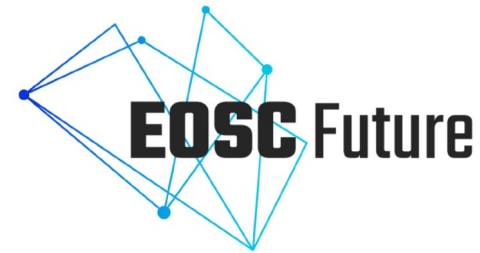# Integrating the VISA portal into DESY infrastructure

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DMA-ST1, Jan 20 2025, Hamburg

HELMHOLTZ | RESEARCH FOR GRAND CHALLENGES

DESY.

Overview

- VISA portal originally developed by Institut Laue-Langevin (ILL) during PaNOSC
- Adopted by member institutes of the project itself as well as by ExPaNDS members
- Currently setting up an MoU to
  - Build a community for further development of the portal software and exchange experiences
  - Ensure sustainable reuse of the portal software at multiple institutes
  - Disseminate the use of VISA to a wider audience
- Visa is currently in productive use at ILL and ESRF
- More institutes to join soon

- VISA allows scientific users to run data analysis tools in their browser on virtual hardware close to their data
- VISA allows to embrace **FAIR** data principles
  - Data catalogue integration in VISA makes data **Findable**
  - Storage integration at the hosting institutes makes data **Accessible**
  - Standardized data formats per scientific discipline make data **Interoperable**
  - Labelling data for open use after embargo periods makes it **Reusable**

VISA
Create an instance

VISA
Work with JupyterLab

Example by Silvan Schön (DESY/FS-SC):
Using CrystFEL Docker Images to run Singularity Container in a Jupyter Notebook (on a Bash Kernel).
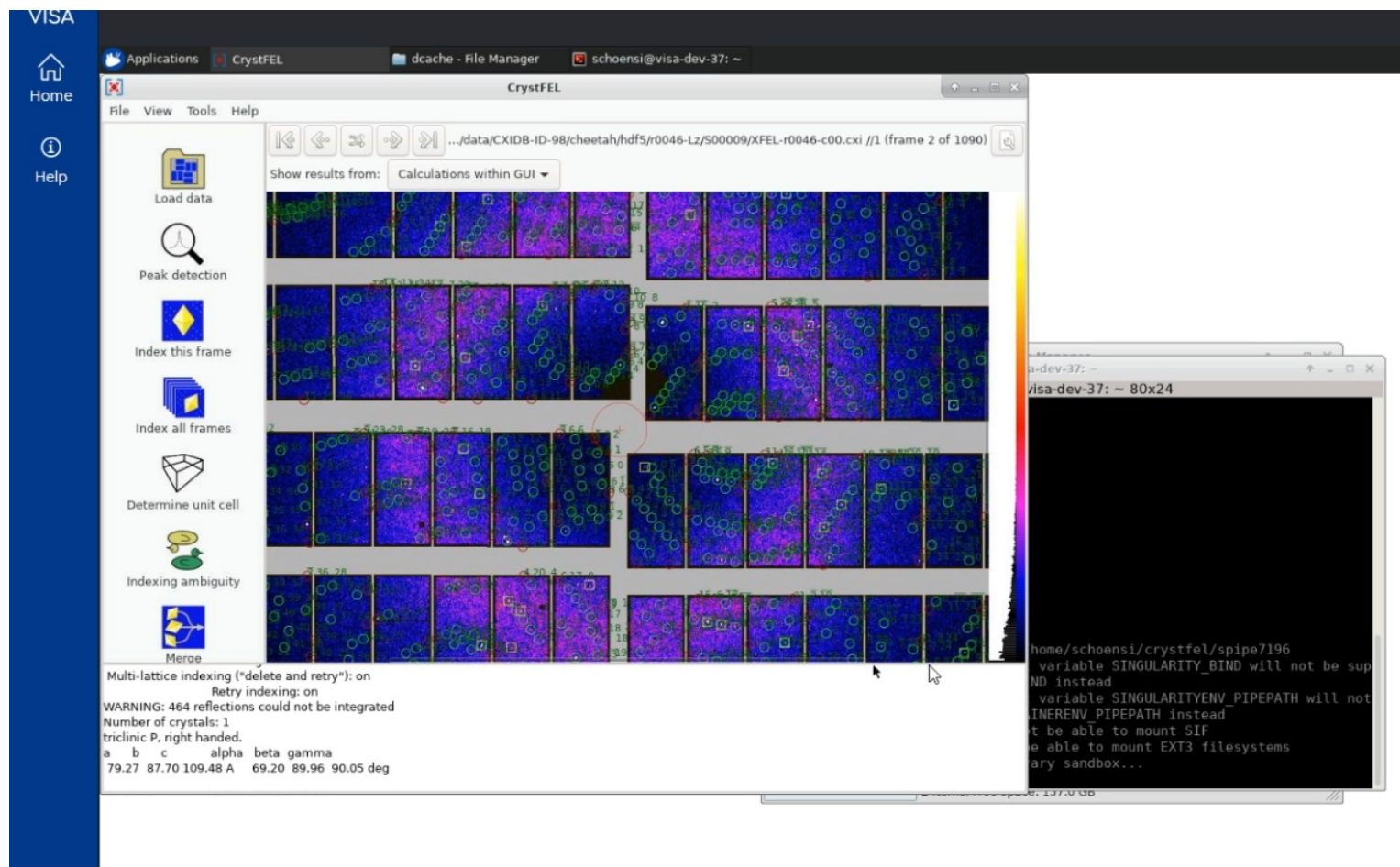
VISA
Work with Remote Desktop

Example by Silvan Schön (DESY/FS-SC)
Using CrystFEL Docker Images to run Singularity Container and work with Crystfel 10 Graphical Interface.

VISA

Interoperable workflow that seamlessly extends to Maxwell HPC Infrastructure
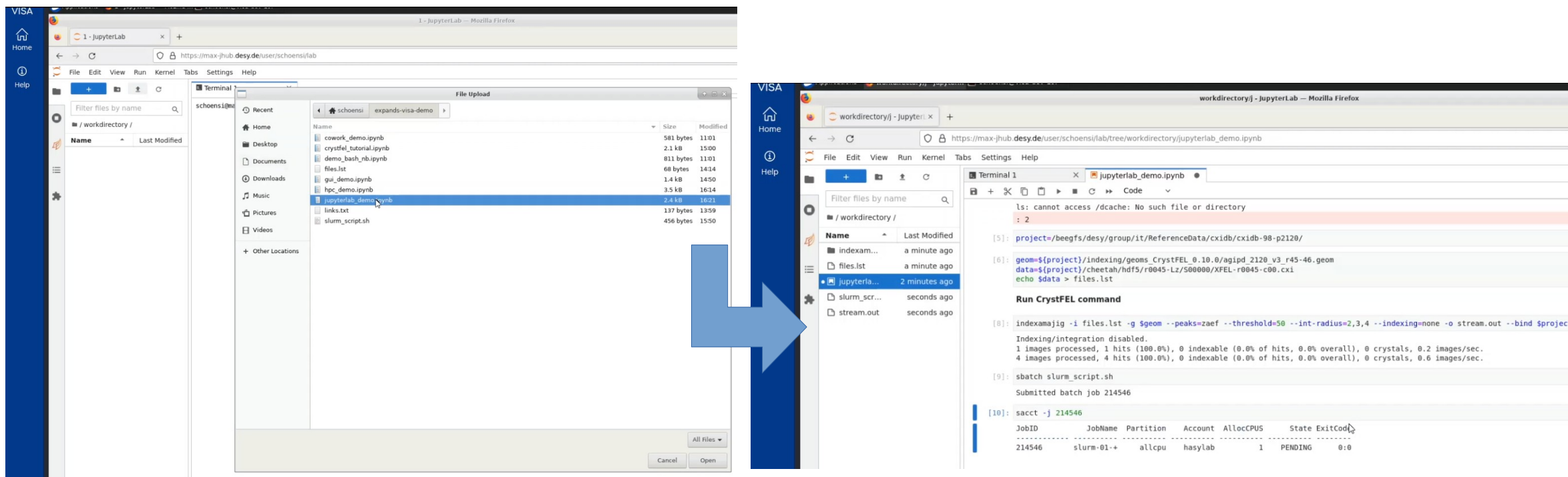
Example by Silvan Schön (DESY/FS-SC)
Use VISA to upload notebook to Maxwell HPC Cluster, Notebook + Slurm Job
Interoperable: Run same analysis, same data (CrystFEL 10 Singularity Container)

VISA hosted at DESY
Architecture Overview (Data Analysis Platform)
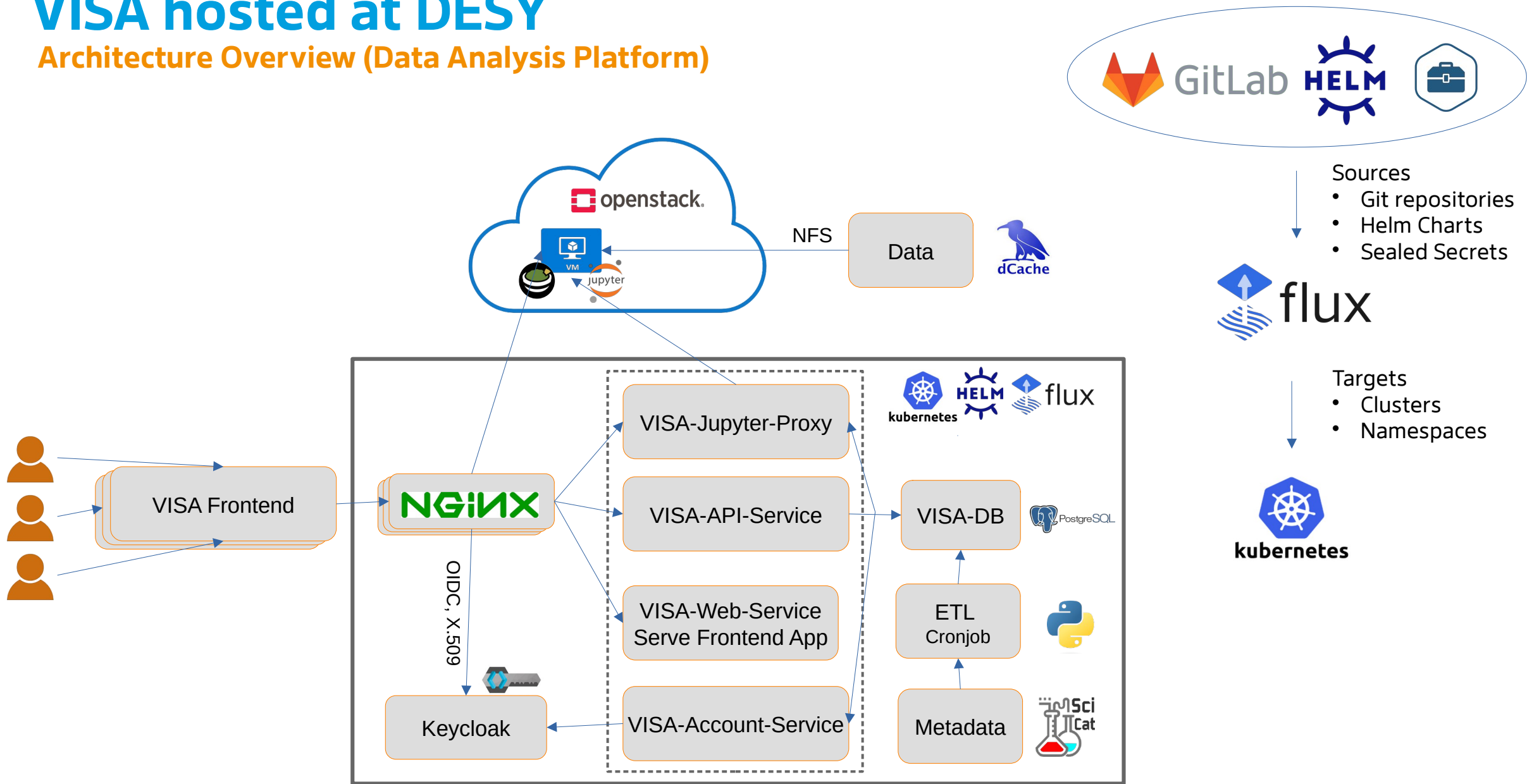
AAI
Keycloak


```
dn: uid=******-dlr-f,ou=people,ou=rgy,o=desy,c=de
[...]
displayName: ******, ****** (******-dlr-f)
mail: ******@dlr.de
uid: ******-dlr-f       ←--- persistent UIDs
uidNumber: 1001234      ←--- persistent UID numbers
```

- keycloak.desy.de as SSO solution for DESY
- Local:
  - DESY Registry Accounts (LDAP)
  - DOOR accounts
- Integration with federations:
  - Helmholtz AAI
  - EGI Check-in
  - Github
- Importing accounts and assigning persistent UIDs
- OIDC clients managed on-premise

Software deployment
Via Apptainer images built in Gitlab CI/CD
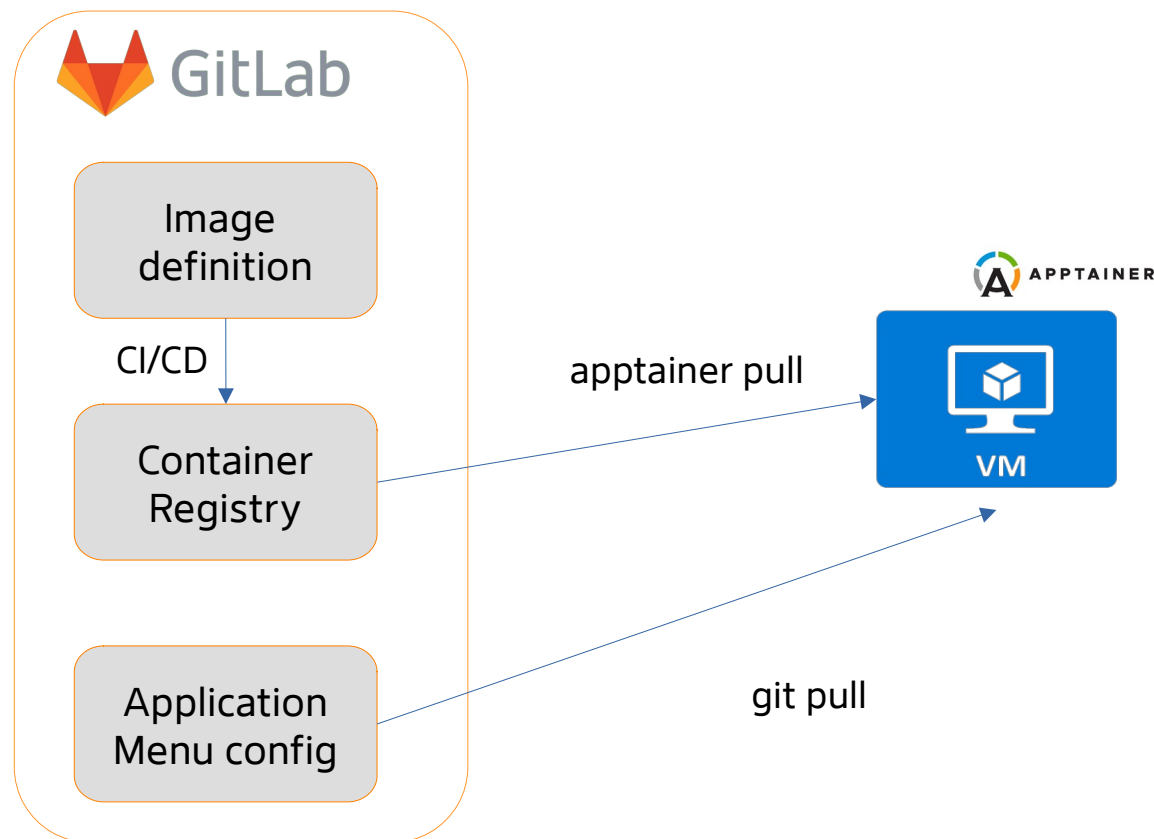
- Software in Apptainer images
  - Many applications already available as Apptainer image from HPC workflows
- Built from .def file in CI/CD pipeline
- Image publicly available in Gitlab registry
- Pulled on application startup

- Application menu entries defined separately in git repository
- Seamless integration into the OS applications
- Menu entries updated from menu config by cronjob pulls the repository regularly
- Updates to the menu by admins

Metadata integration

Custom ETL process
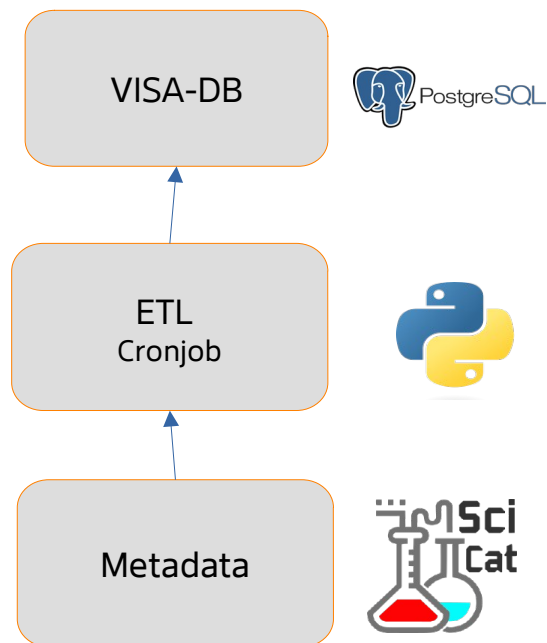
- Python script
- Customizable depending on the metadata source (catalogue API format, authN/Z, …)
- Can be run once for static data or as a cronjob for dynamic data
- Event-based execution would be nice to have (e.g. webhooks)

- Metadata import
  - Experimental specifications
  - Dataset status (embargoed or public)
  - User access rights
  - Storage paths

- Database backup

DESY Photon Science setup

A high-level view of the world

OAI-PMH

Users

PUBLIC DATA

HIFIS-Storage
dCache

OpenAIRE B2FIND

DOI creation
DataCite

Data exploration
silx VISA jupyter

DOI resolution
DataCite

HELMHOLTZ ID

Firewall

Sci Cat

Access controlled data

DESY-dCache
dCache

Only use standard protocols for communication between components so they can be exchanged if necessary
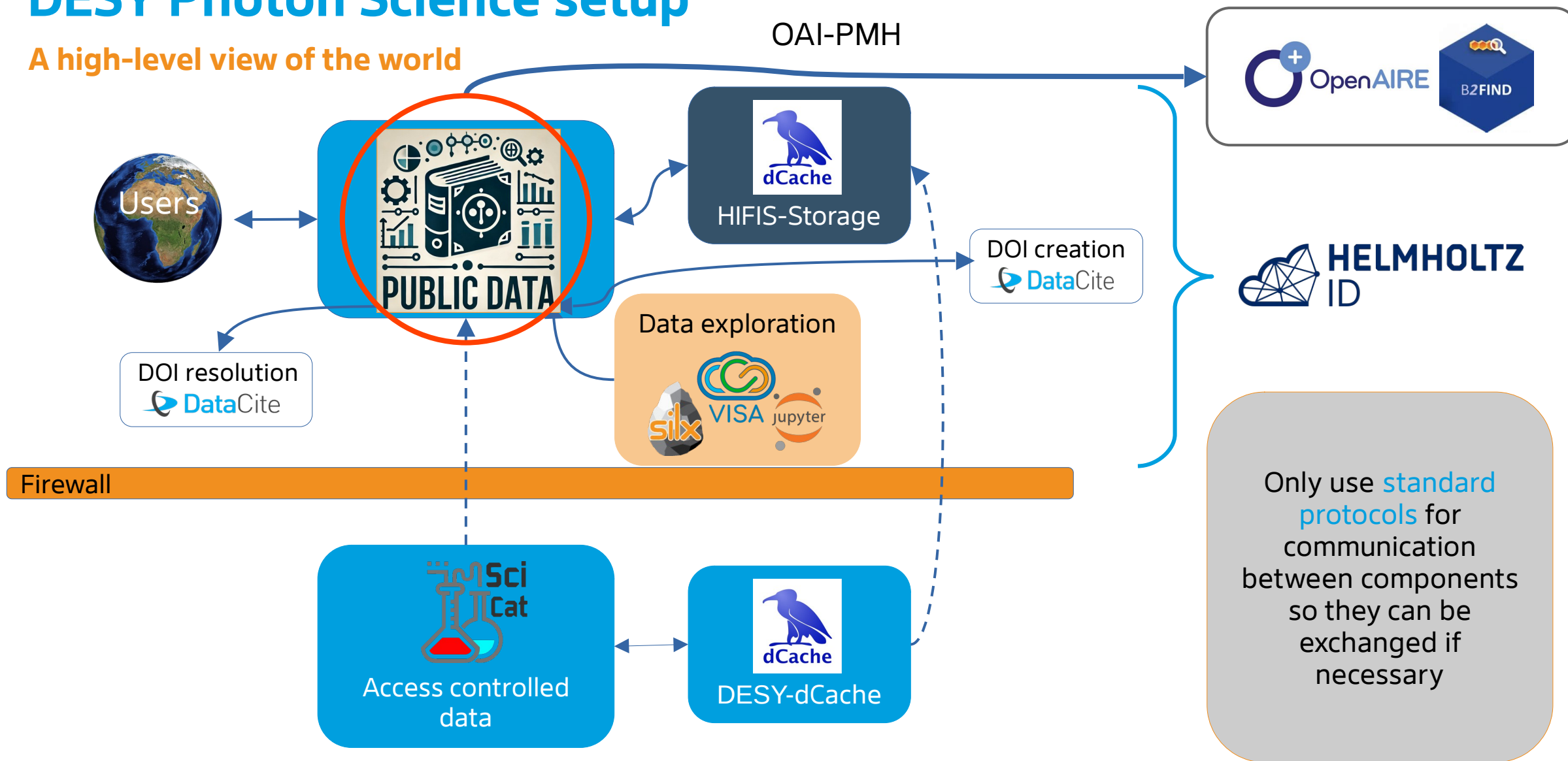
Image adapted from Anton Barty's slide

public-data.desy.de

The metadata catalog!

PUBLIC DATA

Scientific Metadata

🔍 Search   ✕

▼ DIP_1

Experimentalists	Kowark, Stefan
Layer_CAS	188-94-3
Layer_formula	C32H16
Layer_material	Diindenoperylene
Substrate_temperature	303 (K)
instrument	ESRF, ID10b
q_max_fit	0.15 (1/Ang)
year_experiment	2005

▶ DIP_2

Search   ≡ Clear

PID

Text Search

Location

Group

Type

Keywords

Start Date – End Date

+ Add Condition

Name   Source Folder

Reflectometry curves (XRR and NR) and corresponding fits for machine learning   ...do.6497438

spain   .../nfs

📄 General Information

Name	Reflectometry curves (XRR and NR) and corresponding fits for machine learning
Description	This is a compiled dataset of raw X-ray reflectivity (XRR, reflectometry) measurements together with corresponding fit parameters, intentionally published to use as training or test data for machine learning models. (The authors aim to include NR data in further versions of this dataset and plan to include other substrates and materials for XRR. Contributions welcome!)
PID	undefined/10242df2-3868-42cb-bcb2-81c2c44533ec 📋
Type	raw
Creation Time	2024-01-25 18:34
Keywords	

👤 Creator Information

Owner	Linus Pithan
Principal Investigator	linus.pithan@desy.de
Contact Email	linus.pithan@desy.de
Owner Group	fsec
Access Groups	

📁 File Information

Source Folder	/desy/public-data/upload/daphne4nfdi/10.5281_zenodo.6497438

Path   Size

☐ calc_xrr.py	2 KB
☐ conda_env.yml	7 KB
☐ prepare_plot.py	4 KB
☐ README.html	6 MB
☐ README.ipynb	9 MB
☐ requirements.txt	76 B
☐ xrr_dataset.h5	254 KB

Thank you

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    Jamie Hall, Stuart Caunt and Erwan Le Gall (ILL)
    Majid Ounsy, Eric Moge, Alain Buteau and Ryan Perseé (SOLEIL)

Questions?

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