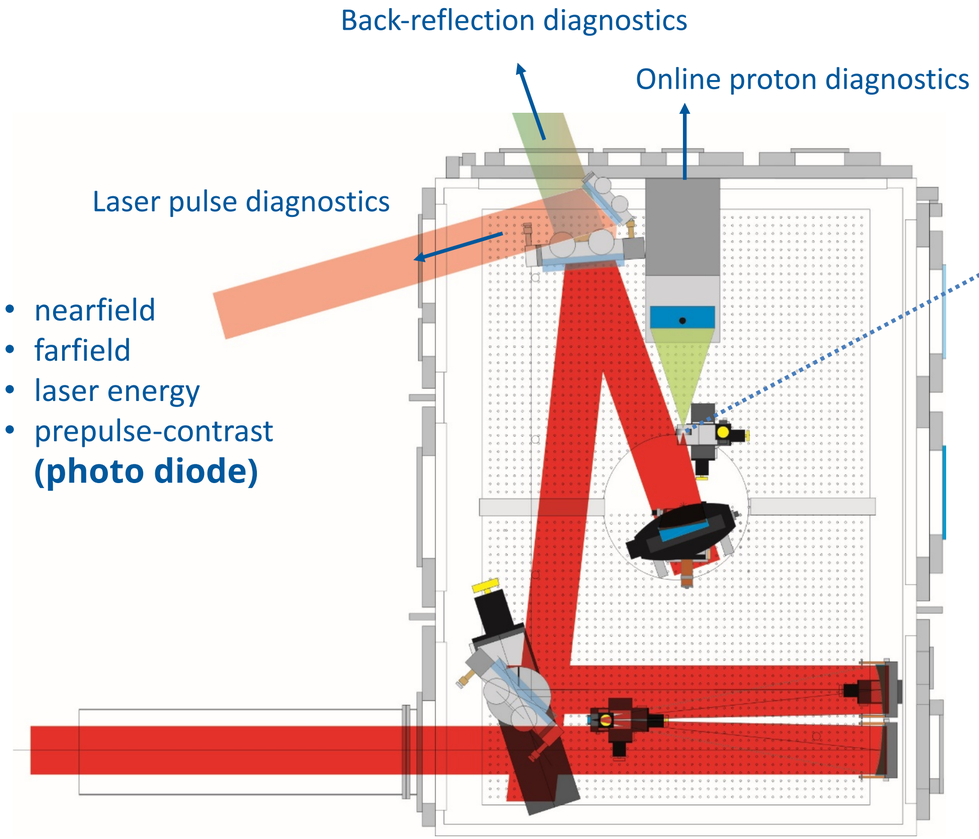


IJ_Vision/HIJ_Vision_Project

HI JENA
Helmholtz Institute Jena

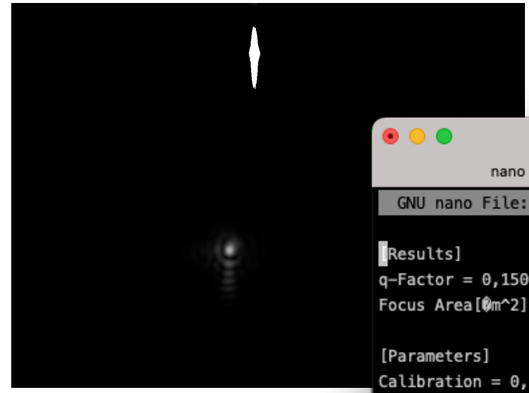
www.hi-jena.de

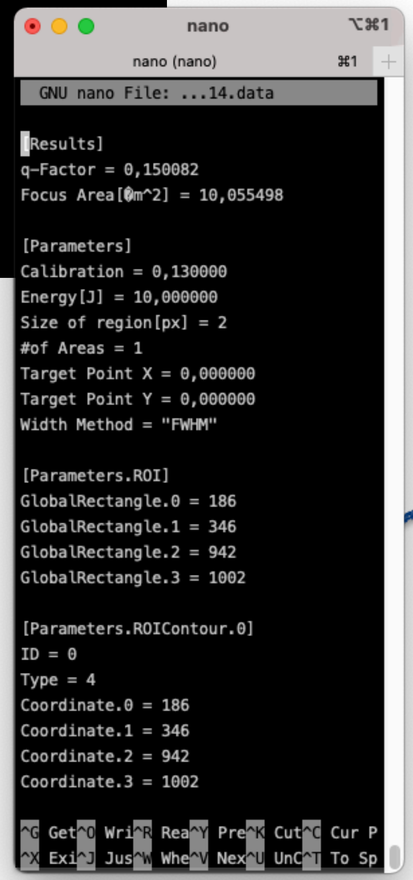
HIL typical experimental Setup



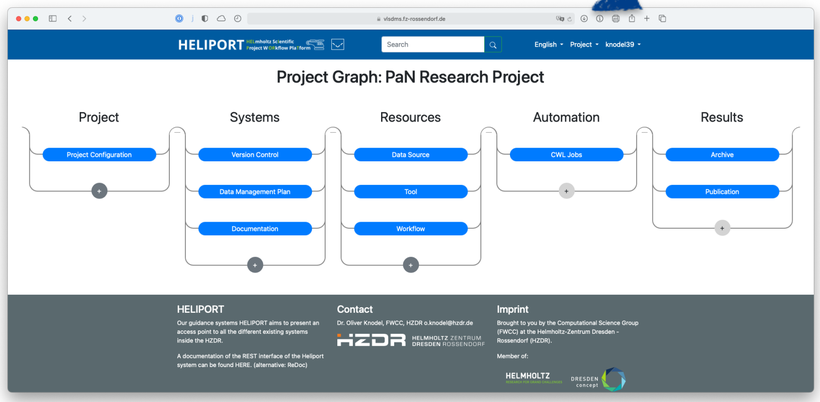
- nearfield
- farfield
- laser energy
- prepulse-contrast **(photo diode)**

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.

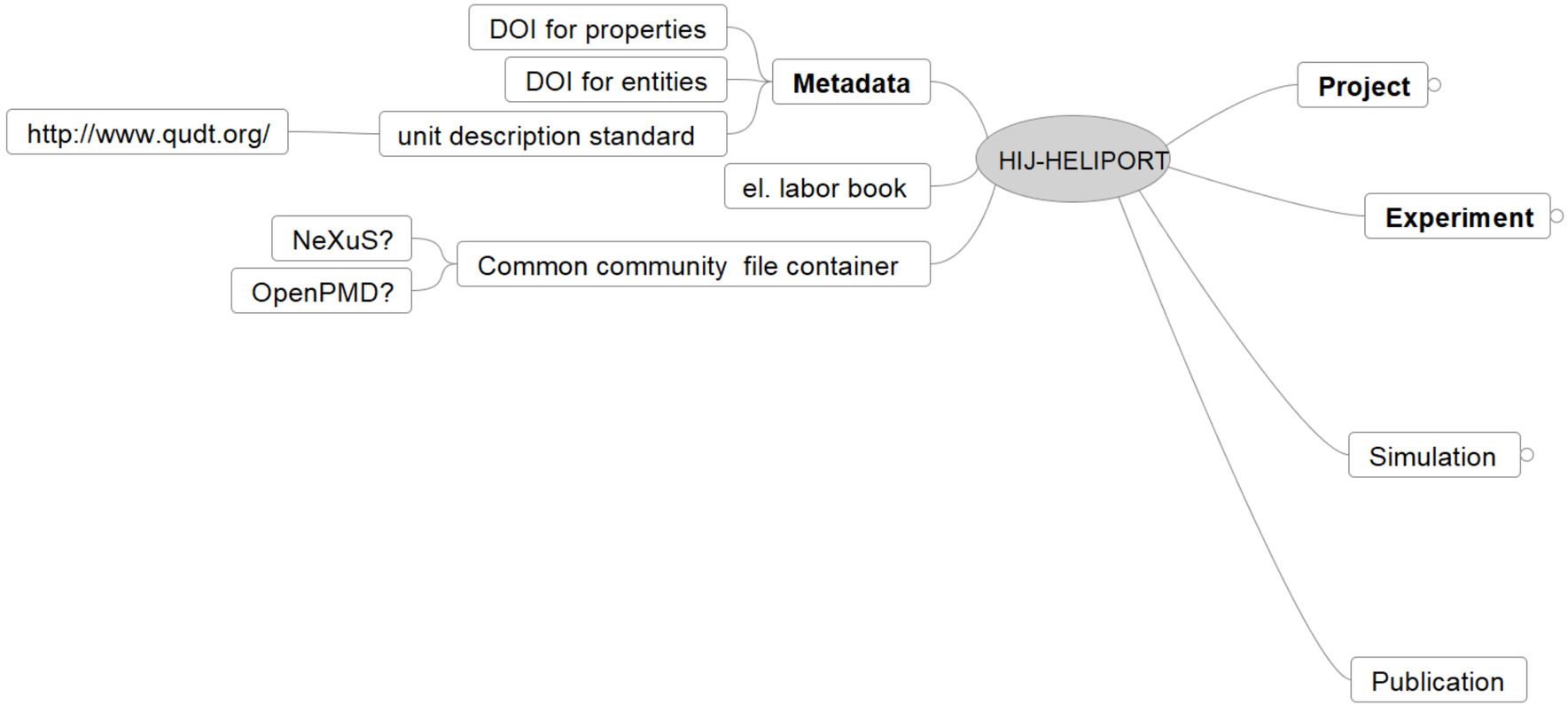


HI JENA
Helmholtz Institute Jena

www.hi-jena.de

Topics to be described by Meta Data

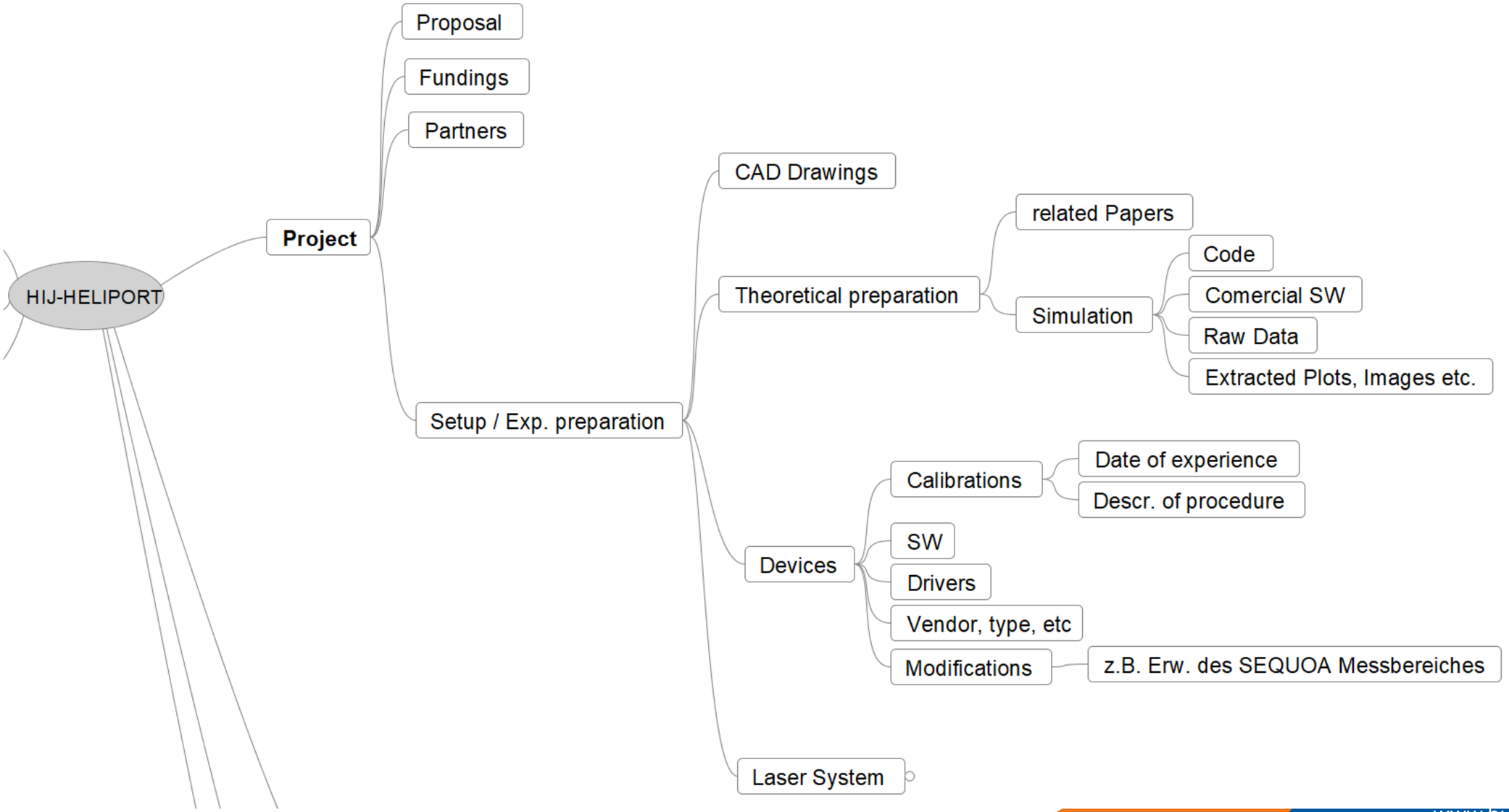
A mind map in order to get overview about topics to be described

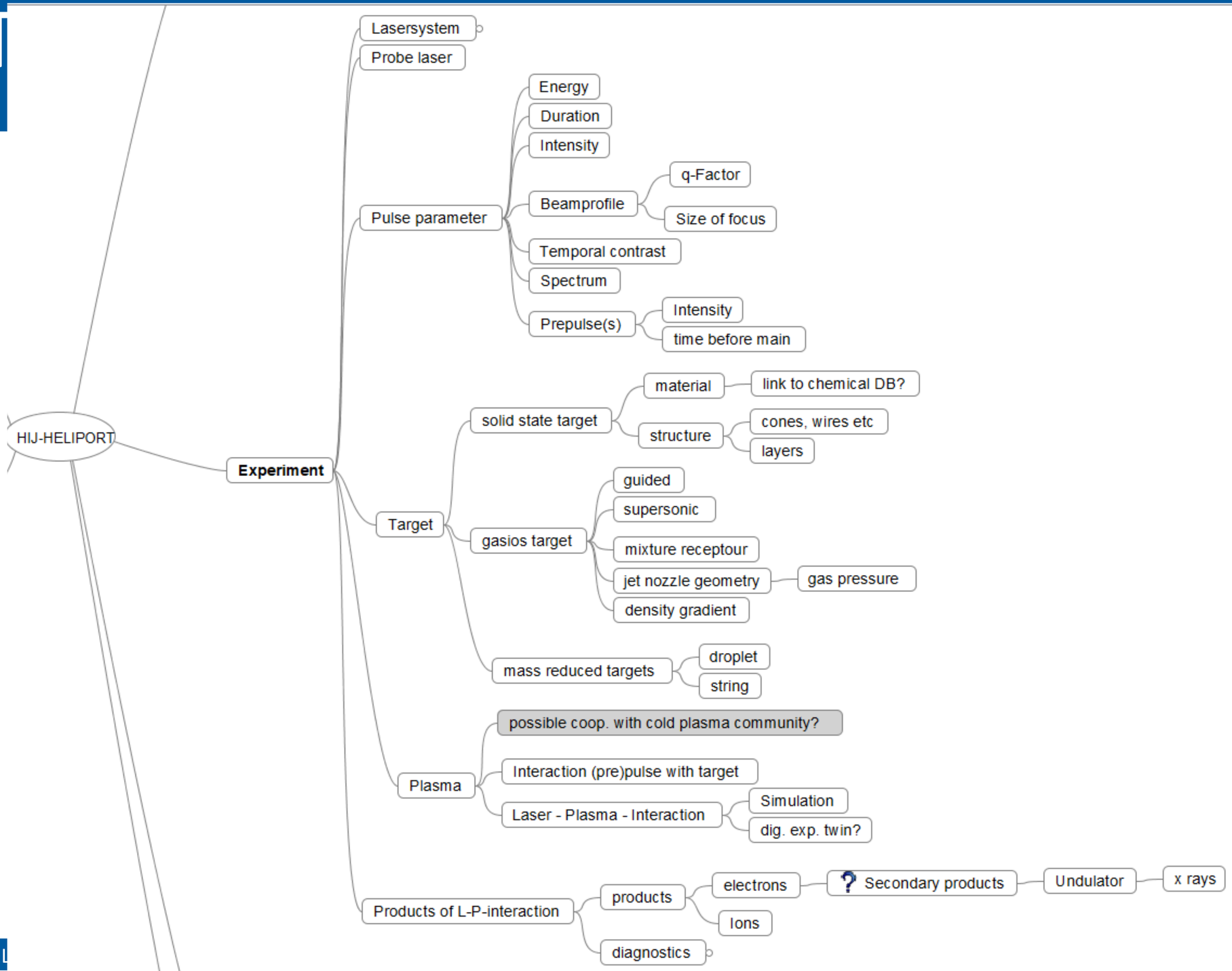


HI JENA
Helmholtz Institute Jena

www.hi-jena.de

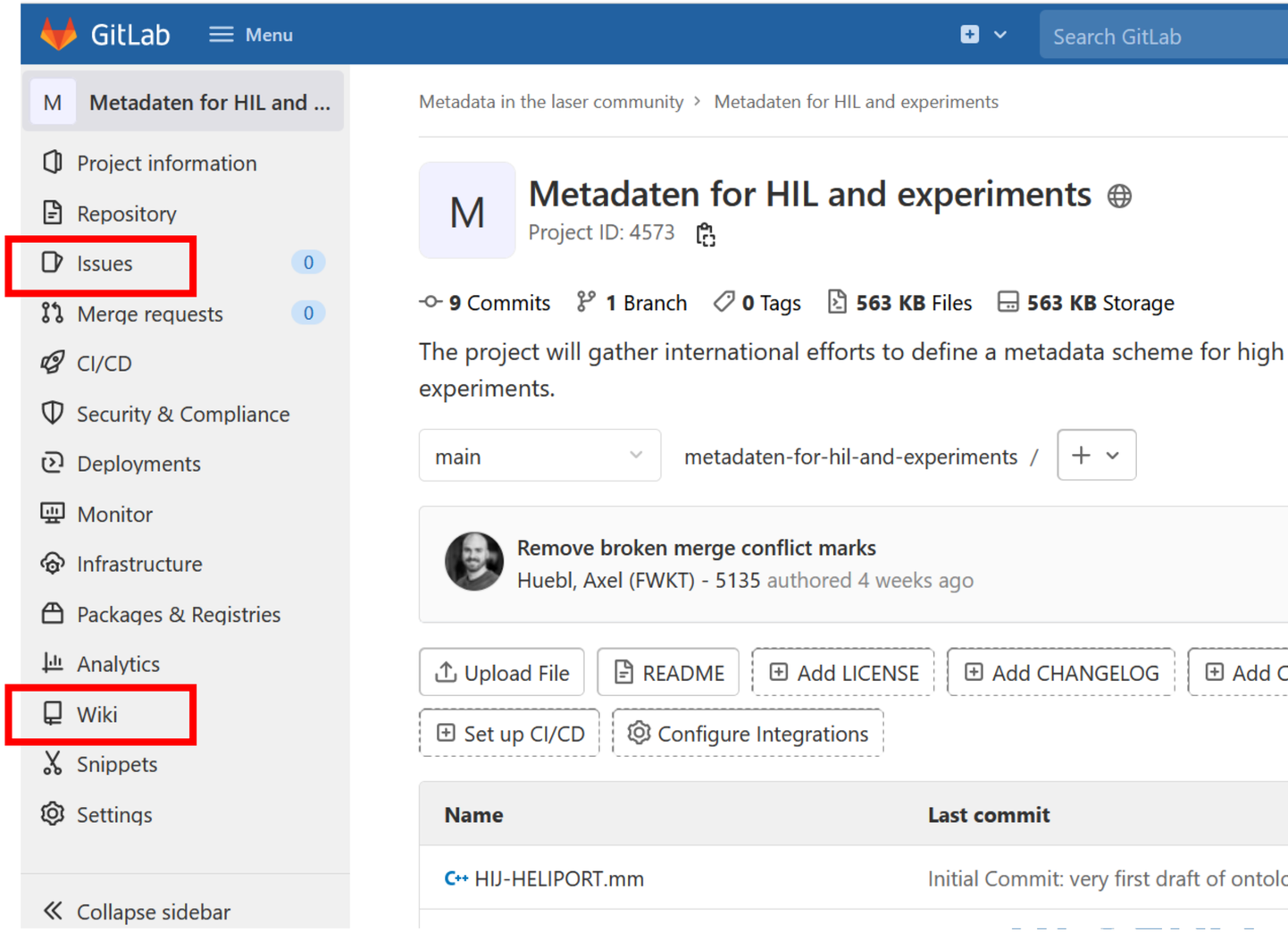
Topics to be described by Meta Data




HIJ-HELIPORT
Experiment
Lasersystem
Probe laser
Pulse parameter
Energy
Duration
Intensity
Beamprofile
q-Factor
Size of focus
Temporal contrast
Spectrum
Prepulse(s)
Intensity
time before main
Target
solid state target
material
link to chemical DB?
structure
cones, wires etc
layers
gasios target
guided
supersonic
mixture receptour
jet nozzle geometry
gas pressure
density gradient
mass reduced targets
droplet
string
Plasma
possible coop. with cold plasma community?
Interaction (pre)pulse with target
Laser - Plasma - Interaction
Simulation
dig. exp. twin?
Products of L-P-interaction
products
electrons
Secondary products
Undulator
x rays
Ions
diagnostics

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...

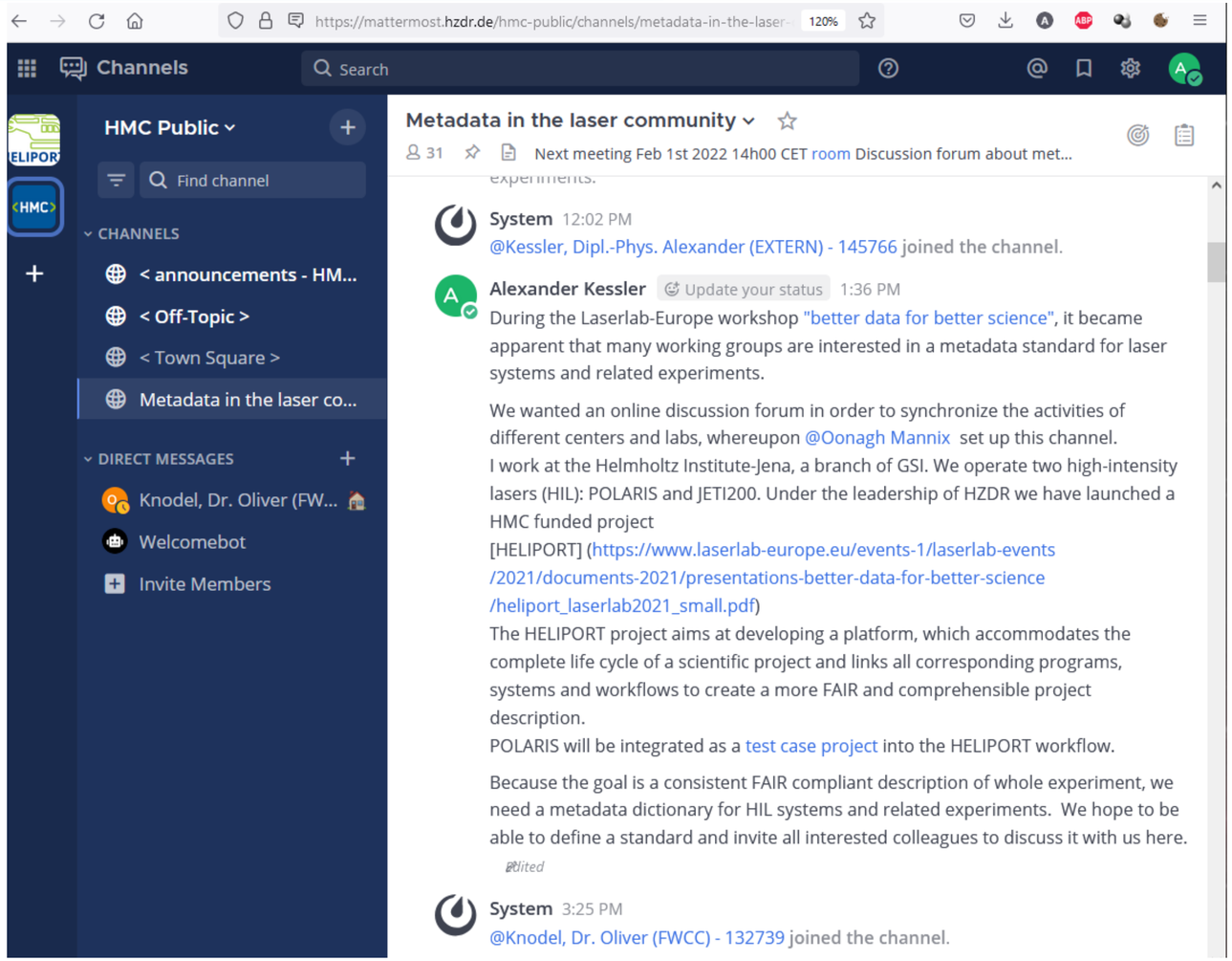


Collaboration for MD Standard

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

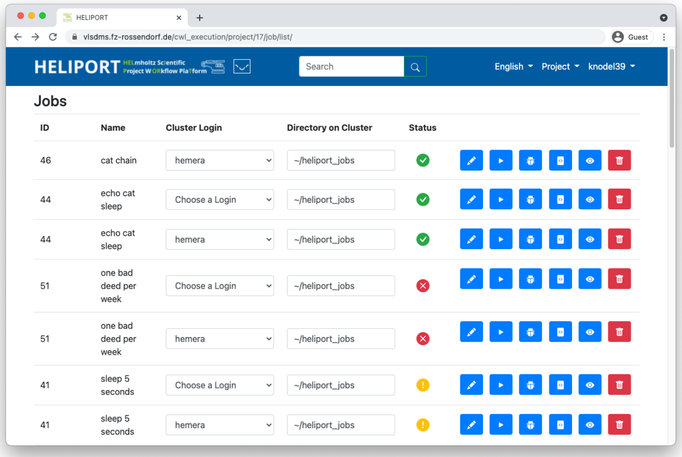


* https://mattermost.hzdr.de/hmc-public/channels/metadata-in-the-laser-community

HI JENA
Helmholtz Institute Jena

www.hi-jena.de

HELIPORT and Digital Tweens



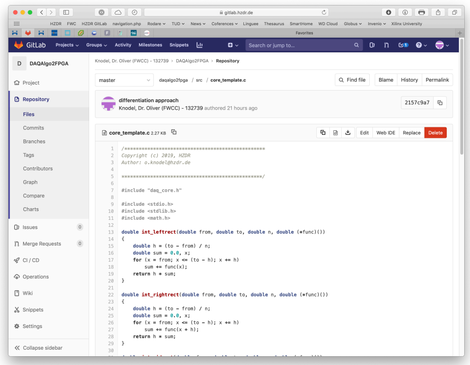
- Analysis and Pre-/Postprocessing steps needs to be:
  - Documented and
  - Reproducible
- Capsuling every step in a workflow adapts the F.A.I.R. principles.

COMMON WORKFLOW LANGUAGE

Workflow Engine

Version Control

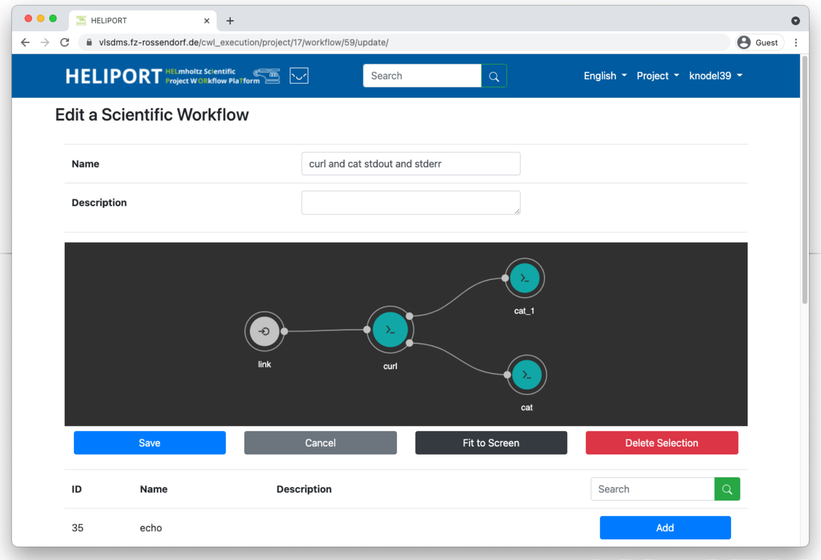
Compute (HPC, OpenStack)



GitLab

slurm workload manager

UNICORE



HI JENA
Helmholtz Institute Jena

www.hi-jena.de

Expected Benefit

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 ¾ Year vacant…

HI JENA
Helmholtz Institute Jena

www.hi-jena.de

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