

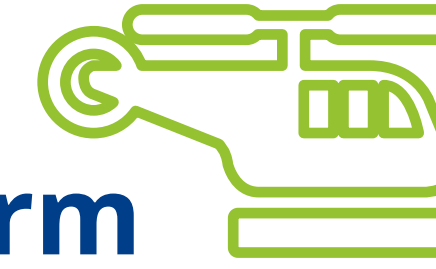
HELIPORT use case POLARIS: Integration of a High Intensity Laser in a complete data life cycle workflow

Better Data for Better Science - Research Data Management Workshop, 28-29 October 2021

Oliver Knodel, Joachim Hein, Alexander Kessler // contact: o.knodel@hzdr.de



HELIPORT HELmholtz Scientific Project WORKflow PlaTform



“ The HELIPORT project 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 **FAIR** and comprehensible project description.

Project Members:



Founded by:



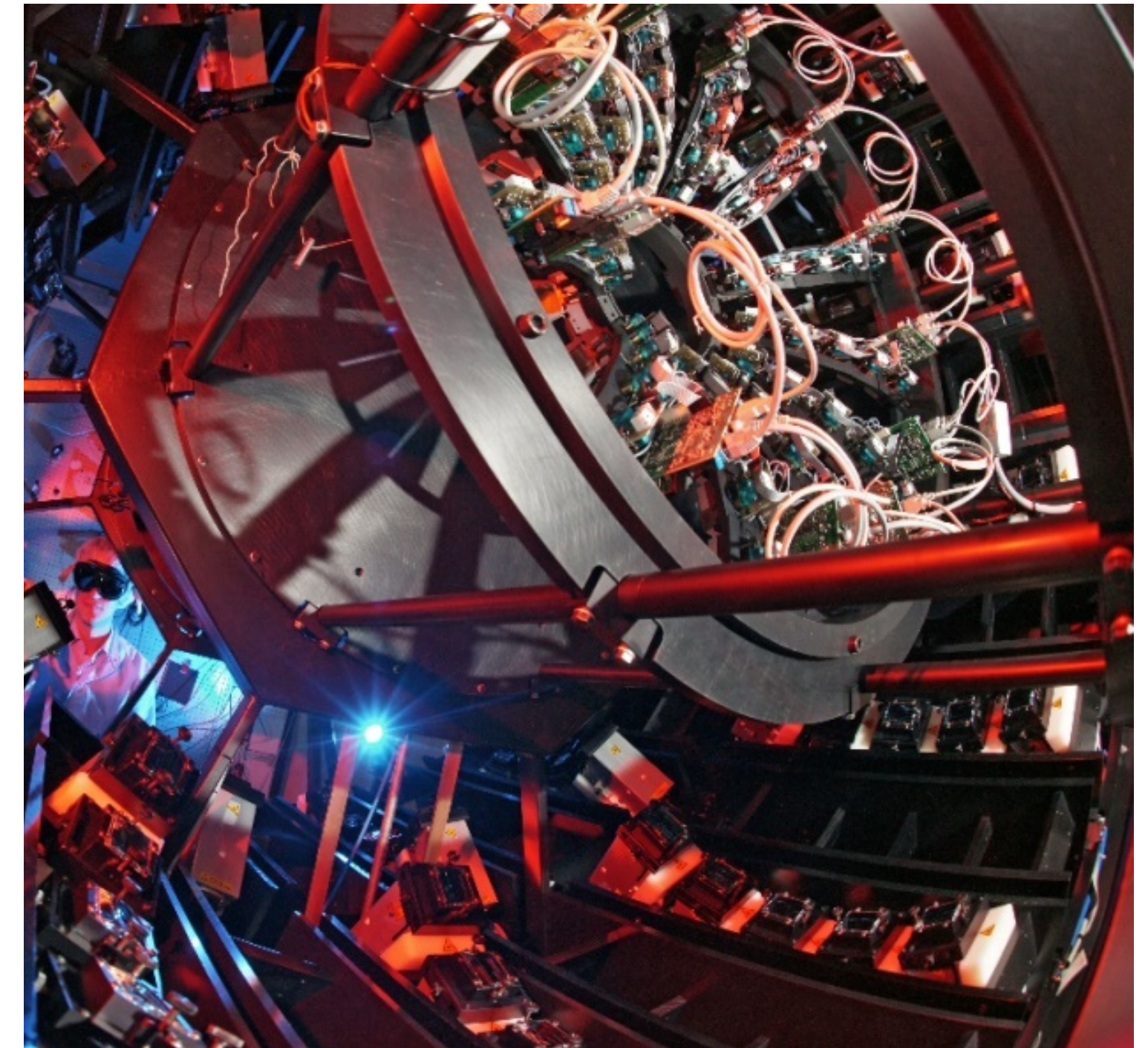
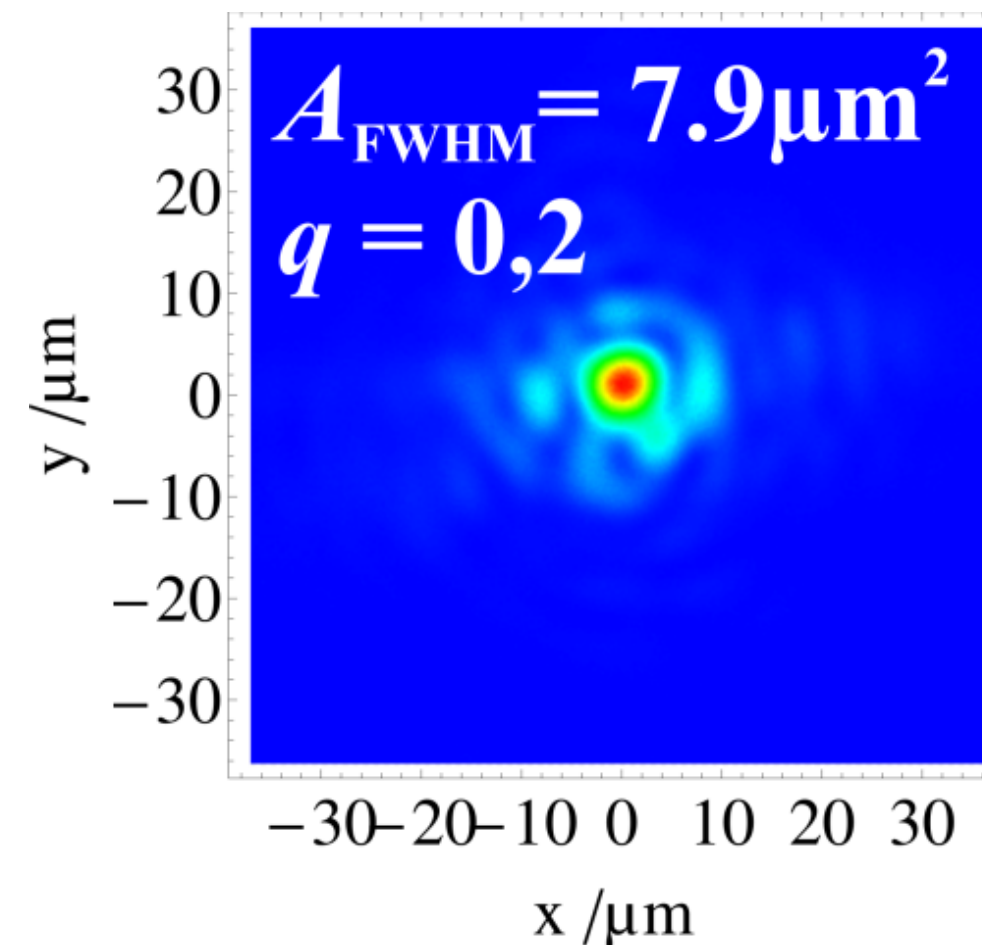
```

{
  "namespaces": {
    "datacite": "http://purl.org/spar/datacite/",
    "rdfs": "http://www.w3.org/2000/01/rdf-schema#",
    "heliport": "https://heliport/schema/",
    "time": "http://www.w3.org/2006/time#",
    "dc": "http://purl.org/dc/terms/"
  },
  "heliport:project_id": 28,
  "datacite:hasIdentifier": "HZDR.FWCC.2021.84769",
  "heliport:uuid": "09779261-200c-48c4-be9c-f298369d6a1c",
  "datacite:handle": "https://hdl.handle.net/None",
  "heliport:project_name": "PaN Research Project",
  "time:hasBeginning": "2021-04-01 09:14:34.296524+00:00",
  "datacite:hasDescription": "",
  "heliport:group": "FWCC",
  "heliport:owner": {
    "datacite:hasIdentifier": "132739",
    "datacite:orcid": null,
    "rdfs:label": "Knodel, Dr. Oliver (FWCC) - 132739"
  },
  "heliport:has_VersionControl": [
    {
      "heliport:version_control_id": 15,
      "datacite:uri": "https://ddd",
      "rdfs:label": "Test"
    }
  ],
  "heliport:has_DataManagementPlan": [
    {
      "heliport:data_management_plan_id": 6,
      "datacite:uri": "https://dddd",
      "datacite:hasDescription": "dddd"
    }
  ],
  "heliport:has_Documentation": [
    {
      "heliport:documentation_id": 7,
      "datacite:uri": "https://dddd",
      "heliport:documentation_system": "MediaWiki",
      "datacite:hasDescription": "dddd"
    }
  ],
  "heliport:has_DataSource": [
    {
      "heliport:data_source_id": 11,
      "datacite:uri": "http://ddd",
      "heliport:use_computer": null,
      "rdfs:label": "ddd",
      "datacite:hasDescription": ""
    }
  ]
}

```

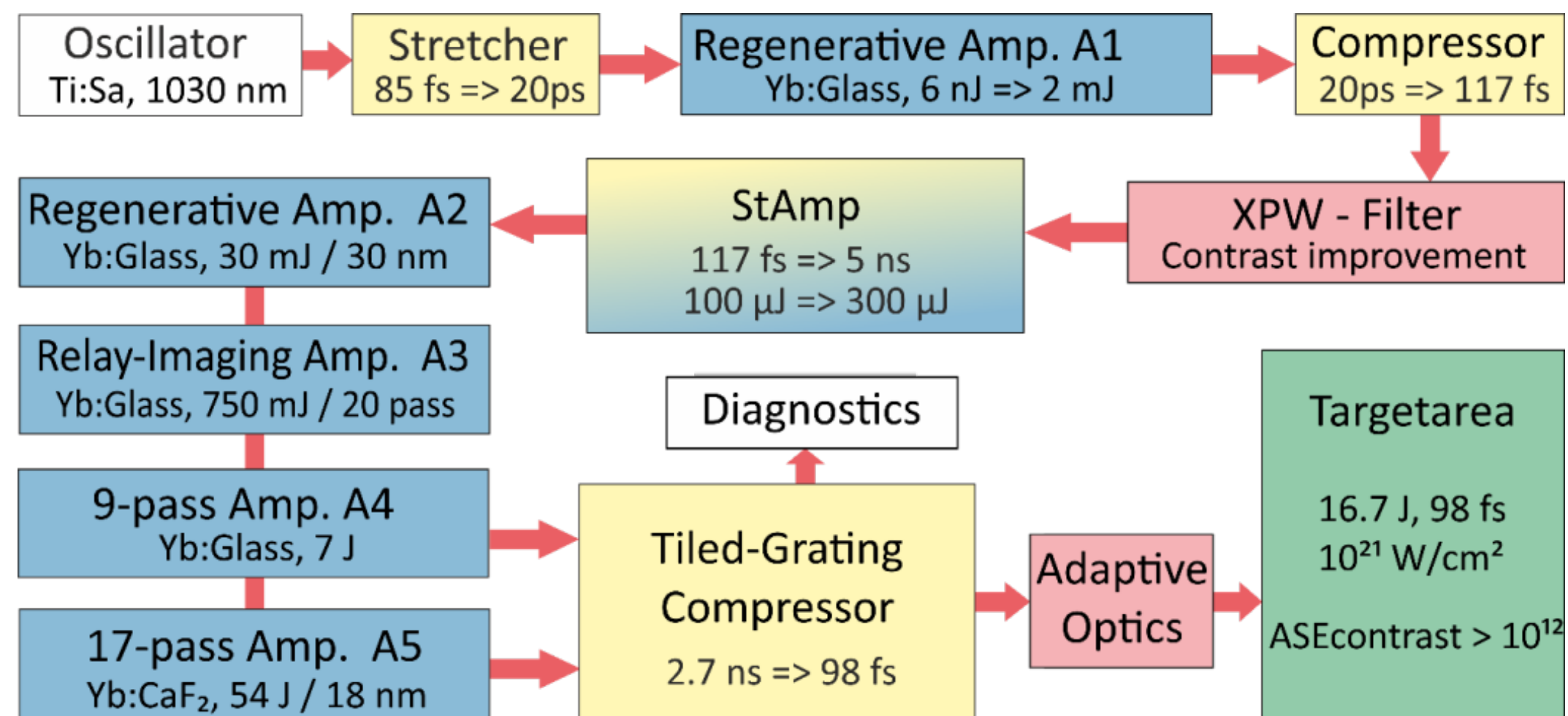

The POLARIS Experiment @ HI Jena

- The **P**etawatt **O**ptical **L**aser **A**mplifier for **R**adiation **I**ntensive **E**xperiments (**POLARIS**) is the only fully diode-pumped, double-CPA laser system worldwide.
- Used for Laser Particle Acceleration Experiments
- Research project of the Faculty of Physics and Astronomy at the University of Jena and the Helmholtz Institute Jena (HI-Jena).
- Key features:
 - Energy on target: $E_L = 16.7 \text{ J}$, $t_L < 100 \text{ fs}$
 - Repetition rate: 1/50 Hz
 - Optimized peak intensity
 - Full suppression of short pre-pulses



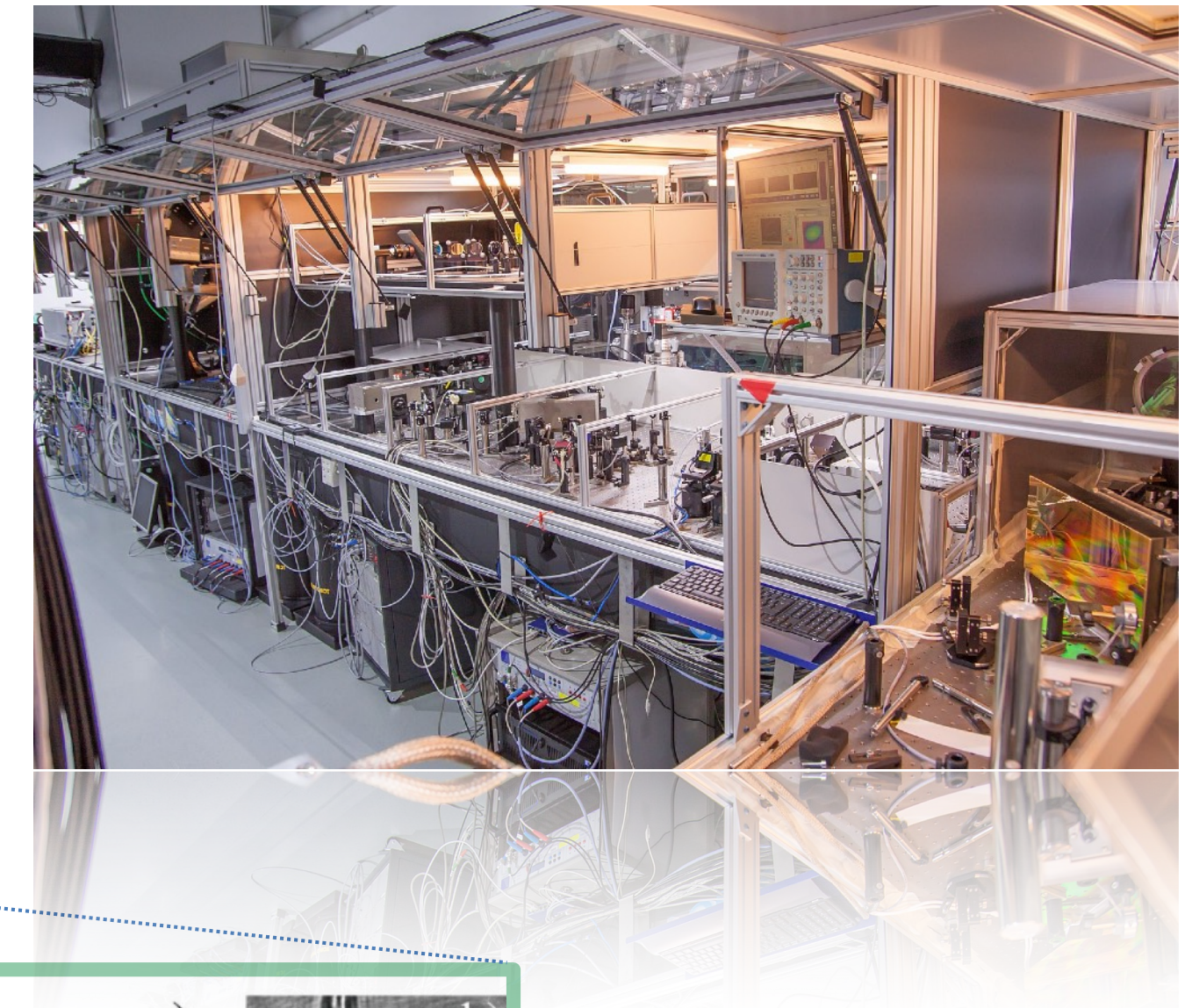
Malte C. Kaluza, Contrast Dependence of Laser-Driven Proton Acceleration, 18th Advanced Accelerators Concepts Workshop, Breckenridge, US, (2018)

The POLARIS Experiment Chain



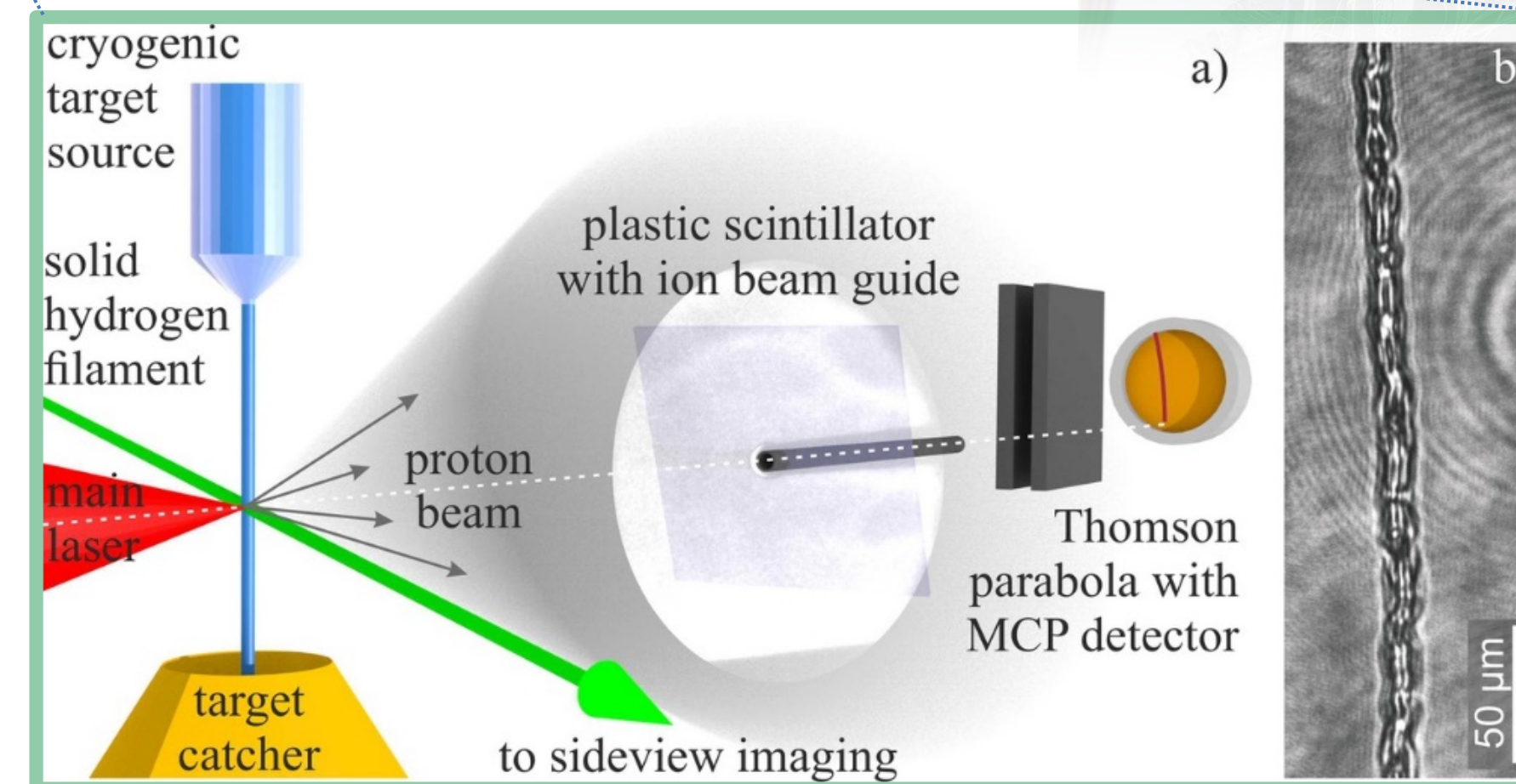
Malte C. Kaluza, Contrast Dependence of Laser-Driven Proton Acceleration, 18th Advanced Accelerators Concepts Workshop, Breckenridge, US, (2018)

View from oscillator to A4



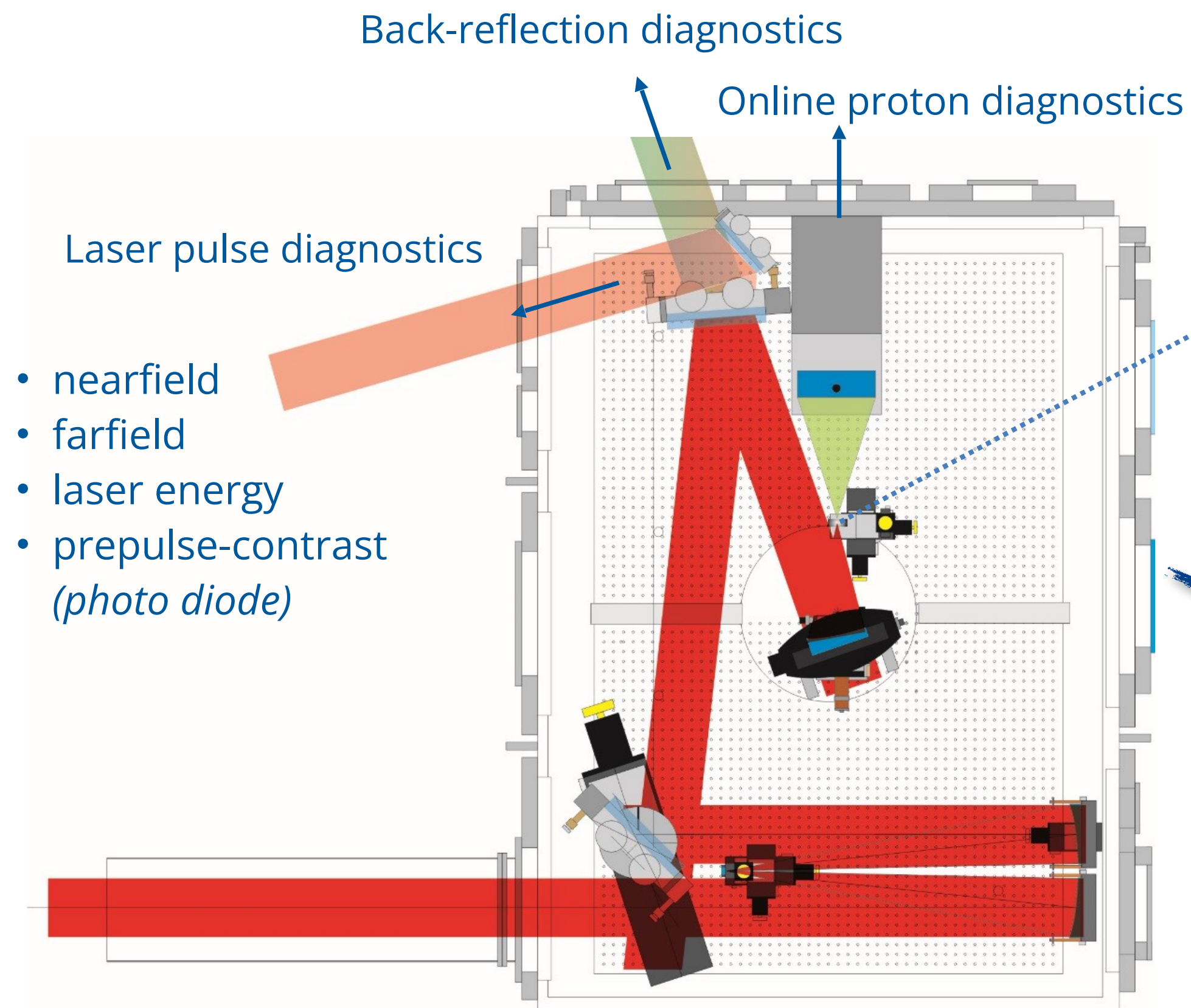
Important Diagnostics:

- CCD cameras
- Photodiodes
- oscilloscopes
- Spectrometer
- energy meter

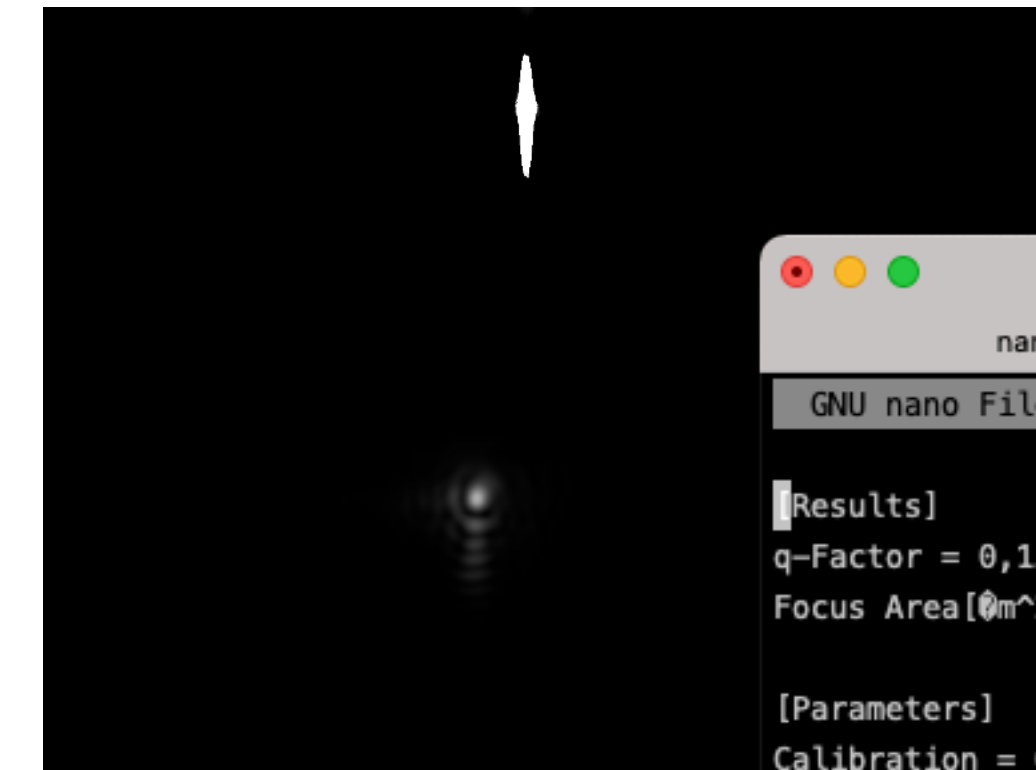
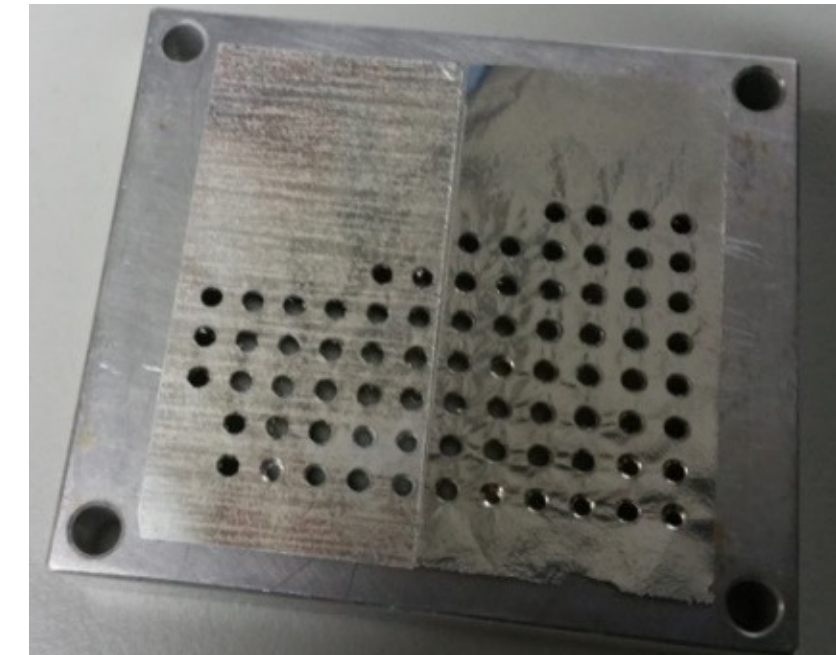


Polz, J., Robinson, A.P.L., Kalinin, A. *et al.* Efficient Laser-Driven Proton Acceleration from a Cryogenic Solid Hydrogen Target. *Sci Rep* 9, 16534 (2019).
<https://doi.org/10.1038/s41598-019-52919-7>

POLARIS Experimental Setup



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



```

nano
nano (nano)
GNU nano File: ...14.data

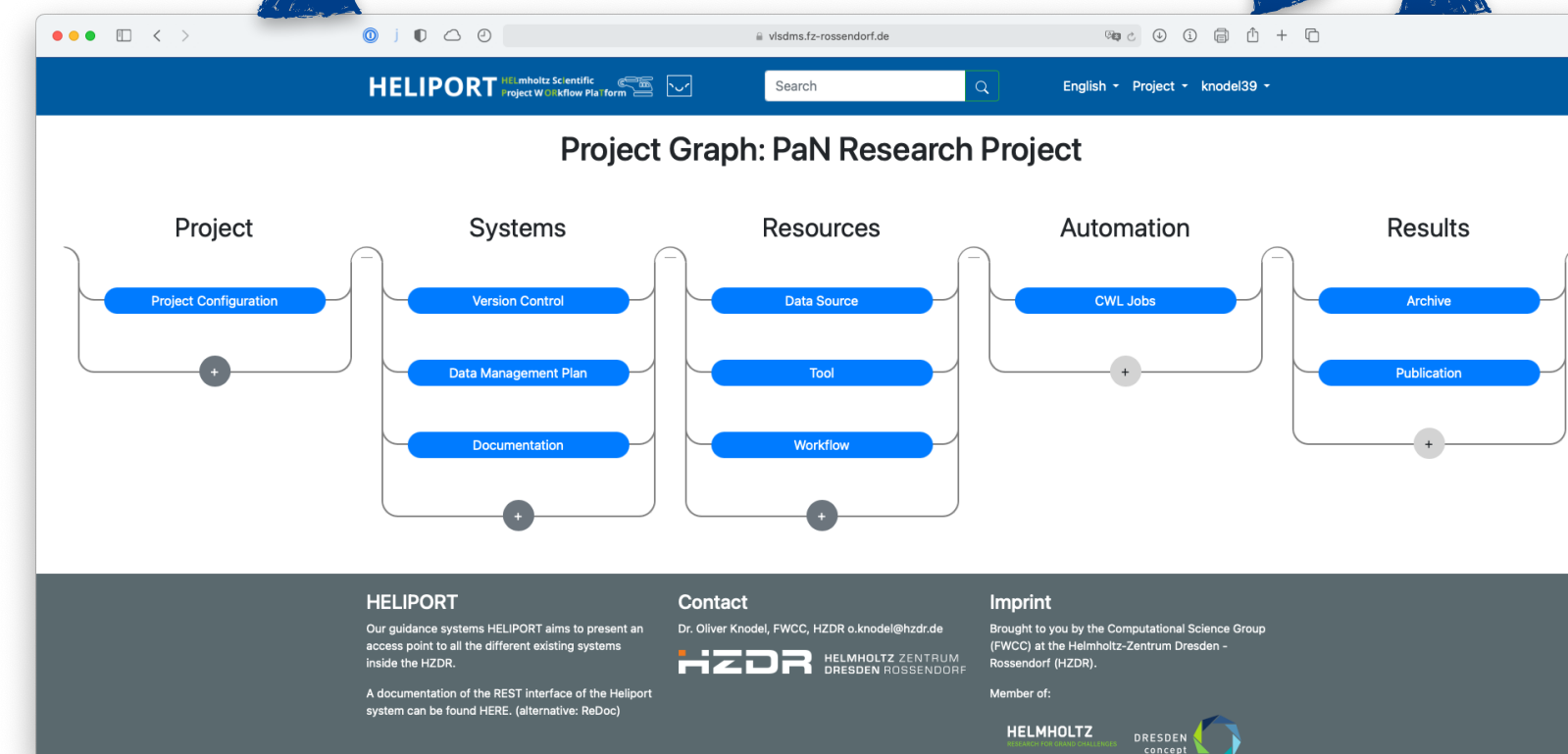
[Results]
q-Factor = 0,150082
Focus Area[0m^2] = 10,055498

[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.R0I]
GlobalRectangle.0 = 186
GlobalRectangle.1 = 346
GlobalRectangle.2 = 942
GlobalRectangle.3 = 1002

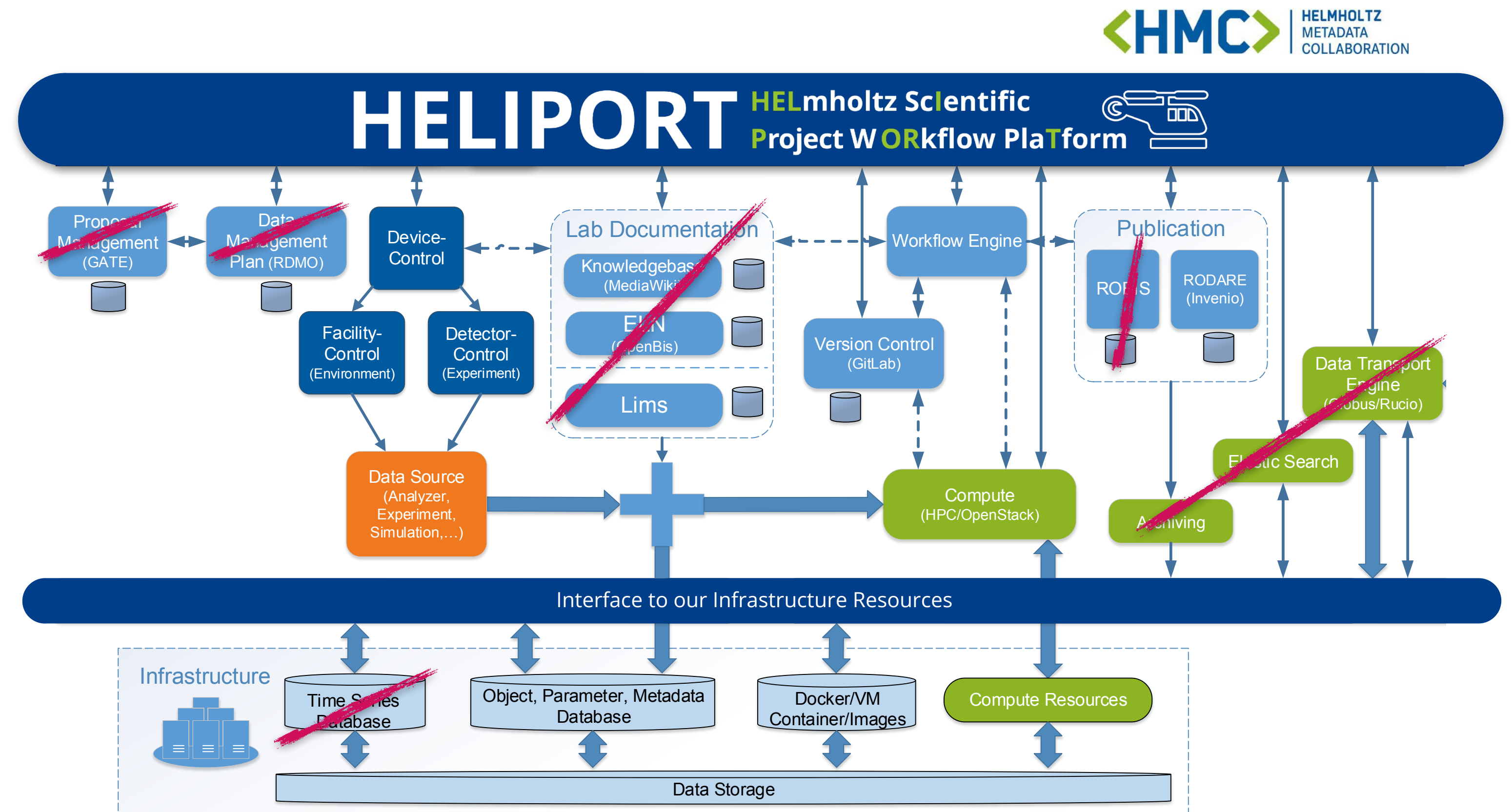
[Parameters.R0IContour.0]
ID = 0
Type = 4
Coordinate.0 = 186
Coordinate.1 = 346
Coordinate.2 = 942
Coordinate.3 = 1002
    
```

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



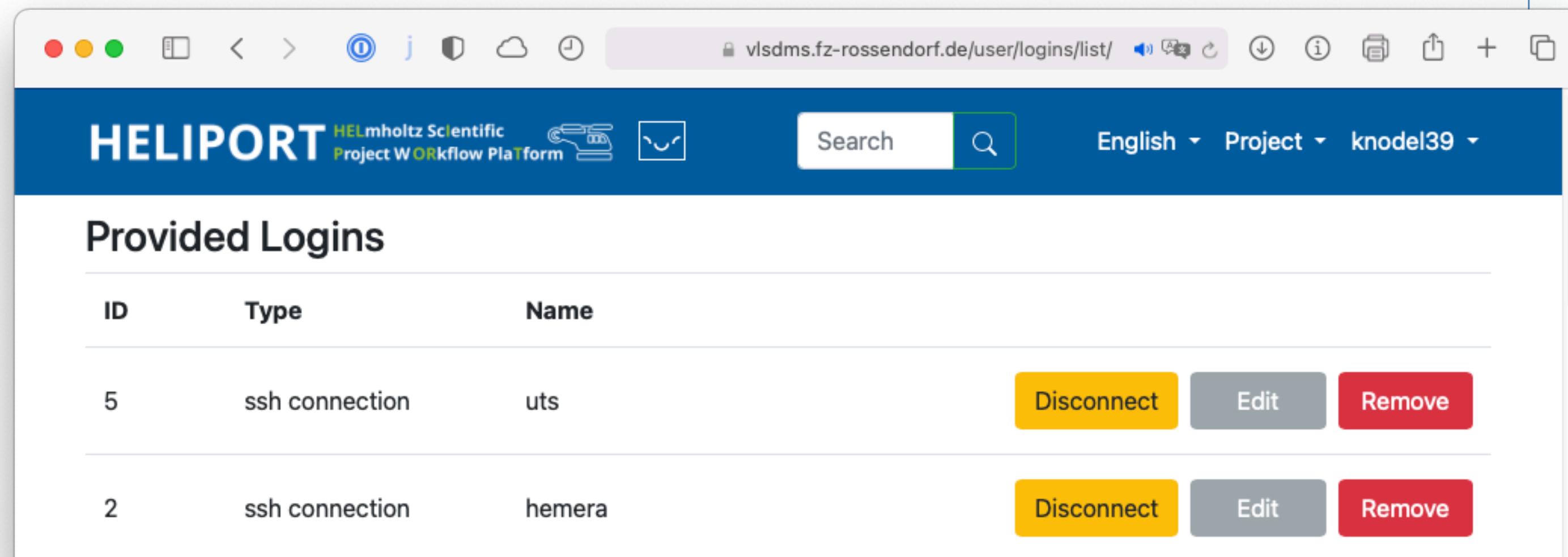
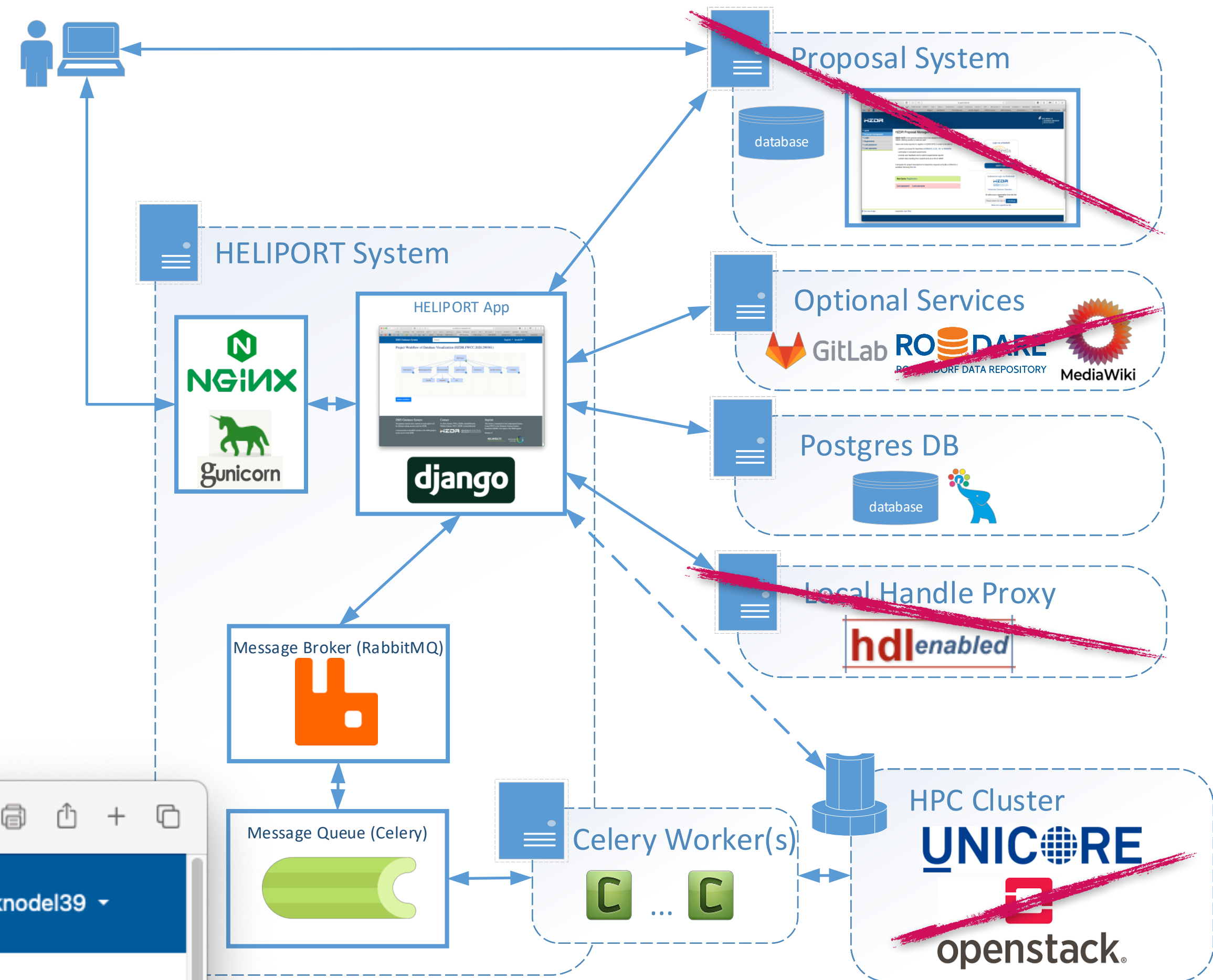
HELIPORT and the Infrastructure at Helmholtz Institute Jena

- HELIPORT was initially developed to provide access to the computing Infrastructure at the HZDR.
- The infrastructure at Jena is different, but the important systems are available:
 - HPC Infrastructure and Data Management*
 - Data Acquisition
 - Git Repositories
- And others are in development:
 - Lab Documentation
 - Data Repository



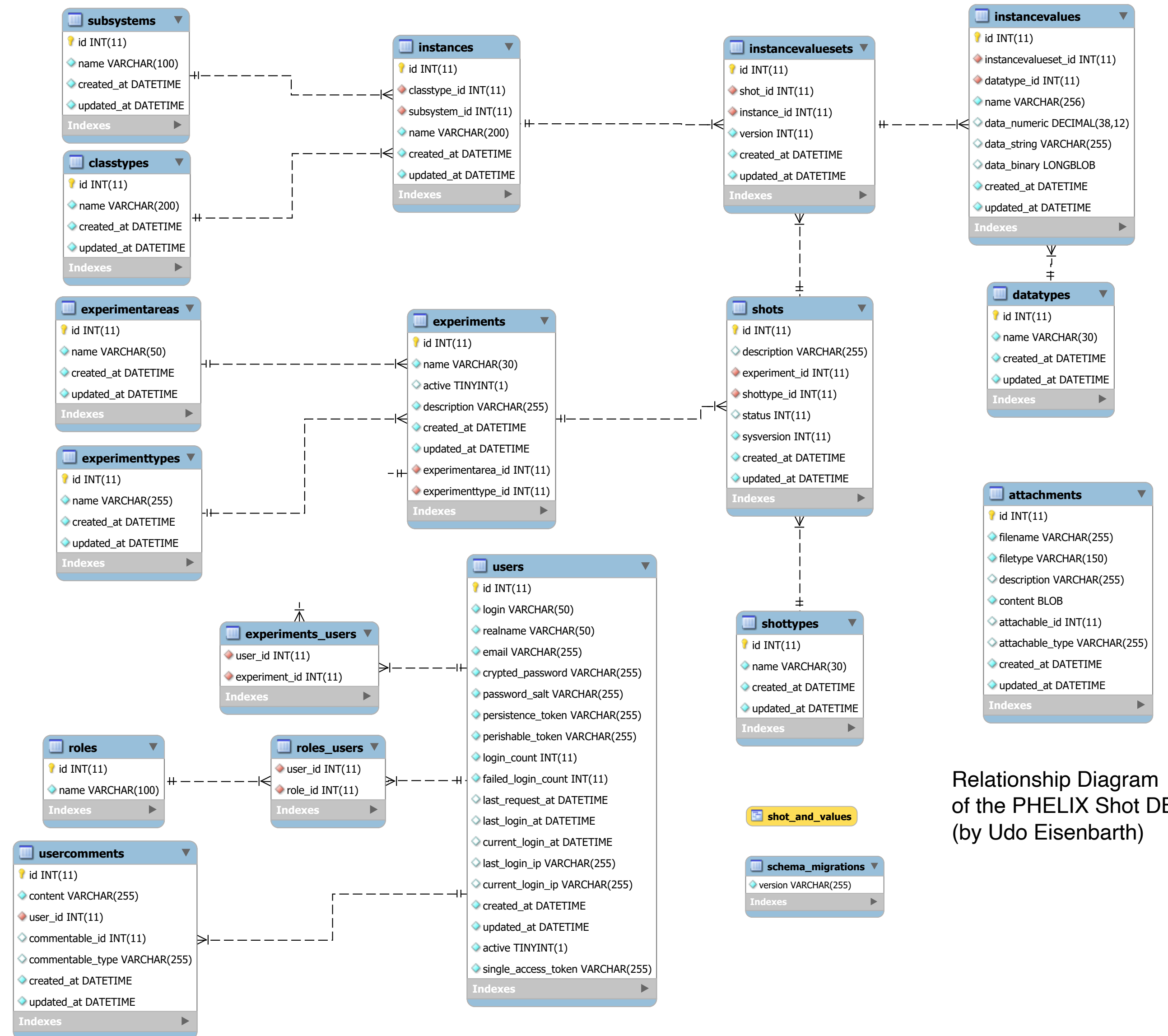
HELIPORT System Infrastructure for POLARIS

- HELIPORT is a future service on a HII server.
- Other services or systems are configurable.
- The HELIPORT Web-App itself is based on Django:
 - HELIPORT communicates with various system through REST APIs,
 - The metadata is stored in a PostgreSQL database.
 - The HELIPORT graph and integrated systems are configurable.
- The CWL workflows are managed in HELIPORT and can be executed on various machines using SSH:



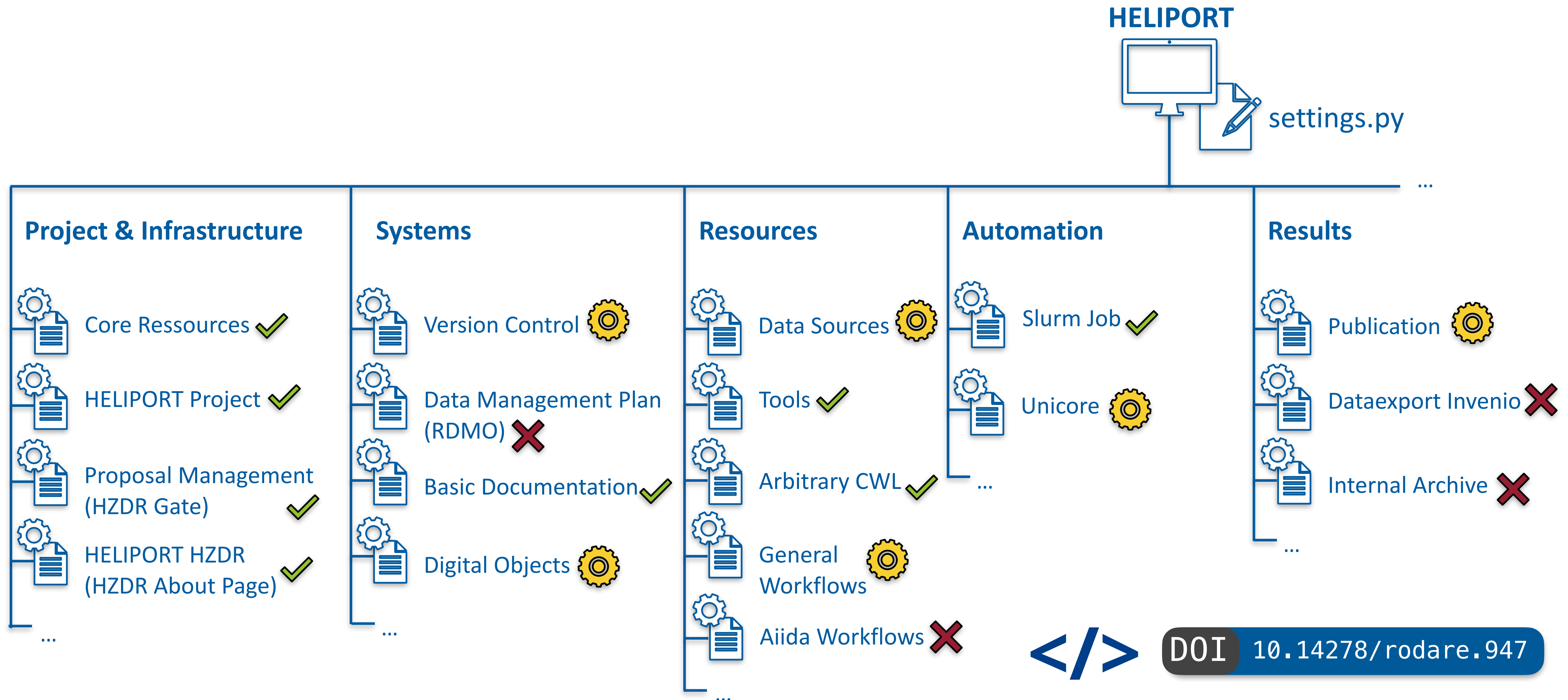
POLARIS Experiment Database

- The Metadata of the POLARIS experiment is managed by a modified version of the **PHELIX Shot DB**.
- Top-level project metadata is available within HELIPOINT.
- Additionally a separate (POLARIS) **Laser Metadata Plugin** in HELIPOINT is required:
 - (Meta)Data can be exchange with various system through REST APIs,
 - The experiment specific metadata will be exchanged with the PHELIX Shot DB and referenced in HELIPOINT.
- The **Laser Metadata Plugin** provides a view in HELIPOINT to configure laser specific metadata.



Relationship Diagram of the PHELIX Shot DB (by Udo Eisenbarth)

Modular HELIPOINT Design (Django Apps)

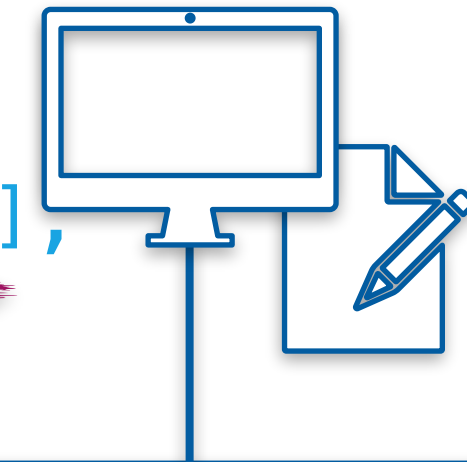


Integration of a Custom Plugin

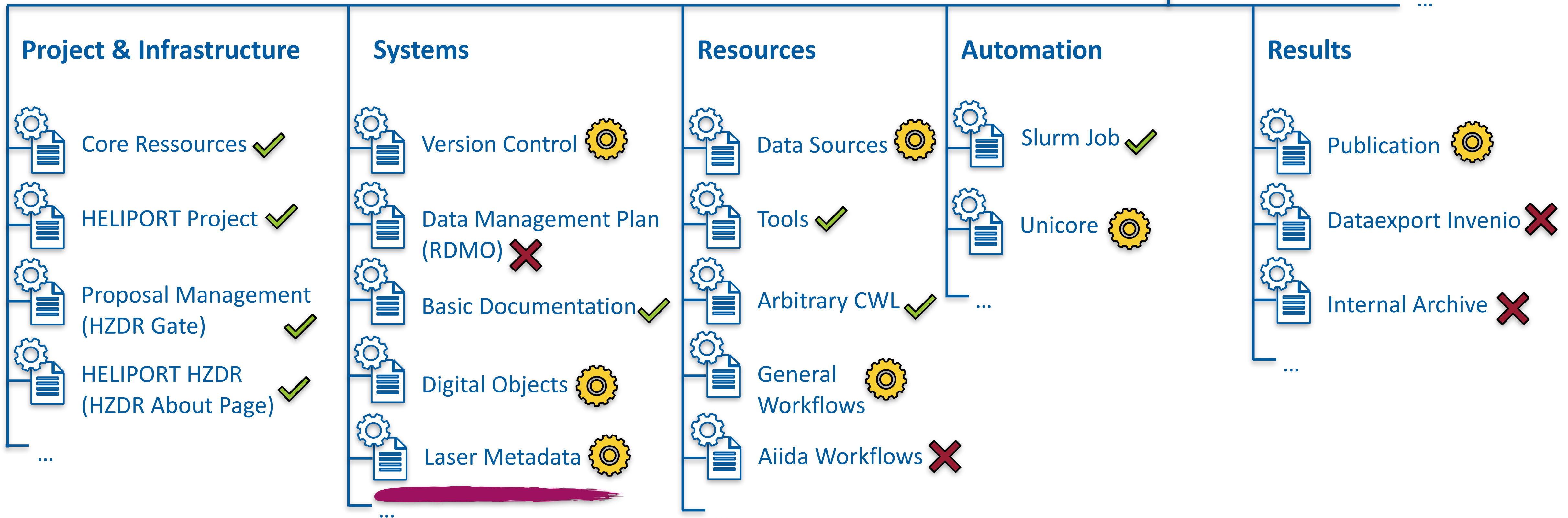
```

GRAPH = {
  'Project': ['project_configuration', 'gate_connection'],
  'Systems': ['version_control', 'data_management_plan', 'documentation',
             'digital_objects', 'sharelatex', 'lasermeta'],
  ...
}
    
```

HELIPORT



settings.py



POLARIS Metadata — Laser Metadata Plugin

- The idea is to collect the experiment specific metadata with a flexible **Laser Metadata Plugin**
- The data columns are can be configured flexible using the HELIPORT website:
 - An extendable vocabulary for specific field can be extended during the experiment
 - Rows can be added using web interface or REST API.
 - Fields can be configured with pre-filled (but editable) content.
- The resulting schema can be used in other future projects and also published in a data repository using a workflow in Heliport.

HELIPORT HELmholtz Scientific Project Workflow Platform

Projects > Polaris Shot 2020.58444

Laser Metadata Table

Search

data_source documentation Namespace publication version_control

detector job proposal tool

Filter **Reset Categories** **All Categories** **Clear Selection**

ID	Handle	Label	
2044	20.500.12865/HELIPORT.Namespace.2044	detector	Edit Remove
2045	20.500.12865/Device.detector.2045	camera	Edit Remove

Add a vocabulary item **Edit Project Relations**

choose category

Property Value

(Meta)data can be exported in an uniform **community standard** and also be exchanged within the HELIPORT components

Enhancing POLARIS Experiments with Simulations (Digital Twins)

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 editor interface showing a step: 'Create supercell from element and structure'. The interface includes a search bar and navigation options.

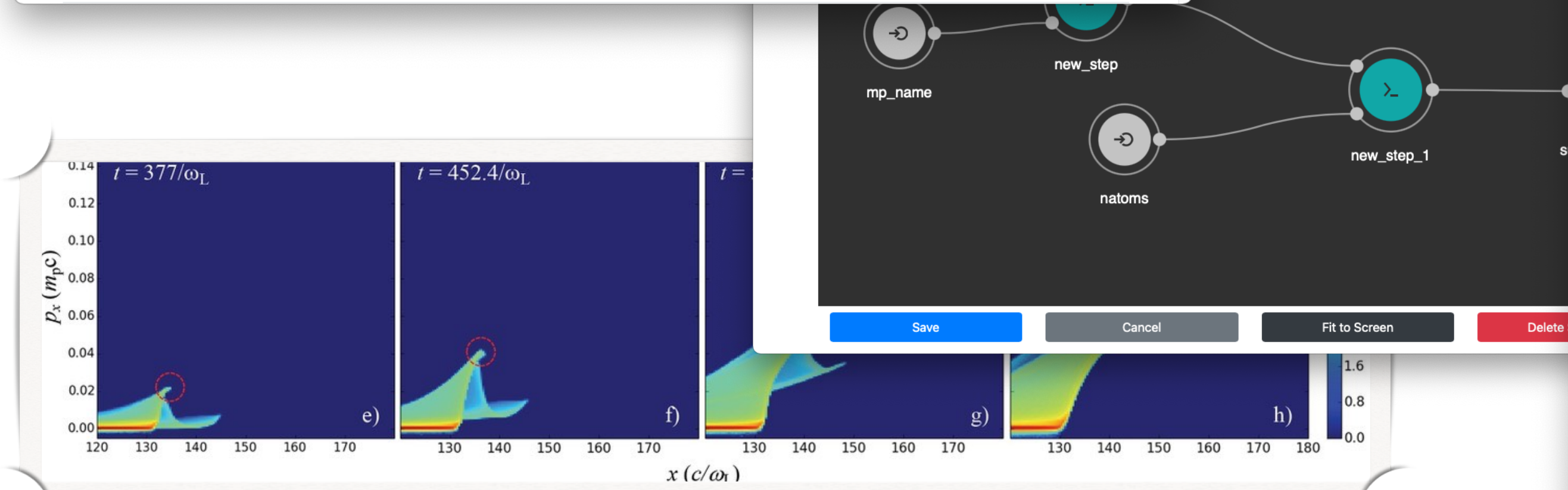
Test job Run Output Details

```

93% |██████████| 1.1MB 9.0MB/s eta 0:00:01
93% |██████████| 1.1MB 11.2MB/s eta 0:00:01
94% |██████████| 1.1MB 11.5MB/s eta 0:00:01
95% |██████████| 1.1MB 10.1MB/s eta 0:00:01
96% |██████████| 1.1MB 11.5MB/s eta 0:00:01
97% |██████████| 1.1MB 12.5MB/s eta 0:00:01
98% |██████████| 1.2MB 10.7MB/s eta 0:00:01
99% |██████████| 1.2MB 11.9MB/s eta 0:00:01
99% |██████████| 1.2MB 11.9MB/s eta 0:00:01
100% |██████████| 1.2MB 650kB/s

[?25hCollecting mpy-extensions (from cwlttool)
Downloading
https://files.pythonhosted.org/packages/5c/eb/975c7c080f3223a5cdaff09612f3a5221e4ba534f7039db34c35d95fa6a5
/mpy_extensions-0.4.3-py2.py3-none-any.whl
Collecting requests>=2.6.1 (from cwlttool)
Cache entry deserialization failed, entry ignored
Downloading
https://files.pythonhosted.org/packages/29/c1/24814557f1d22c56d50280771a17307e6bf87b70727d975fd6b2ce6b014a
/requests-2.25.1-py2.py3-none-any.whl (61kB)
[?25l
16% |██████| 10kB 27.2MB/s eta 0:00:01
33% |██████| 20kB 25.3MB/s eta 0:00:01
50% |██████| 30kB 25.5MB/s eta 0:00:01
66% |██████| 40kB 26.3MB/s eta 0:00:01
83% |██████| 51kB 23.9MB/s eta 0:00:01
100% |██████████| 61kB 994kB/s

[?25hCollecting shellescape<3.5,>=3.4.1 (from cwlttool)
Downloading
https://files.pythonhosted.org/packages/51/b6/986c99a10040beaefca1ad6c93bd7738cb8e4f52f6caed13d3ed1caa7e4
/shellescape-3.4.1-py2.py3-none-any.whl
Collecting psutil (from cwlttool)
Cache entry deserialization failed, entry ignored
Downloading
https://files.pythonhosted.org/packages/e1/b0/7276de53321c12981717490516b7e612364f2cb372ee8901bd4a66a000d7
/psutil-5.8.0.tar.gz (470kB)
[?25l
2% |██| 10kB 11.5MB/s eta 0:00:01
4% |██| 20kB 14.2MB/s eta 0:00:01
6% |██| 30kB 16.6MB/s eta 0:00:01
8% |██| 40kB 18.4MB/s eta 0:00:01
10% |██| 51kB 19.5MB/s eta 0:00:01
13% |██| 61kB 20.7MB/s eta 0:00:01
    
```



Polz, J., Robinson, A.P.L., Kalinin, A. *et al.* Efficient Laser-Driven Proton Acceleration from a Cryogenic Solid Hydrogen Target. *Sci Rep* 9, 16534 (2019). <https://doi.org/10.1038/s41598-019-52919-7>

The Heliport Project-Level Metadata Scheme

```

{
  "namespaces": {
    "datacite": "http://purl.org/spar/datacite/",
    "rdfs": "http://www.w3.org/2000/01/rdf-schema",
    "heliport": "https://heliport/schema/",
    "time": "http://www.w3.org/2006/time#",
    "dc": "http://purl.org/dc/terms/"
  },
  "heliport:project_id": 9,
  "datacite:hasIdentifier": "HZDR.FWCC.2021.95018",
  "heliport:uuid": "8fab8a14-0f2f-414d-bbe0-747c38129bc4",
  "datacite:handle": "https://hdl.handle.net/20.500.12865/HZDR.FWCC.2021.95018",
  "heliport:label": "An Example Project",
  "time:hasBeginning": "2021-05-18 13:03:34.378458+00:00",
  "datacite:hasDescription": "This Project has the sole purpose of demonstrating the functionality of HELIPOINT",
  "heliport:group": "FWCC",
  "heliport:owner": {
    "datacite:hasIdentifier": "141575",
    "datacite:orcid": "https://orcid.org/0000-0001-5556-838X",
    "rdfs:label": "Voigt, Martin (FWCC) - 141575"
  },
  "heliport:co_owners": [
    {
      "datacite:hasIdentifier": "132739",
      "datacite:orcid": "https://orcid.org/0000-0001-8174-7795",
      "rdfs:label": "Knodel, Dr. Oliver (FWCC) - 132739"
    },
    . . .
  ],
  "heliport:has_GATEProject": [
    {
      "heliport:gate_id": 283747364,
      "dc:title": "An Example GATE Project",
      "heliport:status": "Continuesly Improving",
      "dc:abstract": "There is an urgent need to ... (ref.: 10.1038/sdata.2016.18)",
      "datacite:hasIdentifier": "sdata.2016.18",
      "dc:accessRights": true,
      "dc:creator": {
        "datacite:hasIdentifier": "141575",
        "datacite:orcid": "https://orcid.org/0000-0001-5556-838X",
        "rdfs:label": "Voigt, Martin (FWCC) - 141575"
      },
      "heliport:responsible_experimentalist": {
        . . .
      },
      . . .
    }
  ],
  . . .
}

```



The screenshot shows the HELIPOINT web interface for project 9. The page title is "Project Properties". The interface includes a search bar and a language selector set to "English". The project details are as follows:

HZDR-ID	HZDR.FWCC.2021.95018
Handle	20.500.12865/HZDR.FWCC.2021.95018
Digital Object ID	73
uuid	8fab8a14-0f2f-414d-bbe0-747c38129bc4
serialization url	https://vlsdms.fz-rossendorf.de/project/9/serialize/
Owner	Voigt, Martin (FWCC) - 141575
Created	May 18, 2021, 1:03 p.m.
Group	FWCC
Title	An Example Project
Description	This Project has the sole purpose of demonstrating the serialization functionality of HELIPOINT using vocabularies like datacite, rdfs or custom terms.

There is an "Edit" button below the description. The "Members" section below shows the following member:

Name	Knodel, Dr. Oliver (FWCC) - 132739
-------------	------------------------------------

Conclusions

- HELIPOINT provides a comprehensible top-level view on the project and all corresponding systems
- With plugins additional services or systems can be integrated
- The metadata can be used in integrated workflows to enable high interoperability
- With our **Laser Metadata Plugin** we can collect and customize metadata and publish it in a data repository like Rodare.

