Technical Talk - ESRF

9th of October 2020

The ExPaNDS project has received funding from the *European Union's Horizon 2020 research and innovation programme* under grant agreement No 857641.
The PaNOSC project has received funding from the *European Union's Horizon 2020 research and innovation programme* under grant agreement No 823852.

Overview

- The Portal Architecture test experience
- COVID and the impact on the team’s roadmap
- ESRF Use Cases – what we need and what we offer

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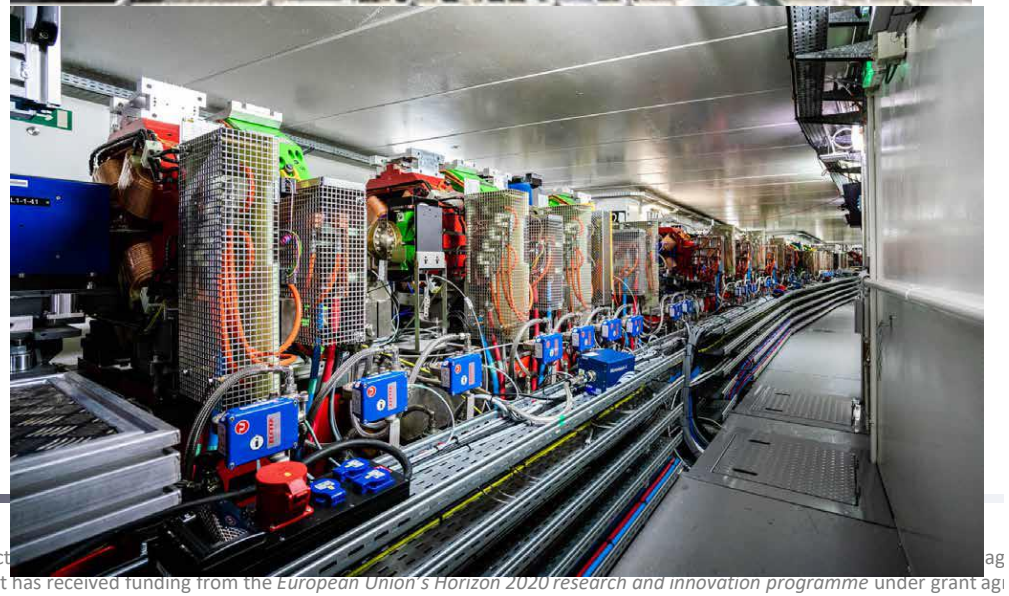
ESRF EBS



EBS Operation status

Beam Current

196.241 mA (0 – 200)

7/8 multibunch

20:13:01 Lifetime

1.4e-9 mBar Average Pressure

Status

Thu 08 Oct 2020 17:25:18

User Service

Delivery since 17:01

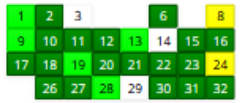
00:34:42 Countdown

157.815 pm EmittanceH

9.545 pm EmittanceV

Beamlines

IDs

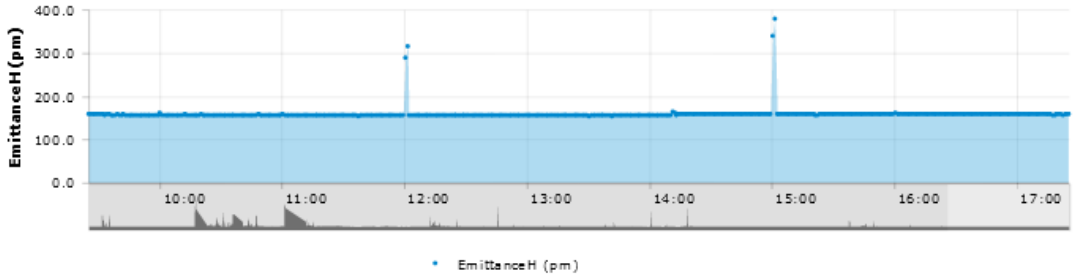


Bendings

Oct 8 17:01 Delivery:Next Refill at 18:00;

last messages

Current | Lifetime | EmittanceH | EmittanceV



Injector

0.0 mA (0 – 0.5)

Linac	SY PS	SY RF
SY inj	SY ext	SR inj
PSS-INJ	INJ-PERM	RF-CAV
---	SR-VAC	RF-TRA

Scan me (Lite view)

Scan me (Detailed view)

Any feedback please email to mstatus-contact@esrf.fr

The ExPaNDS project
The PaNOSC project has received funding from the *European Union's Horizon 2020 research and innovation programme* under grant ag

ESRF PaNOSC Team

Axel Bocciarelli
Software Engineer – Software Group
Expertise in web technologies (React, UX,…)
Will contribute to WP4 + WP5, data portal, Nexus/HDF5 visualization, graphical workflows

Loic Huder
Scientific software Engineer – Software Group
Expertise in visualization, HDF5, Jupyter
Will contribute to WP4 Nexus/HDF5 visualization, Jupyter notebooks

Hire #1 + Hire #2
System administrator – Systems Group
Devops
Will contribute to WP6 + WP4 system infrastructure

Thomas Vincent
Software Engineer – Software Group
Visualisation + Jupyter notebooks
Will contribute to WP4 visualization + coordination

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ESRF PaNOSC Team

Alex de Maria
Software Engineer – Software Group
Expertise in data management, web technologies (React, UX, mongo, camel, SQL, …)
Will contribute to WP3 + WP4, ESRF data portal, data policy implementation

Maxime Chaillet + Hire #3
Software developer –
Software Group
Web developer
Will contribute to WP3 + WP4
e-logbook, DOIs,

Jean-Francois Perrin
Manager – Systems Group
AAI + WP6 leader

Jordi Bodera
Project management – ISDD Office
PaNOSC project manager

Rudolf Dimper
Manager – Directorate
Will contribute to WP2
EOSC Future ESRF lead

Andy Götz
Manager – Software Group
WP2 leader + PaNOSC coordinator

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The Portal Architecture test experience

- **What went well?**
  - We were able to run containers using Docker and Kubernetes on ESRF infra.
  - We also had ESRF data analysis software installed and usable.
  - We could access all of our data in home directories.

- **What could go better?**
  - Supporting all of the different authentication methods and different plugins like icat and scicat was difficult and leads to a configuration mess with too many settings.
  - Supporting other synchrotrons on their infrastructure was borderline impossible as we didn't know their network, why they were having problems and how to integrate it into their synchrotron.
  - The deployment of the entire portal is still quite difficult with quite a few parts.

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Common Portal front-end
ESRF feedback on codebase

- **Modern, popular stack**
  - React + Create React App, styled-components (CSS-in-JS library), Rebass (CSS framework)
  - Prettier + ESLint for code quality
- **React best practices**
  - Small functional components, one component per file, React hooks, error boundaries, authentication via provider, etc.
- **Great code quality overall**
- **Easy to install and start**

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Common Portal front-end – ESRF feedback on Features

- **Search is crucial**
  - Fully on board with idea of filtering sidebar like on e-commerce sites
  - Need to carefully consider each filter (user need + usability)
  - Filters can be added incrementally as user needs are discovered
- **Drag-and-drop UI**
  - Works great, but need to double check WCAG accessibility and discoverability (for keyboard and screen reader users)
  - May be worth adding a simpler UI (e.g. drop-down menu of available environments on each search result) to complement the drag-and-drop interface
- **Dashboard**
  - Nice to have but not necessary; search can remain the main screen for now

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ESRF needs for the Portal

- What are the main use cases for deploying the portal @ ESRF

1. **Link to the ESRF data portal https://data.esrf.fr**
2. **Browse domain specific data similar to https://paleo.esrf.eu**
3. **Provide an access to local Jupyter-slurm notebook service**
4. **Provide access to standard ESRF data analysis programs**
5. **Link software catalogue to data analysis portal**
6. **Provide a remote desktop integrated experience**
7. **Search for data across domains at ESRF and all PaNOSC sites**
8. **Launch standard notebooks for standard experiments**
9. **Expose COVID-19 and other data in a user friendly browser**
10. **Link data portal to data management KPIs e.g. processing with AI/ML**

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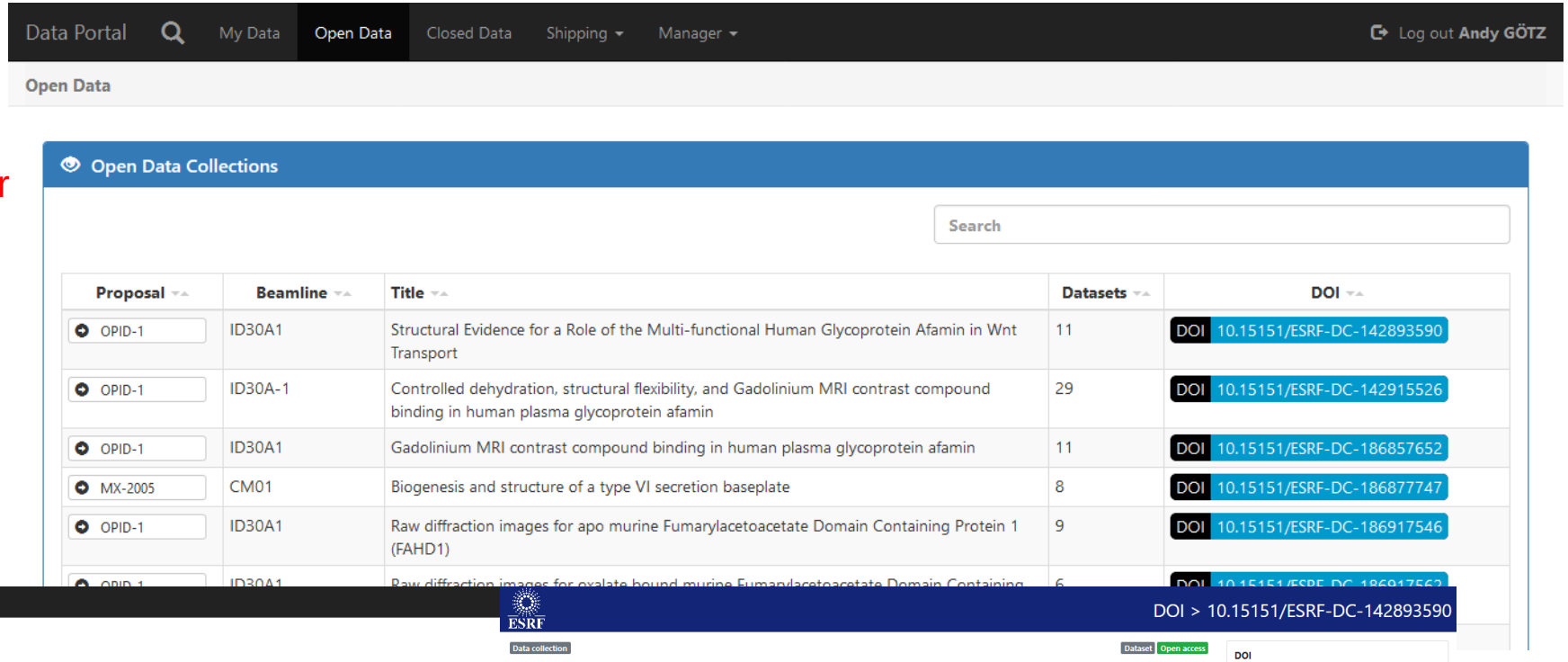
ESRF data portal – https://data.esrf.fr

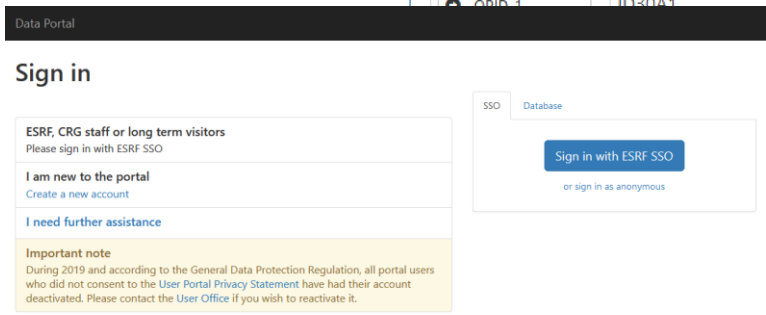
Data policy implemented on **all** ESRF beamlines in 2020

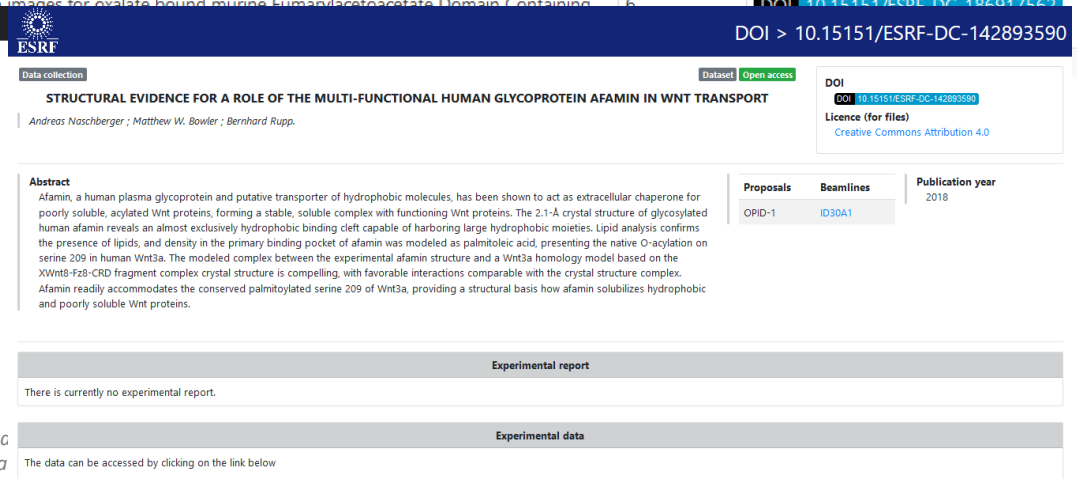
Use Case: integrate https://data.esrf.fr

Users: external users

Expect: common UX







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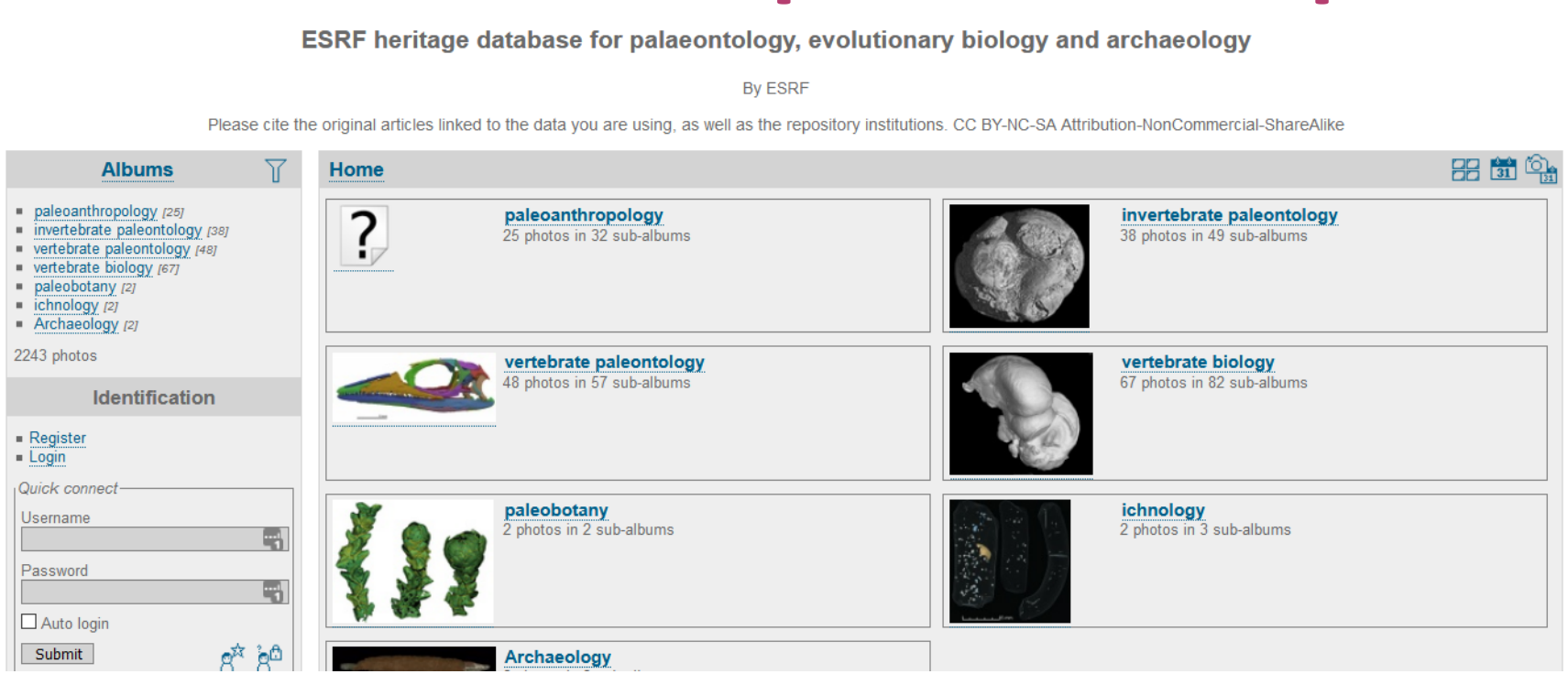
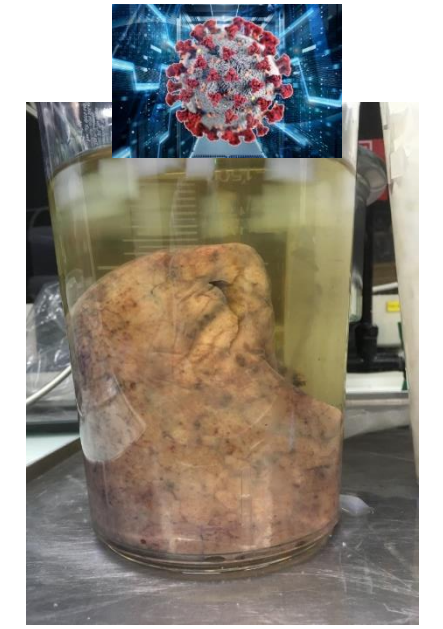
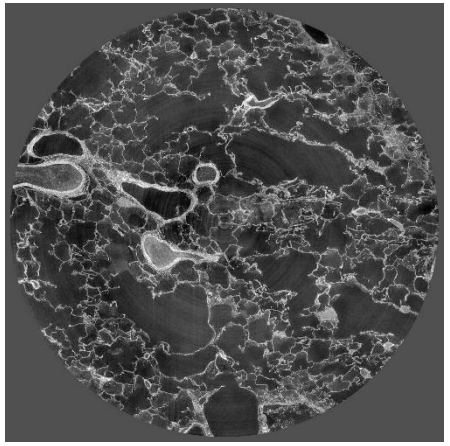
ESRF domain specific data portal(s)







Use Case: provide user friendly way to browse and search for paleontology + COVID-19 data

Users: paleontologists, biologists, medical

Expect: user friendly browser for domain specific categories e.g. paleontology linked to ESRF DOIs

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What ESRF contributes

- High performance **web visualization** of **Nexus/HDF5 (h5web)**
- Integration of visualization of **HDF5** in **Jupyterlab** as 1st class citizen
- **Graphical** visualization of **workflows** in the **web**
- **ICAT integration** and **extensions**
  - Metadata definitions
  - E-logbook
  - Search

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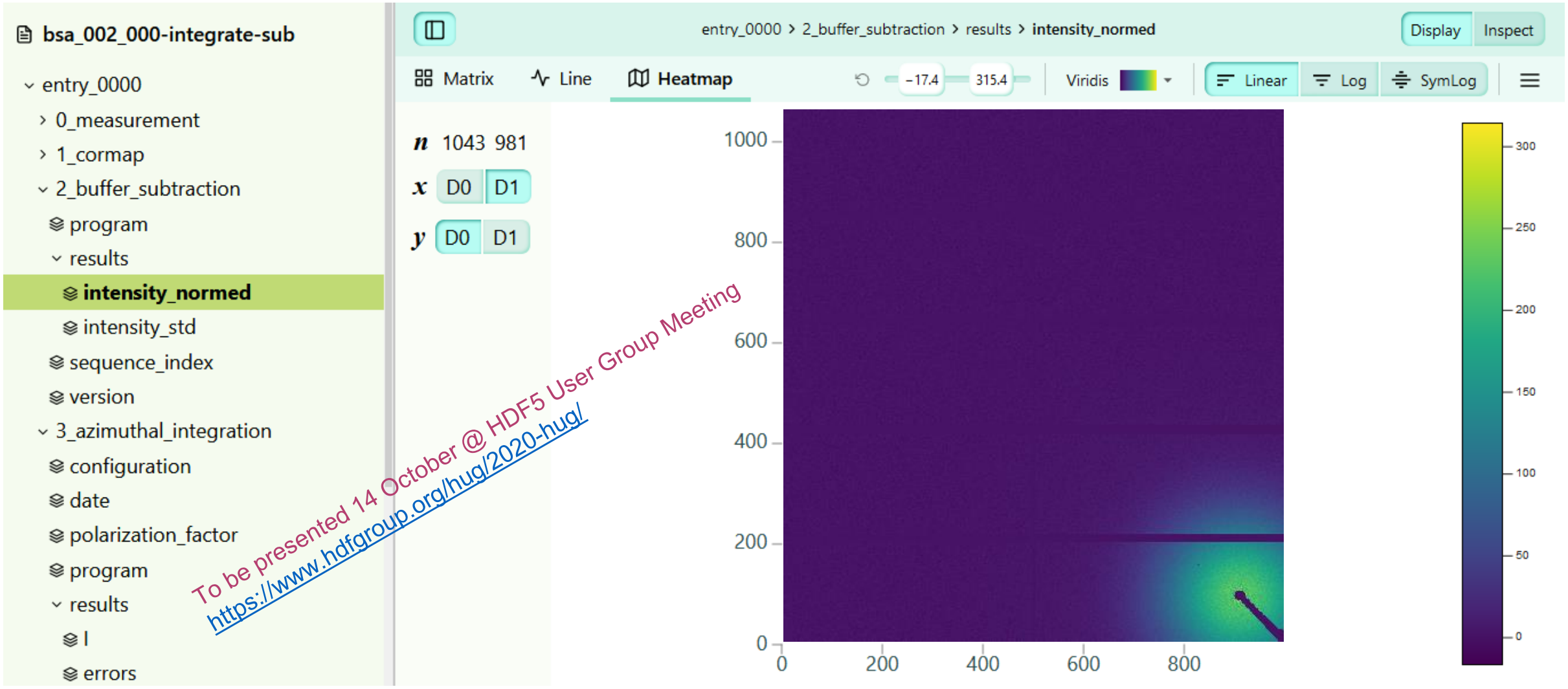
H5web visualisation - https://h5web.panosc.eu



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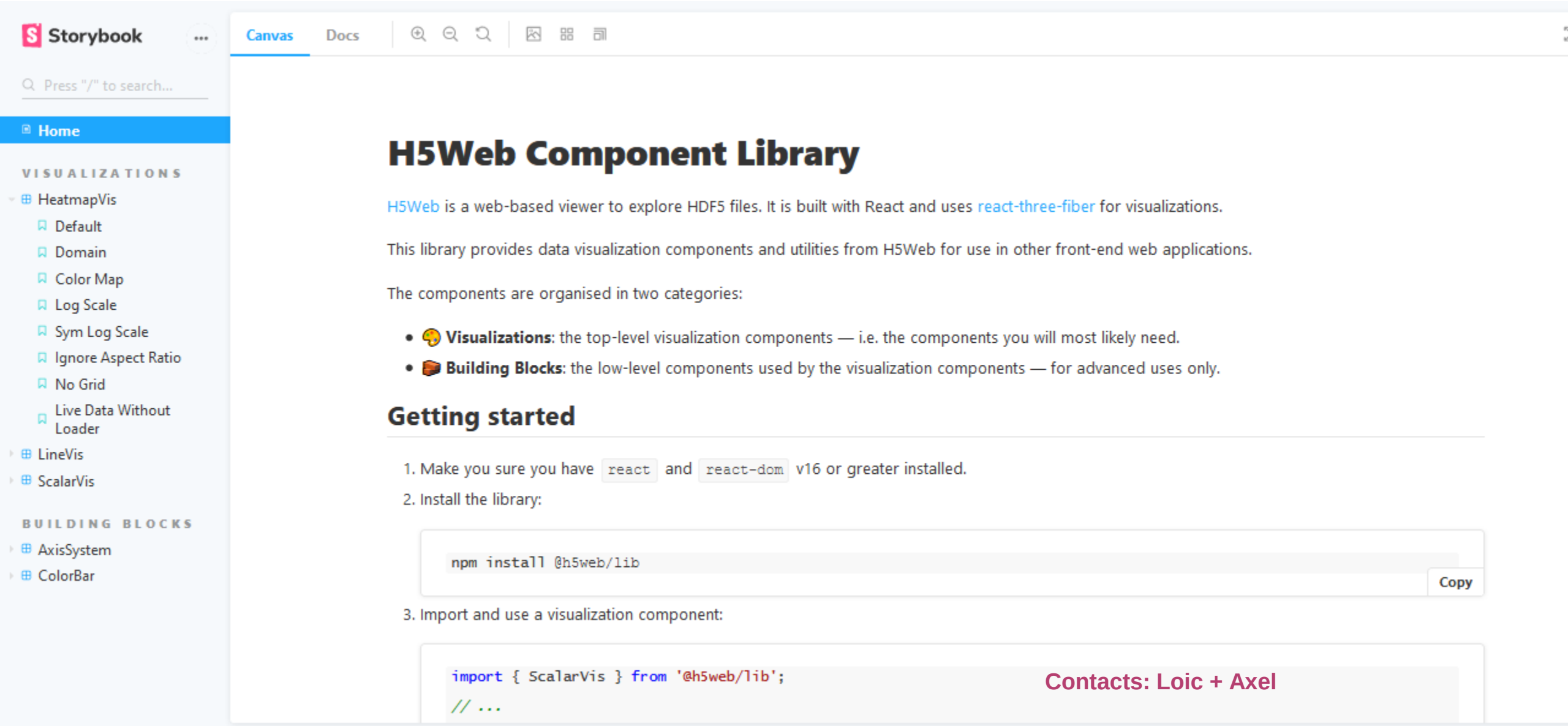
Contacts: Loic + Axel

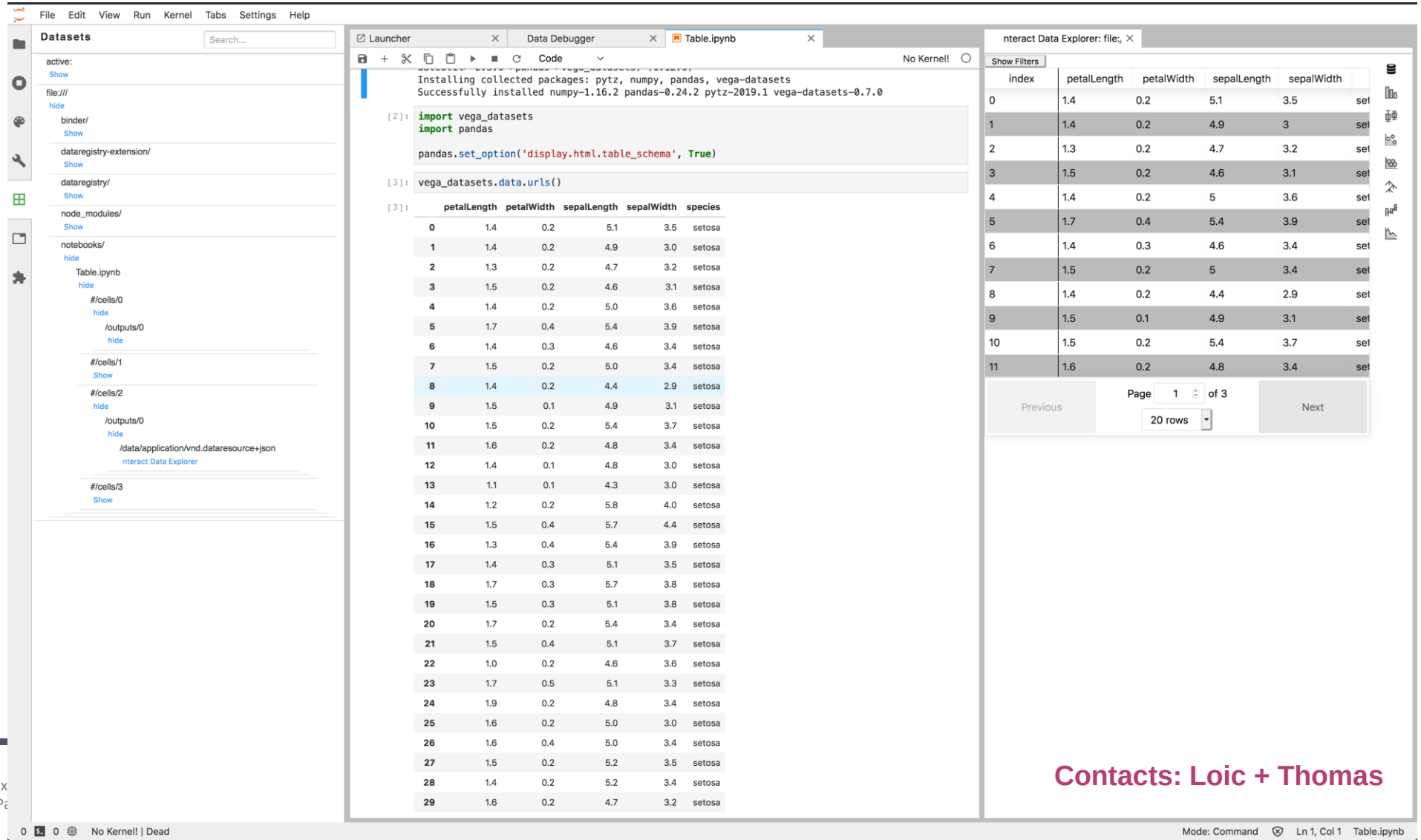
H5web storybook - https://h5web-docs.panosc.eu



Contacts: Loic + Axel

H5web integration in Jupyterlab – Nexus/HDF5 as 1st class citizen

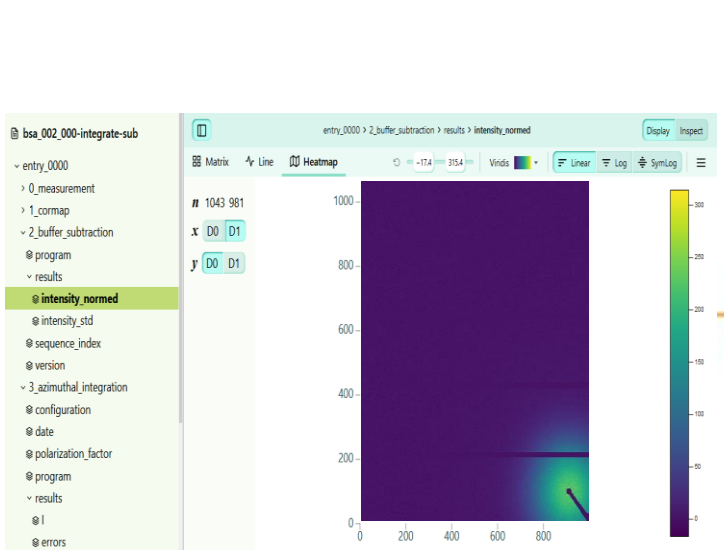
https://github.com/jupyterlab/jupyterlab-data-explorer

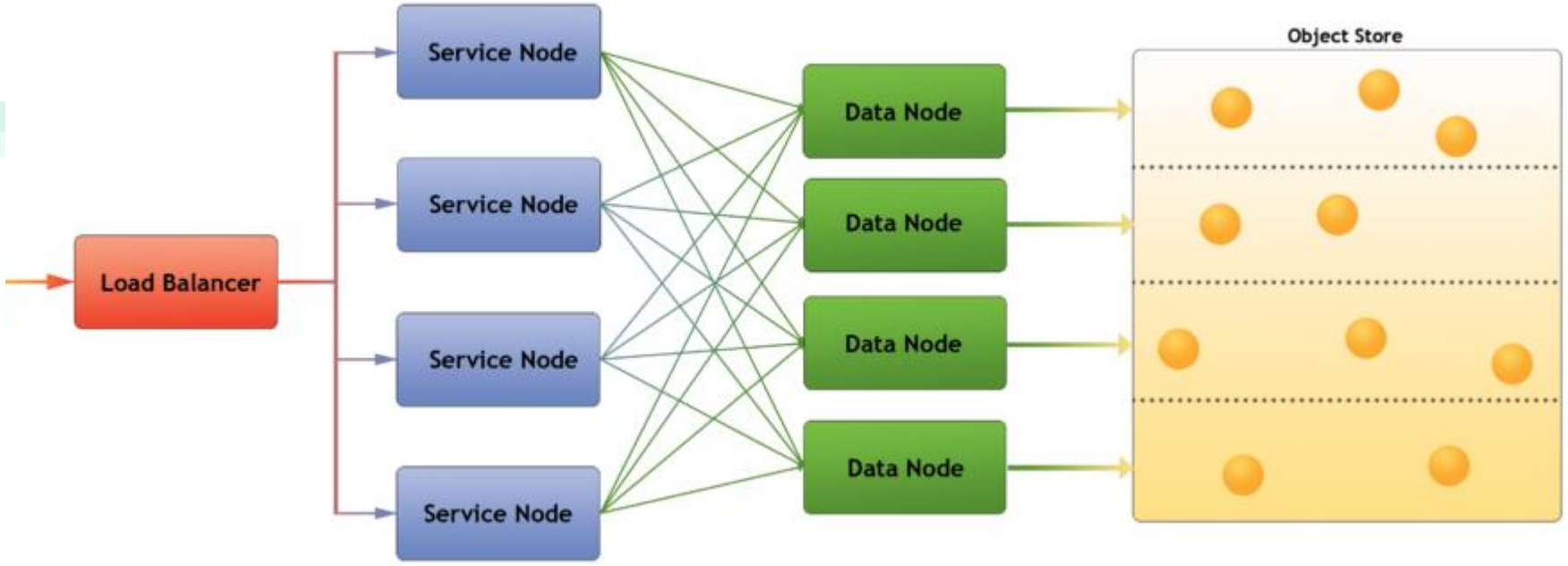


https://github.com/jupyterlab/jupyterlab-hdf5

Contacts: Loic + Thomas

H5web integration in HSDS





https://www.hdfgroup.org/solutions/highly-scalable-data-service-hsds/

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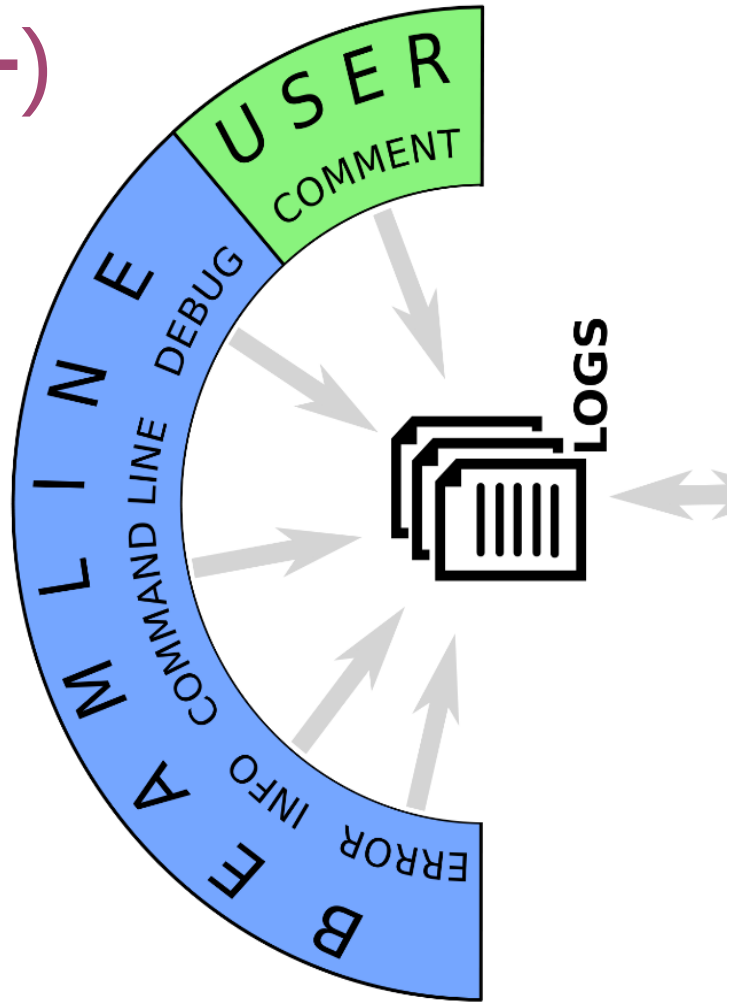
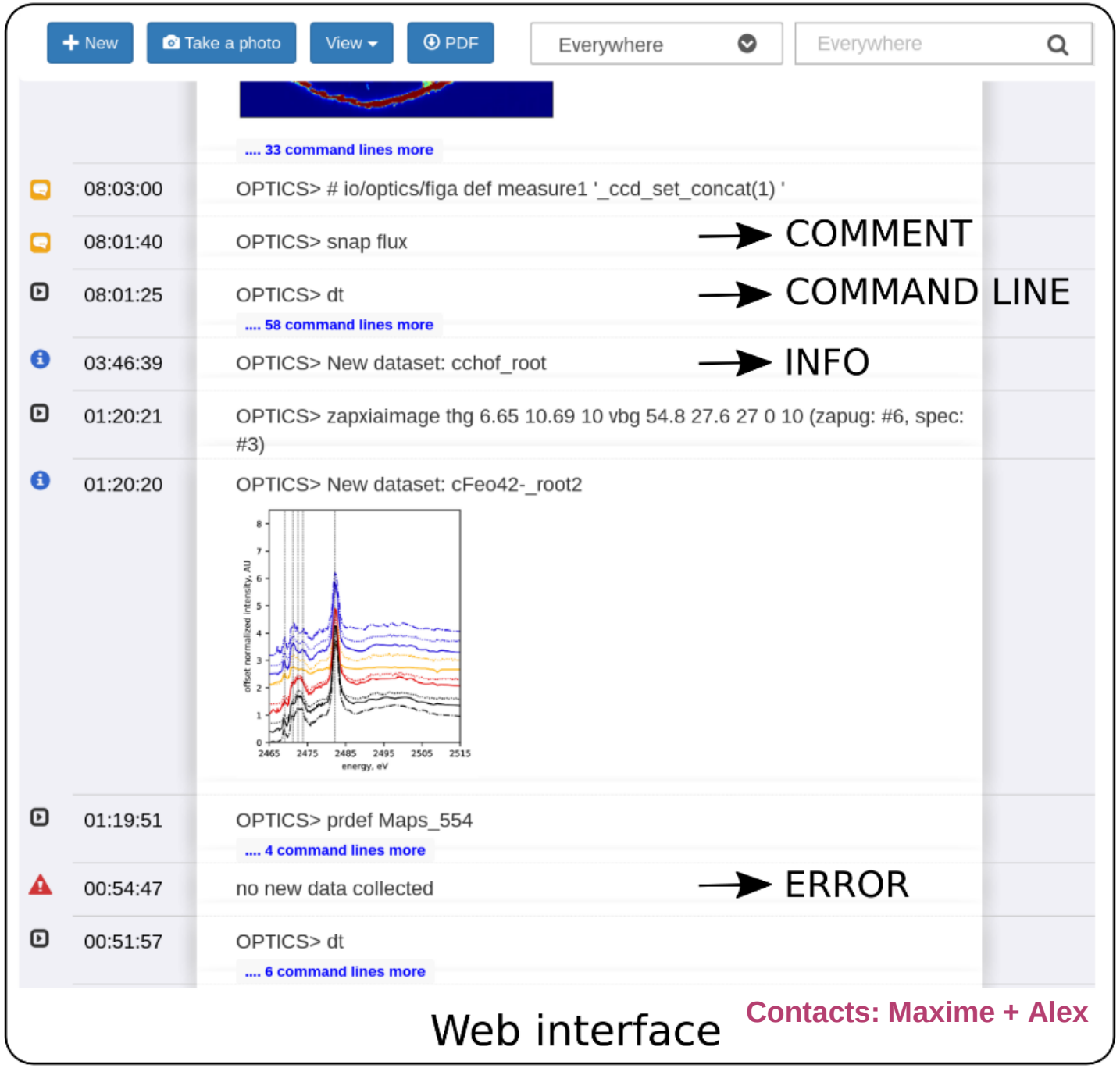
Contacts: Loic

E-logbook makes experiments FAIRer (implemented in ICAT+)





Contacts: Maxime + Alex

Impact of COVID-19 @ ESRF

- All **experiments** are **remote** now
- **Sample tracking** for all beamlines was developed
- Remote analysis via **Jupyter-slurm**
- **Remote access** of experiments via **Guacamole**
- **Downloading** of **data** has become a **critical** issue → **globus+ACLs**

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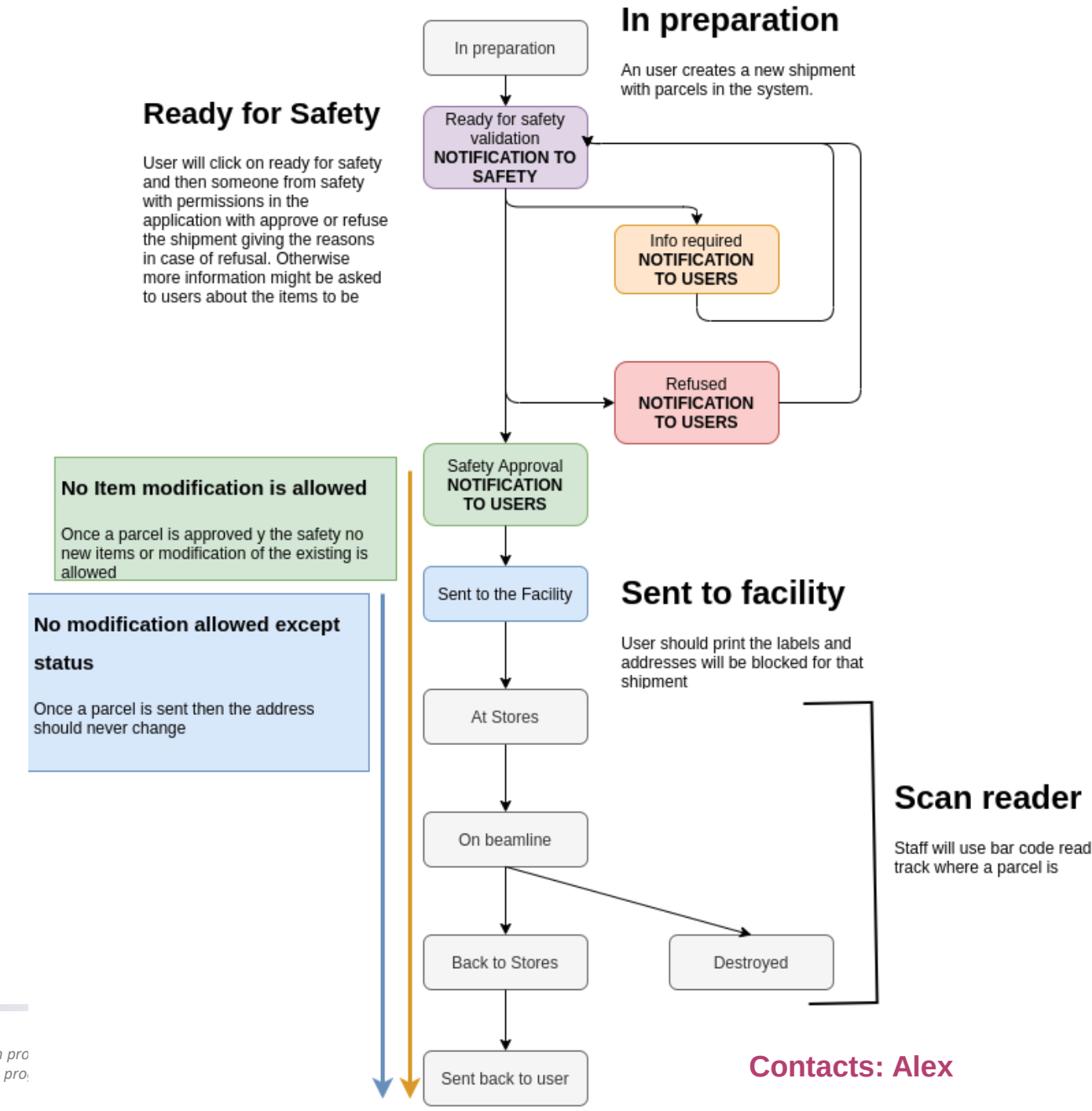
Sample tracking for all Experiments

- ~10 people involved
- 3 months development
- Used for all remote experiments since 25/8/2020
- **121 Shipments** + **672 Samples** in **1 month**
- Implemented in ICAT+



Contacts: Alex

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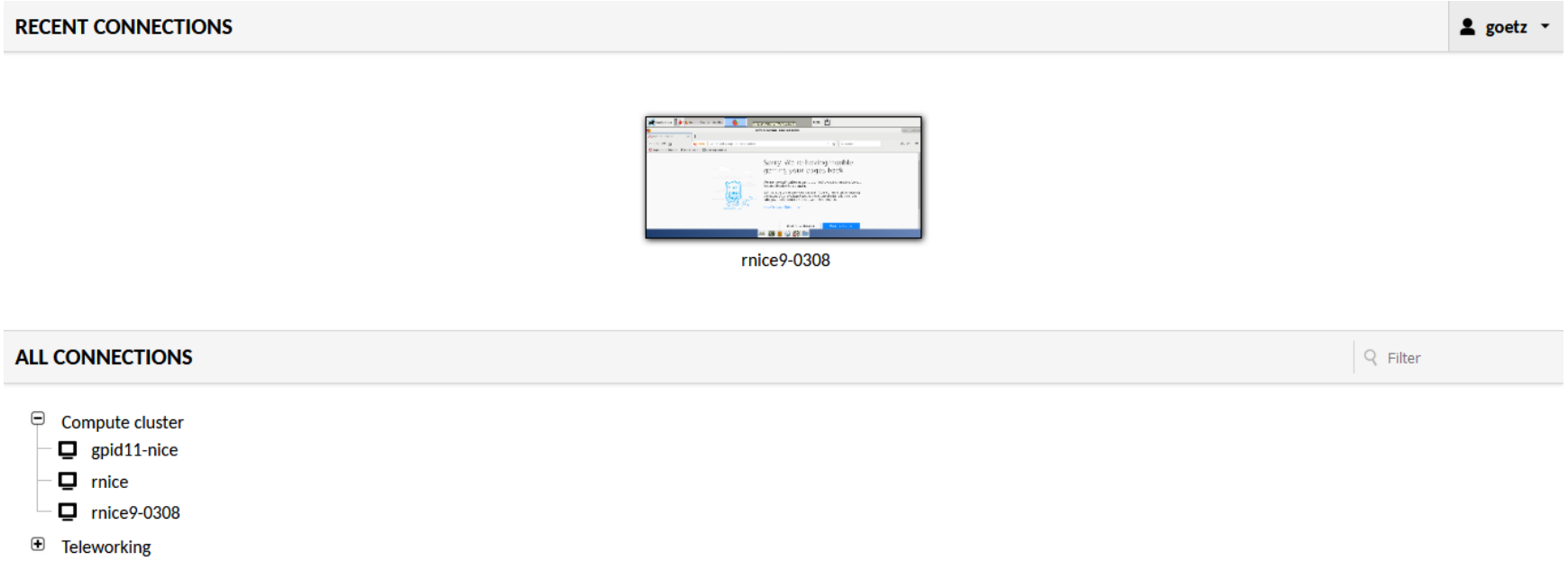
ESRF remote experiment access – Guacamole remote desktop



Use Case: provide remote desktop access for remote experiments

Users: beamline scientists and external users

Expect: VISA would be nice to have

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Contacts: Antoine

Scientific Use Case

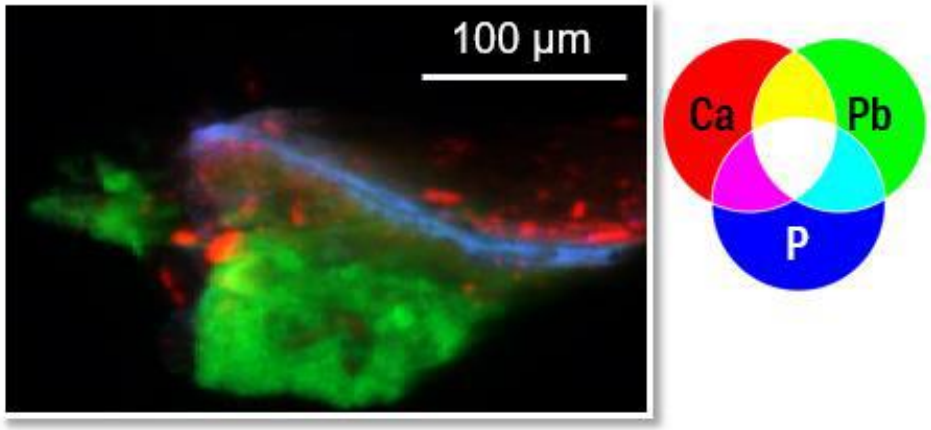

Fig.1 : SR-µ-XRF map (ID21) revealing the presence of a leadfosfate compound in the stratigraphy of a sample from a Leonardo da Vinci painting. SR-µXRD (ID13) analysis revealed the compound to be phosphohedyphane,

- Motivation

  "… improve the efficiency of the experiment (many different users, a possible regular beamtime, remote experiment),

  I think it would help a lot to have a dedicated Jupyter notebook for data processing. It would be a good way i) to save time, ii) to record which map has already been processed and how, iii) and have a coherent data processing between users and between sessions, and also for possible users who would like to reuse data after the embargo period." Scientist

- **Use Case**: provide users with post azimuthal integration maps in hdf5, with Jupyter notebooks taking care of PyFAI integration of 2D maps.
- **Users**: Scientists doing experiments in cultural heritage
- **Contacts**: **Loic + Scientist**

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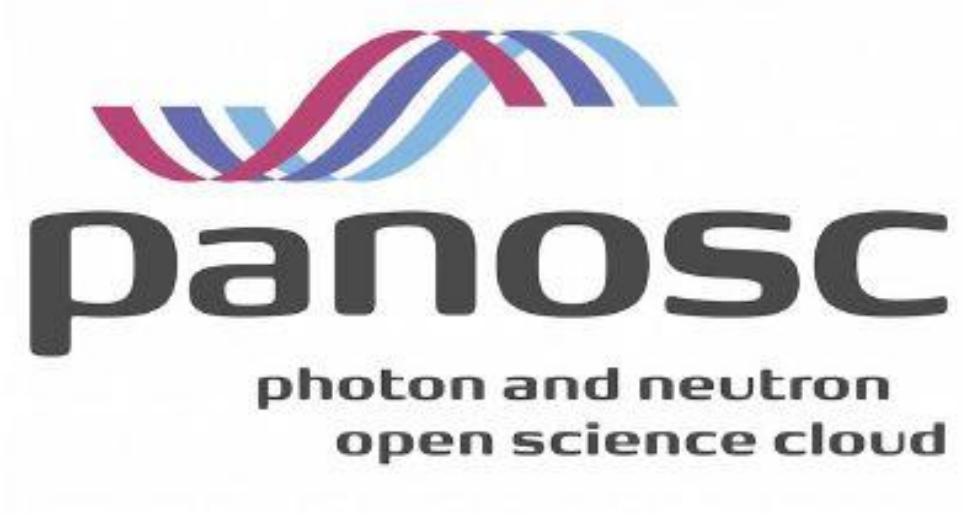

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