DECTRIS
CLOUD

Container Services @ DECTRIS CLOUD

DAPHNE4NFDI Software Practice Workshop
EuXFEL, Germany

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25.02.2025

Overview

Introduction to DECTRIS CLOUD

Why cloud?

Getting data into the cloud

Webapp overview

Implementation Overview

Multicloud approach

Deployment workflow

Container workflow for scientist

Usage of containers @ DECTRIS CLOUD

Environment creation

Environment sharing

Job templates for standardized analysis

Examples

Introduction to DECTRIS CLOUD

DECTRIS Detectors

New!

EIGER2

PILATUS4

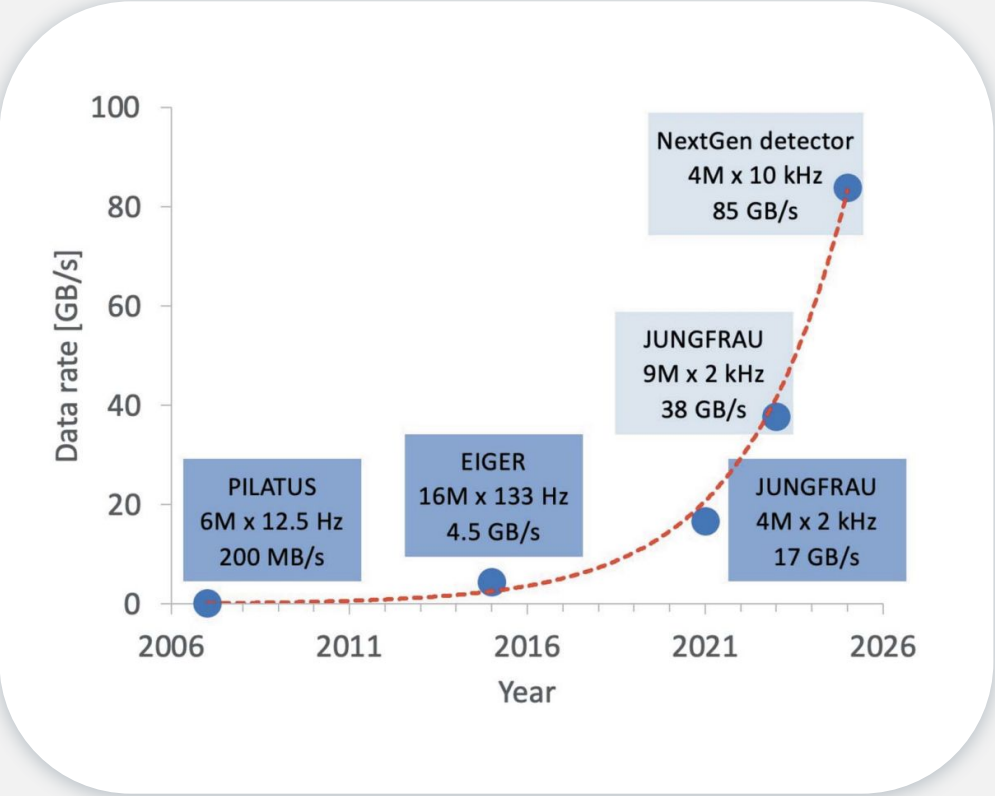
MYTHEN2

New!

SELUN

Fast and reliable instruments for modern experiments

Evolution of Data Rates



"Future detectors targeting frame rates over 100 kHz will have data rates (for raw data) exceeding 1 Tbit/s"

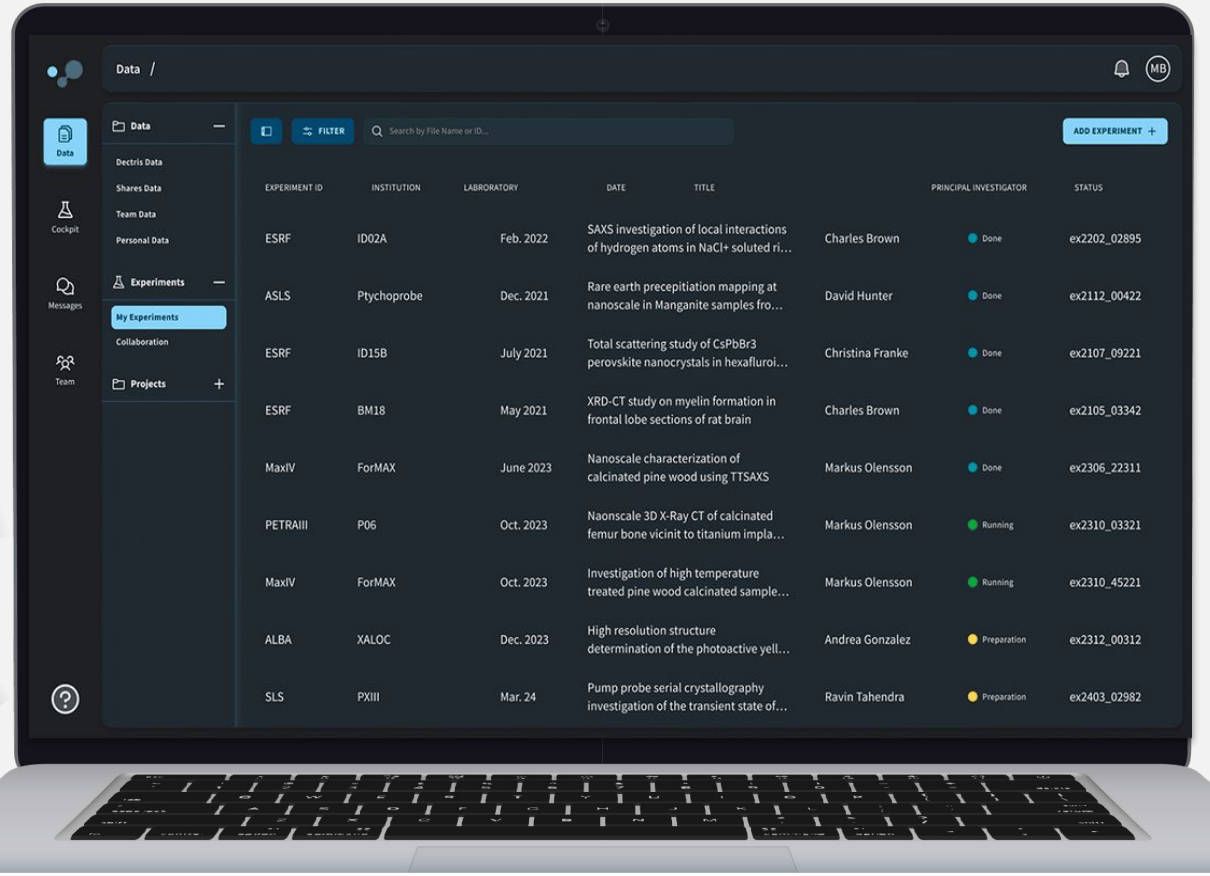
Pennicard et al. Front. Phys., 05 February 2024, Sec. Radiation Detectors and Imaging
Volume 12 - 2024 | https://doi.org/10.3389/fphy.2024.1285854

DECTRIS CLOUD

Processing

Analysis

Data Storage & Archiving



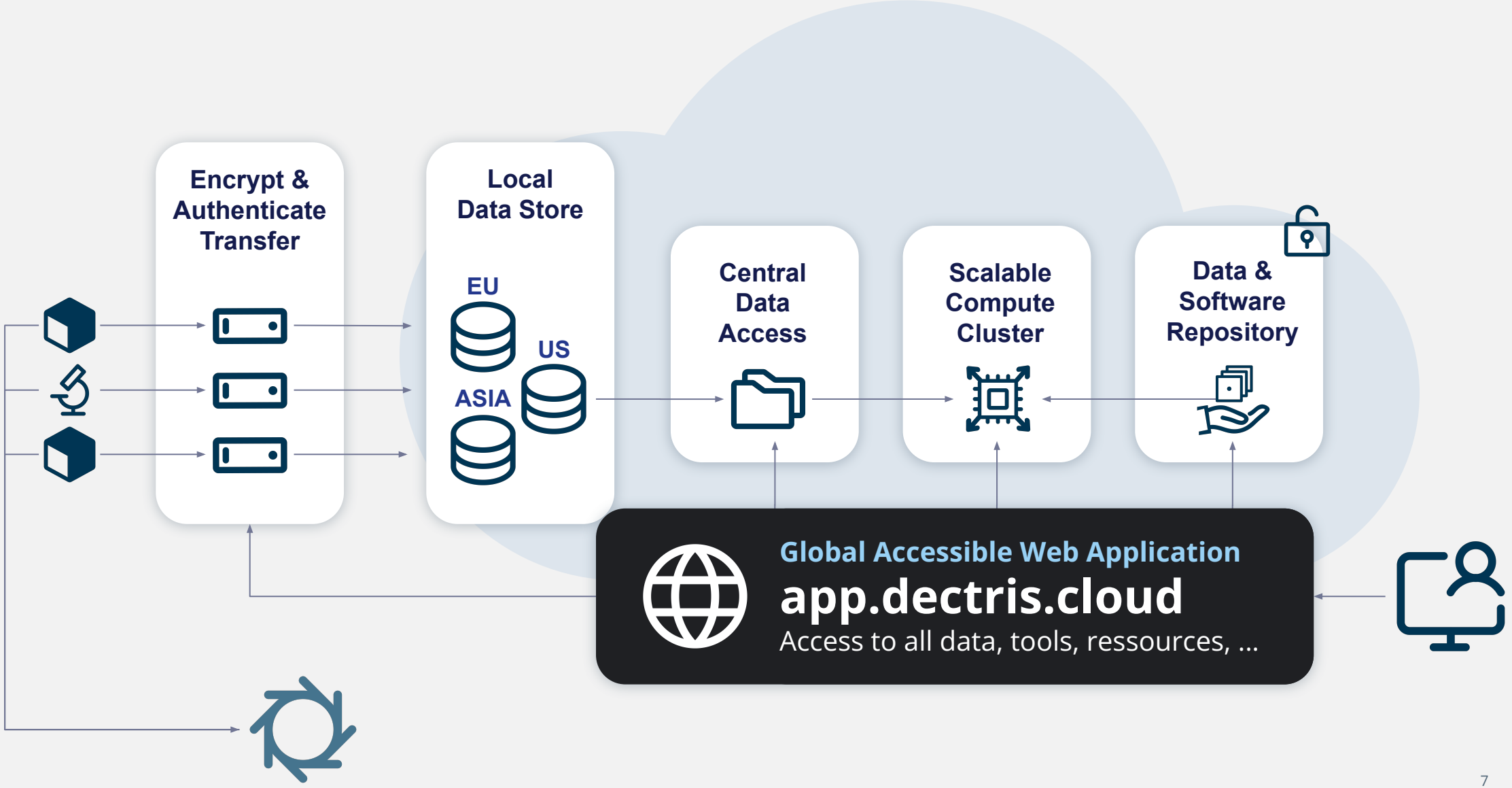
Sharing & Collaboration

FAIR & OPEN Data Access

Global Availability

An open platform to empower scientific collaboration

DECTRIS CLOUD Web Service



A New Experiment

This is you :)

Old Experiment A
(PSI, cSAXS)

Experiment Data

- Raw Data
- Meta Data
- Processed Data
- Results

Old Experiment B
(APS, 8ID)

Experiment Data

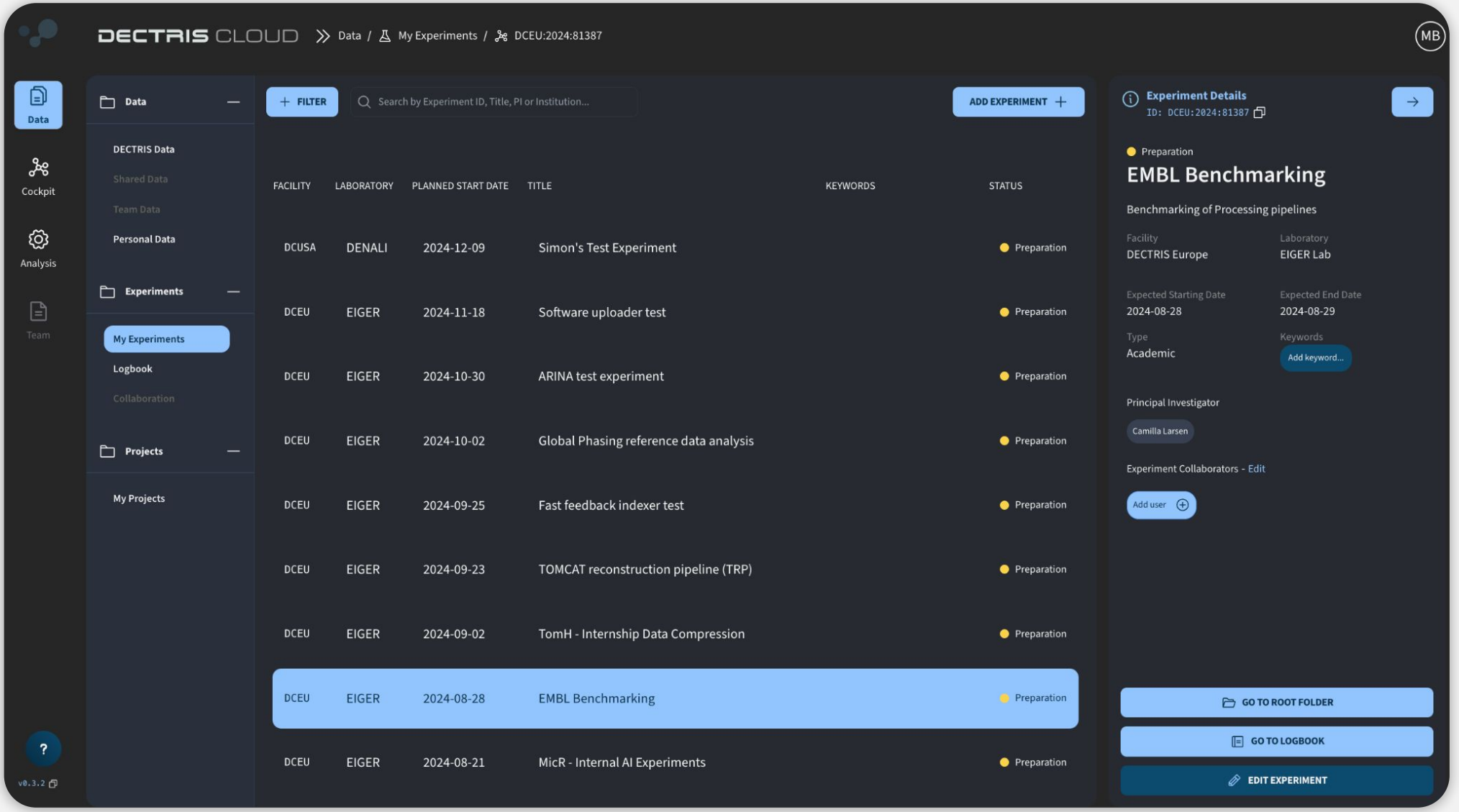
- Raw Data
- Meta Data
- Processed Data
- Results

...

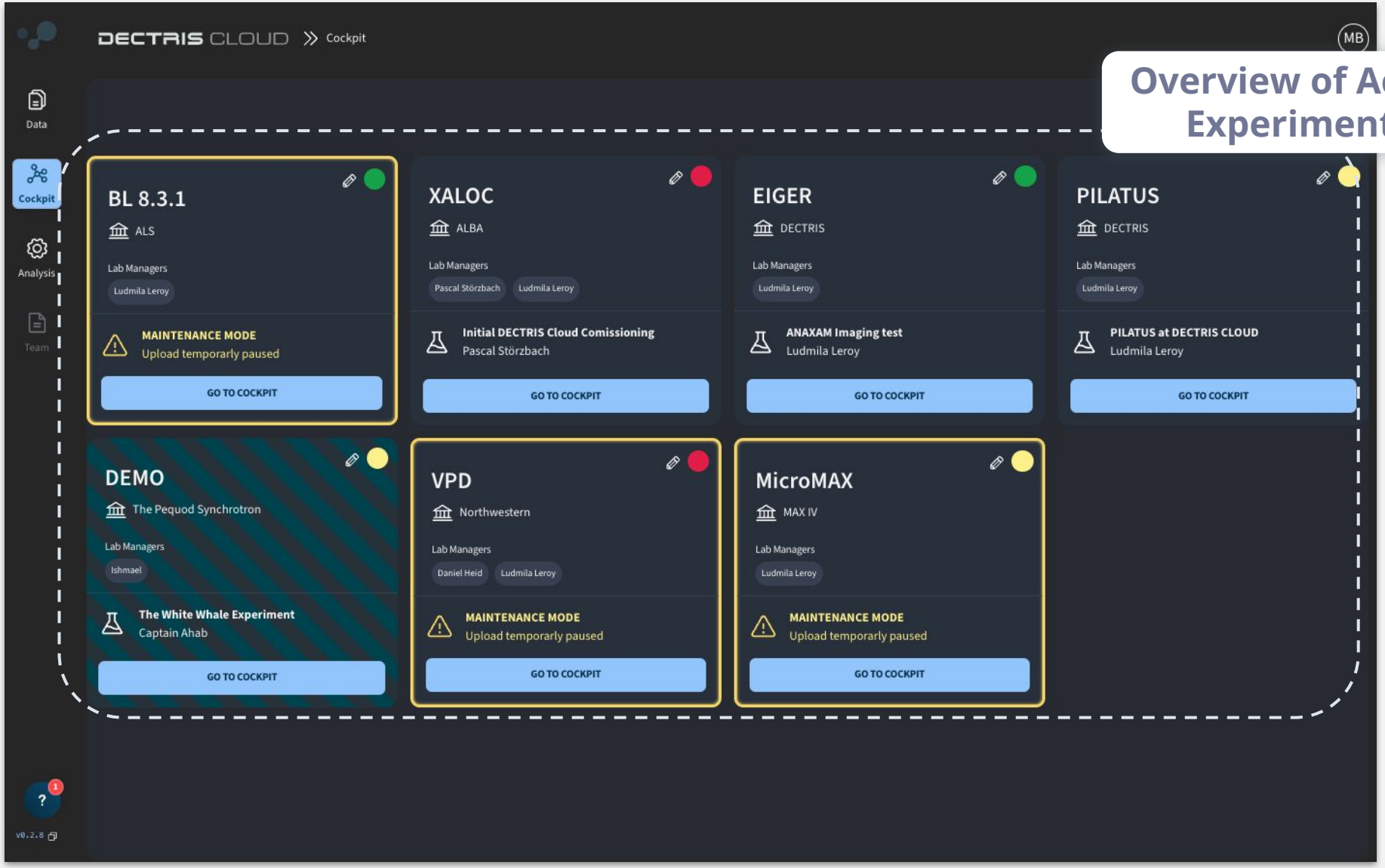
New Experiment B
(MaxIV, NanoMAX)

Experiment Data

- Raw Data
- Meta Data
- Processed Data
- Results

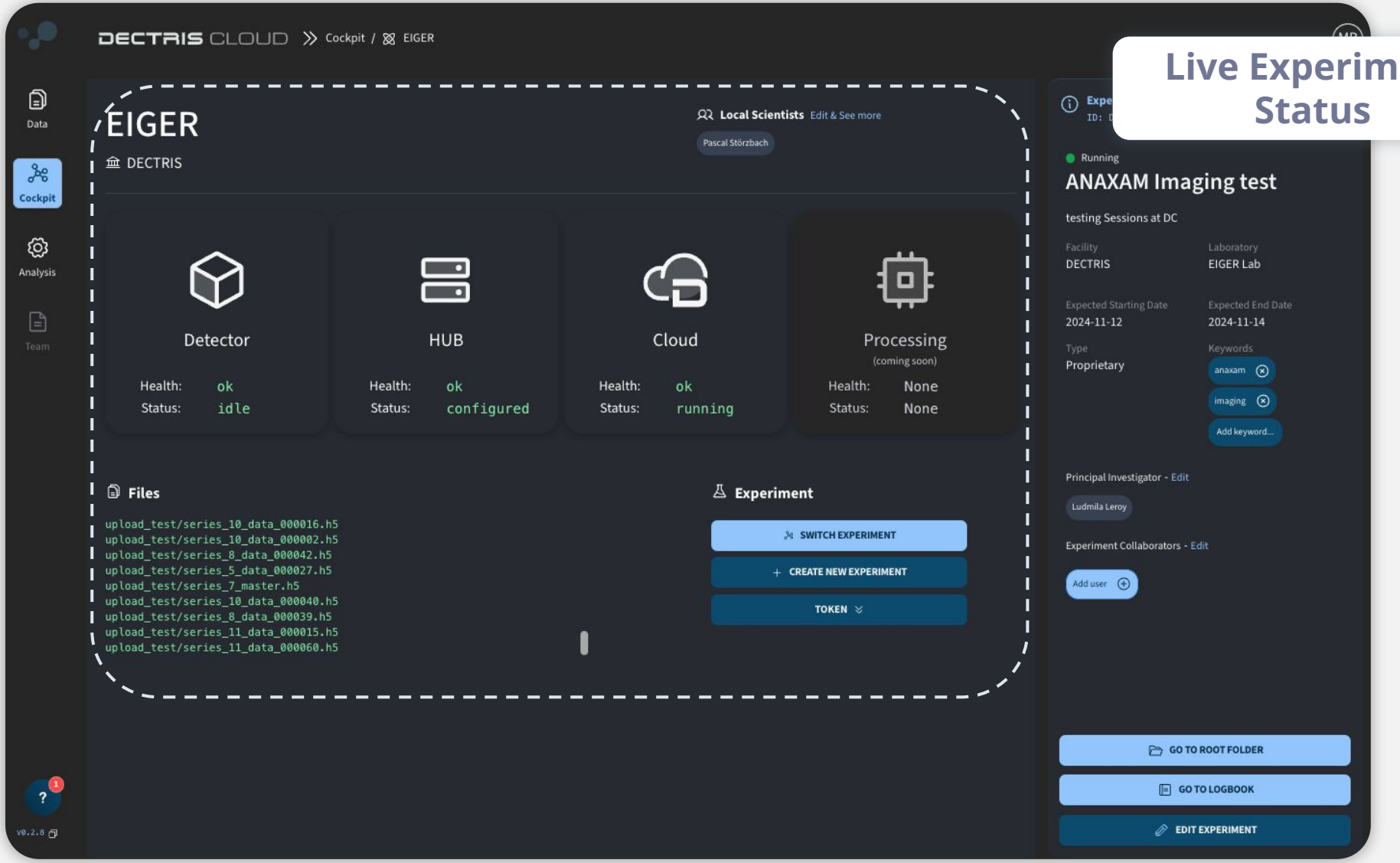

DECTRIS CLOUD
Data / My Experiments / DCEU:2024:81387
MB
Data
Cockpit
Analysis
Team
v0.3.2
Data
DECTRIS Data
Shared Data
Team Data
Personal Data
Experiments
My Experiments
Logbook
Collaboration
Projects
My Projects
FILTER
Search by Experiment ID, Title, PI or Institution...
ADD EXPERIMENT
FACILITY
LABORATORY
PLANNED START DATE
TITLE
KEYWORDS
STATUS
DCUSA DENALI 2024-12-09 Simon's Test Experiment Preparation
DCEU EIGER 2024-11-18 Software uploader test Preparation
DCEU EIGER 2024-10-30 ARINA test experiment Preparation
DCEU EIGER 2024-10-02 Global Phasing reference data analysis Preparation
DCEU EIGER 2024-09-25 Fast feedback indexer test Preparation
DCEU EIGER 2024-09-23 TOMCAT reconstruction pipeline (TRP) Preparation
DCEU EIGER 2024-09-02 TomH - Internship Data Compression Preparation
DCEU EIGER 2024-08-28 EMBL Benchmarking Preparation
DCEU EIGER 2024-08-21 MicR - Internal AI Experiments Preparation
Experiment Details
ID: DCEU:2024:81387
Preparation
EMBL Benchmarking
Benchmarking of Processing pipelines
Facility
DECTRIS Europe
Laboratory
EIGER Lab
Expected Starting Date
2024-08-28
Expected End Date
2024-08-29
Type
Academic
Keywords
Add keyword...
Principal Investigator
Camilla Larsen
Experiment Collaborators - Edit
Add user
GO TO ROOT FOLDER
GO TO LOGBOOK
EDIT EXPERIMENT

DECTRIS CLOUD



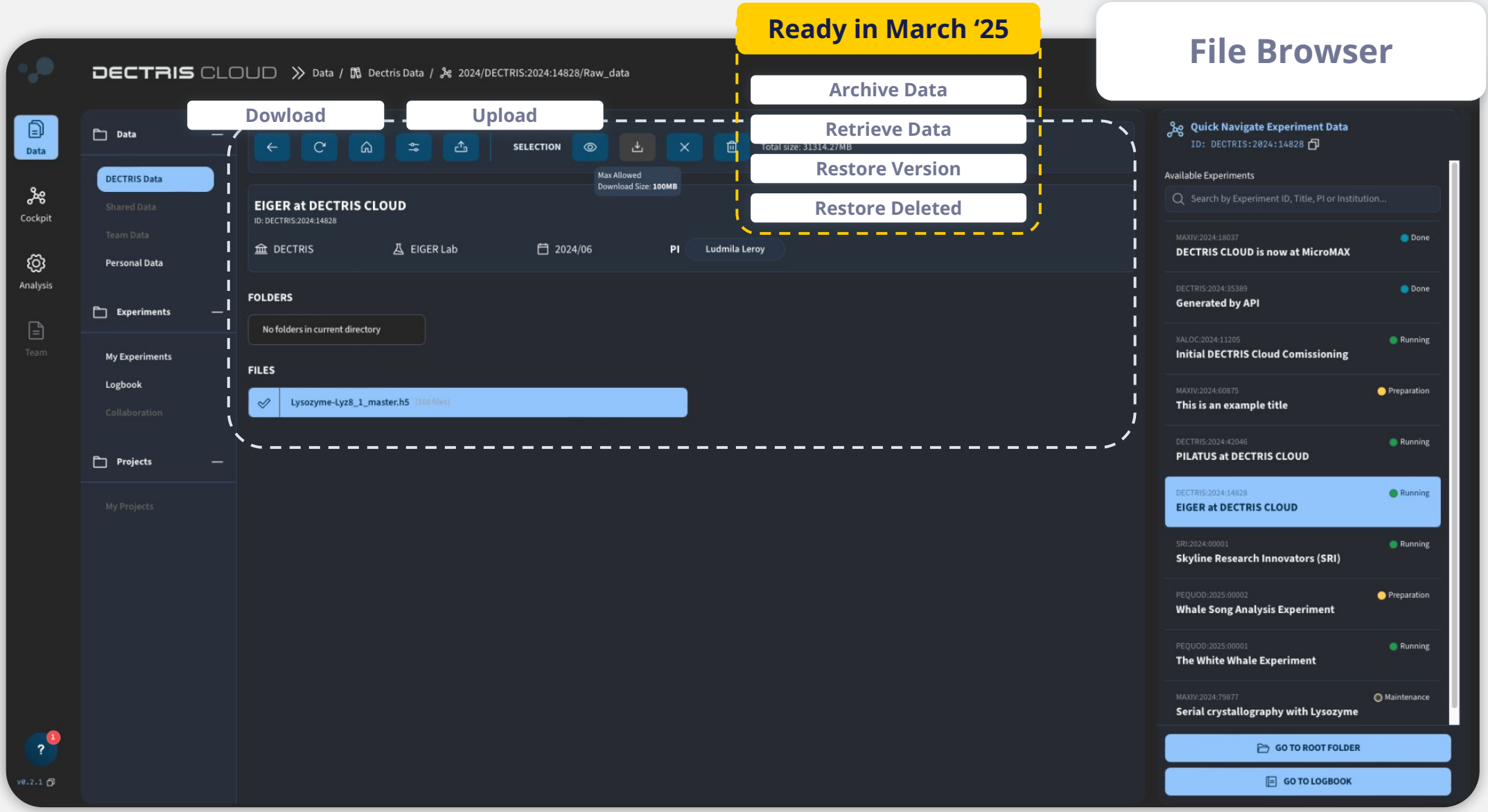
Overview of Active Experiments

Experiment Starts: Activate!

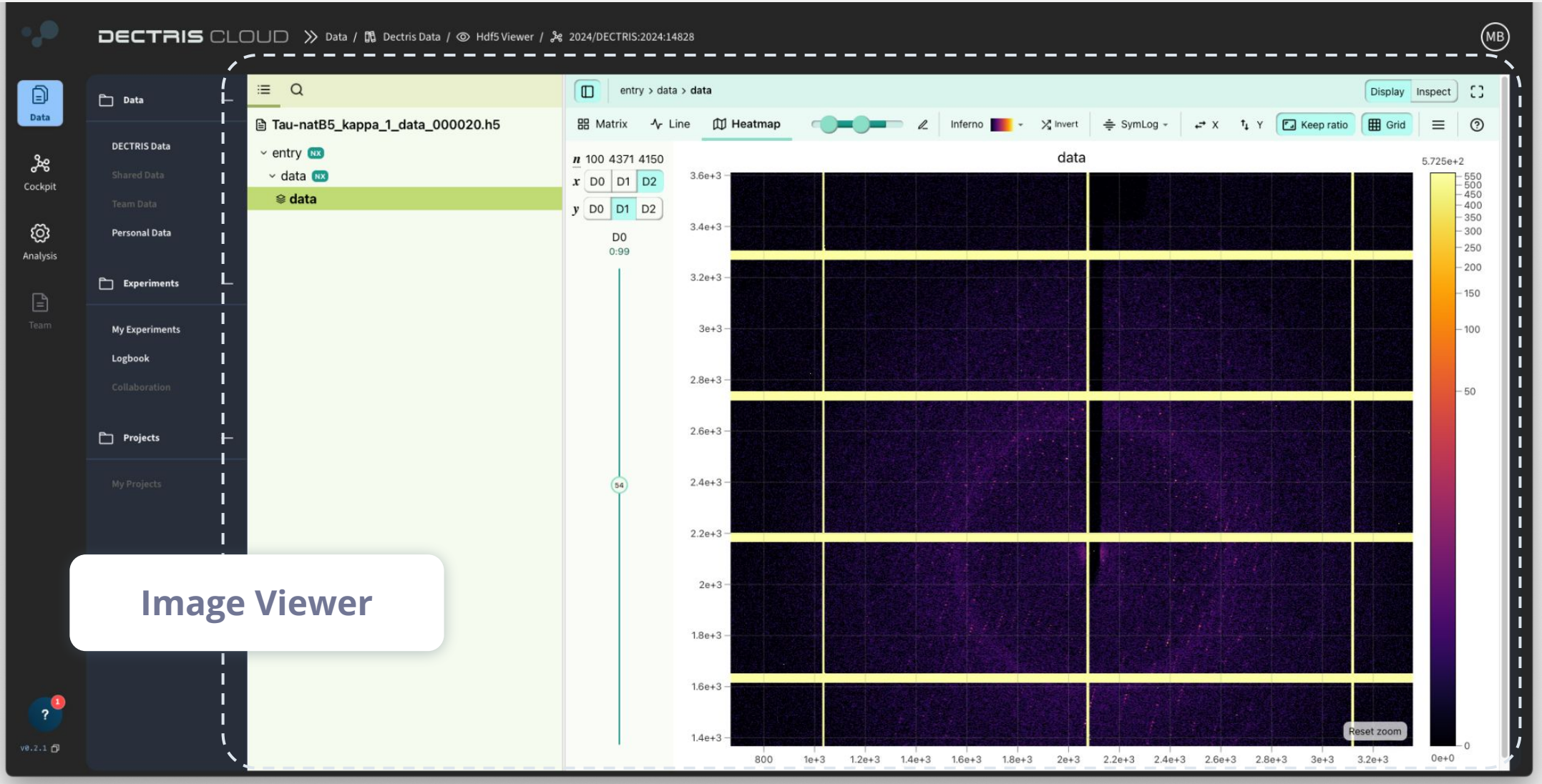


Live Experiment Status

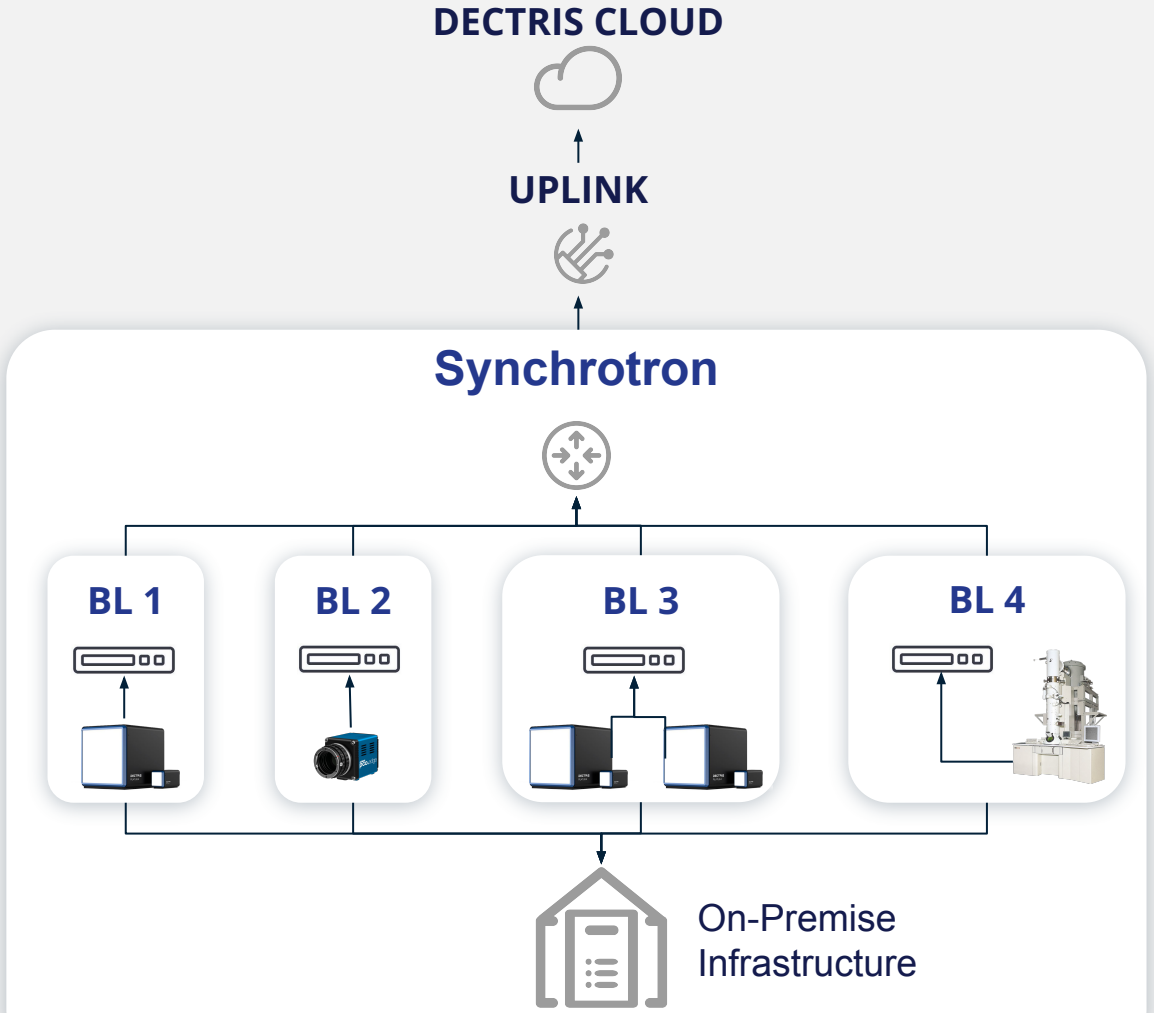
Experiment Data Management



DECTRIS CLOUD

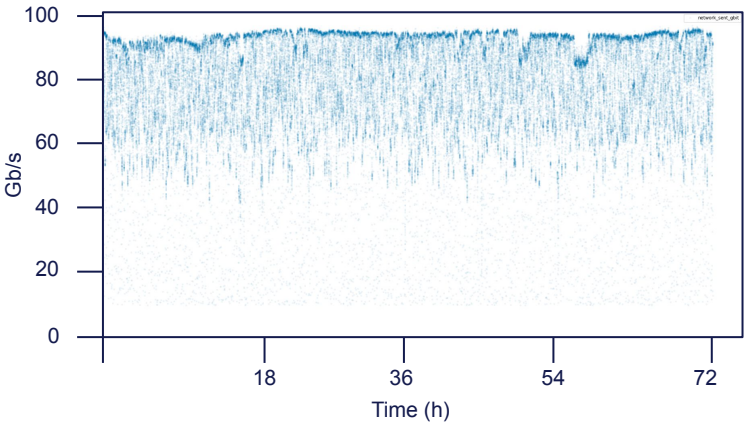


Getting Data into the Cloud



DATA STREAM

Upload Performance

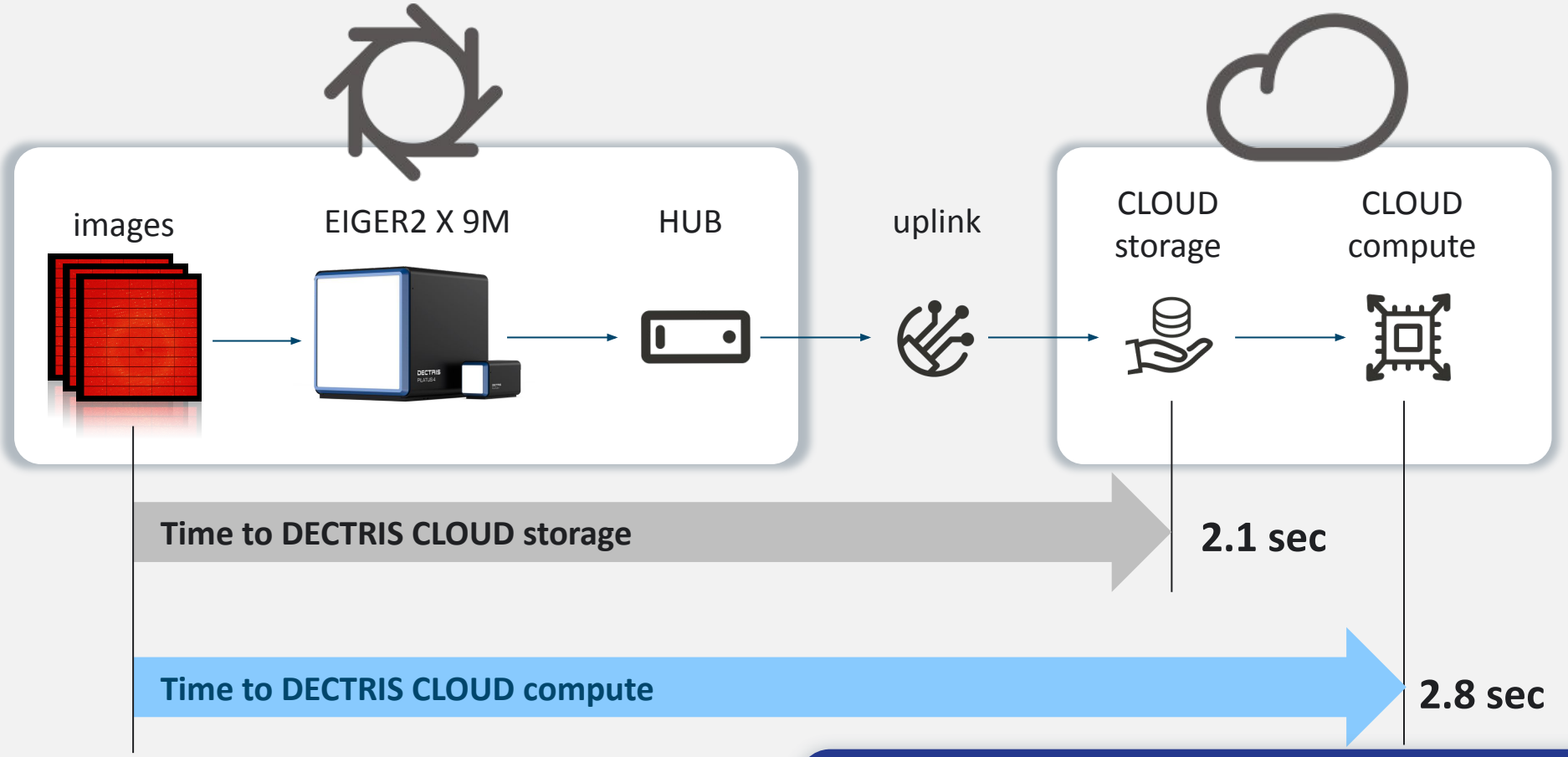


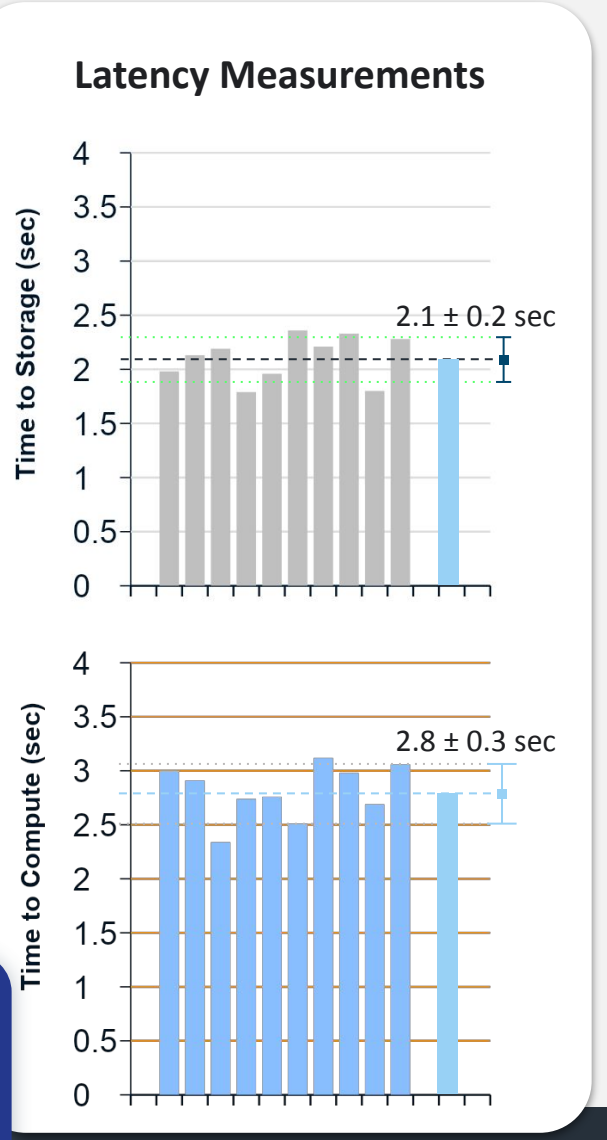
Uninterrupted upload of 1.2 PetaBytes in 72h

Average bandwidth of 92 GBits

2023, ALBA (ESP), XAIRA Beamline

Performance Results: Upload Latency



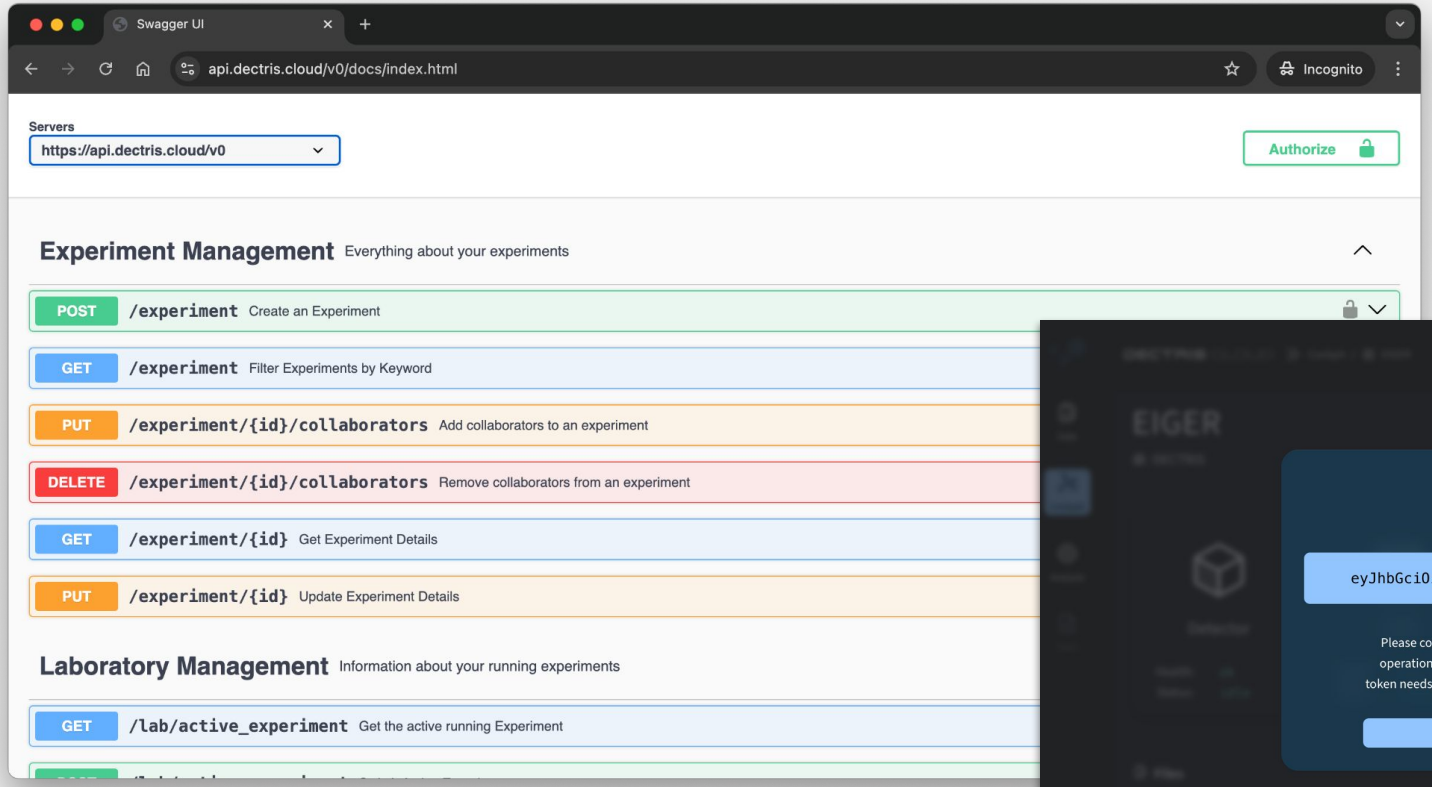


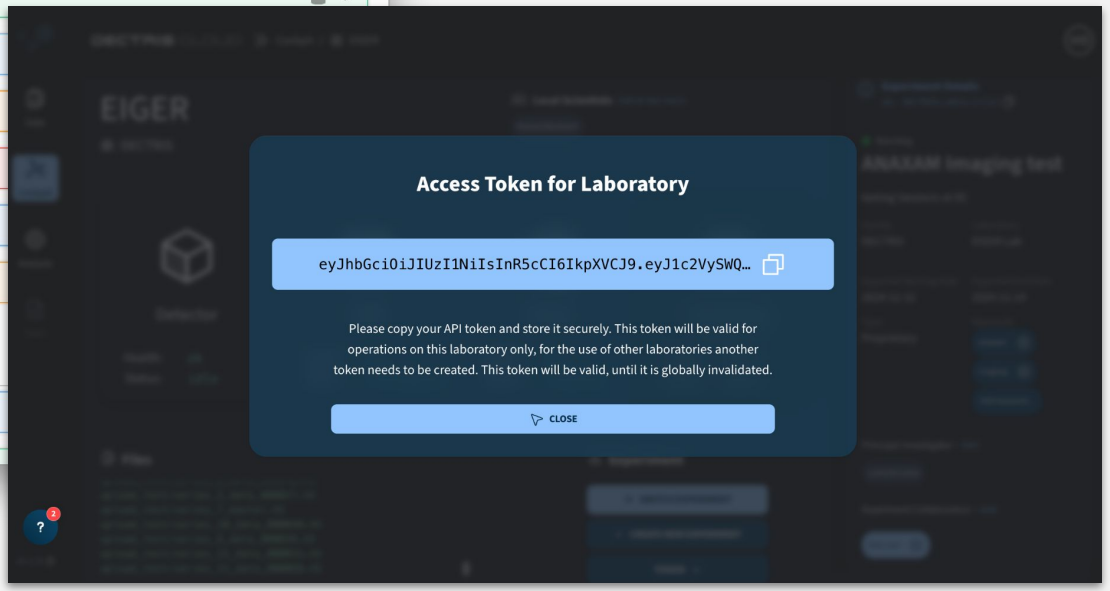
User Benefit:
+ Instant access to data in cloud
+ No manual data copy

Courtesy to T.Ursby & A.Gonzalez, MicroMax, MaxIV

DECTRIS CLOUD

Swagger
Supported by SMARTBEAR





Implementation Overview

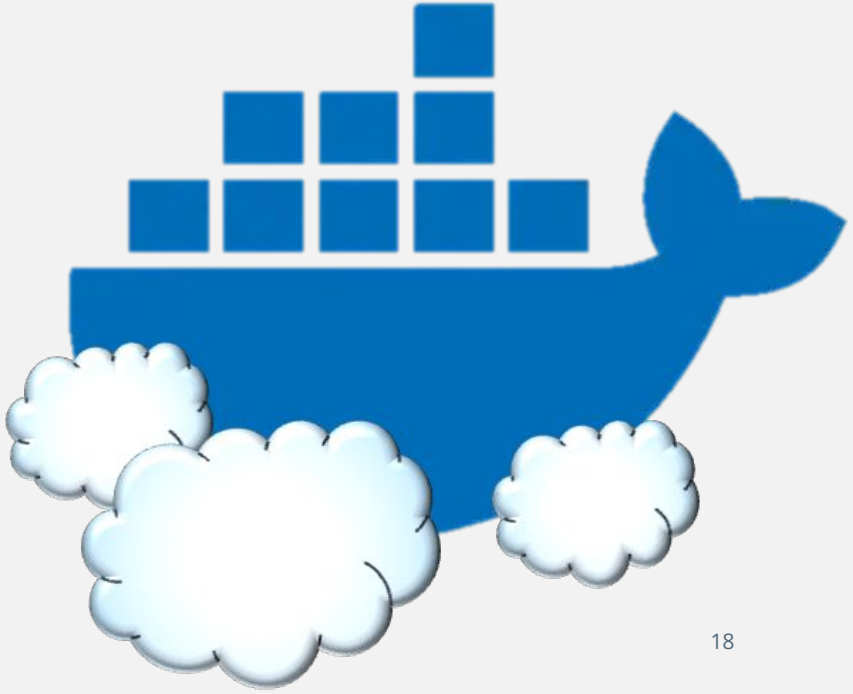
DECTRIS CLOUD Implementation

Containerization

- Uniformity
- Collaboration
- Reproducible workflows

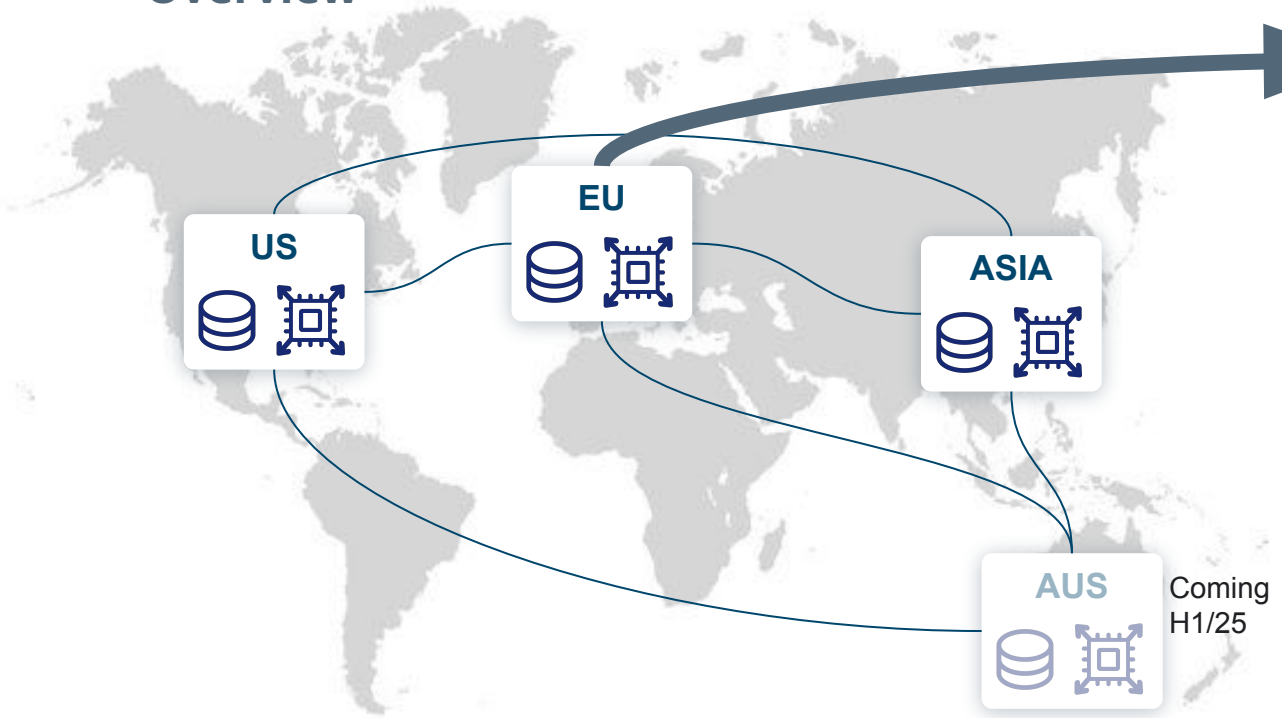
Multi-cloud

- Redundancy
- Optimization
- Scalability



Global Data Bandwidth Capacity

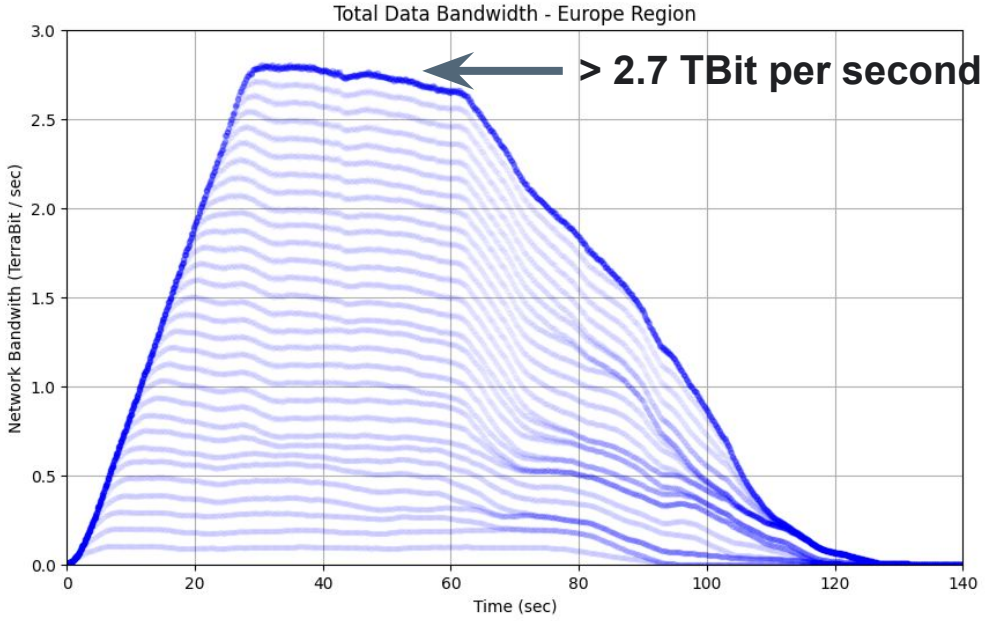
Cloud Architecture Overview



- DECTRIS CLOUD operates in 4 regions of the world.
- Tenant and cluster isolation to ensure data security
- Infrastructure, availability, and SLA provided by hyperscalers

aws Google Cloud

Data Access Bandwidth - EU Region

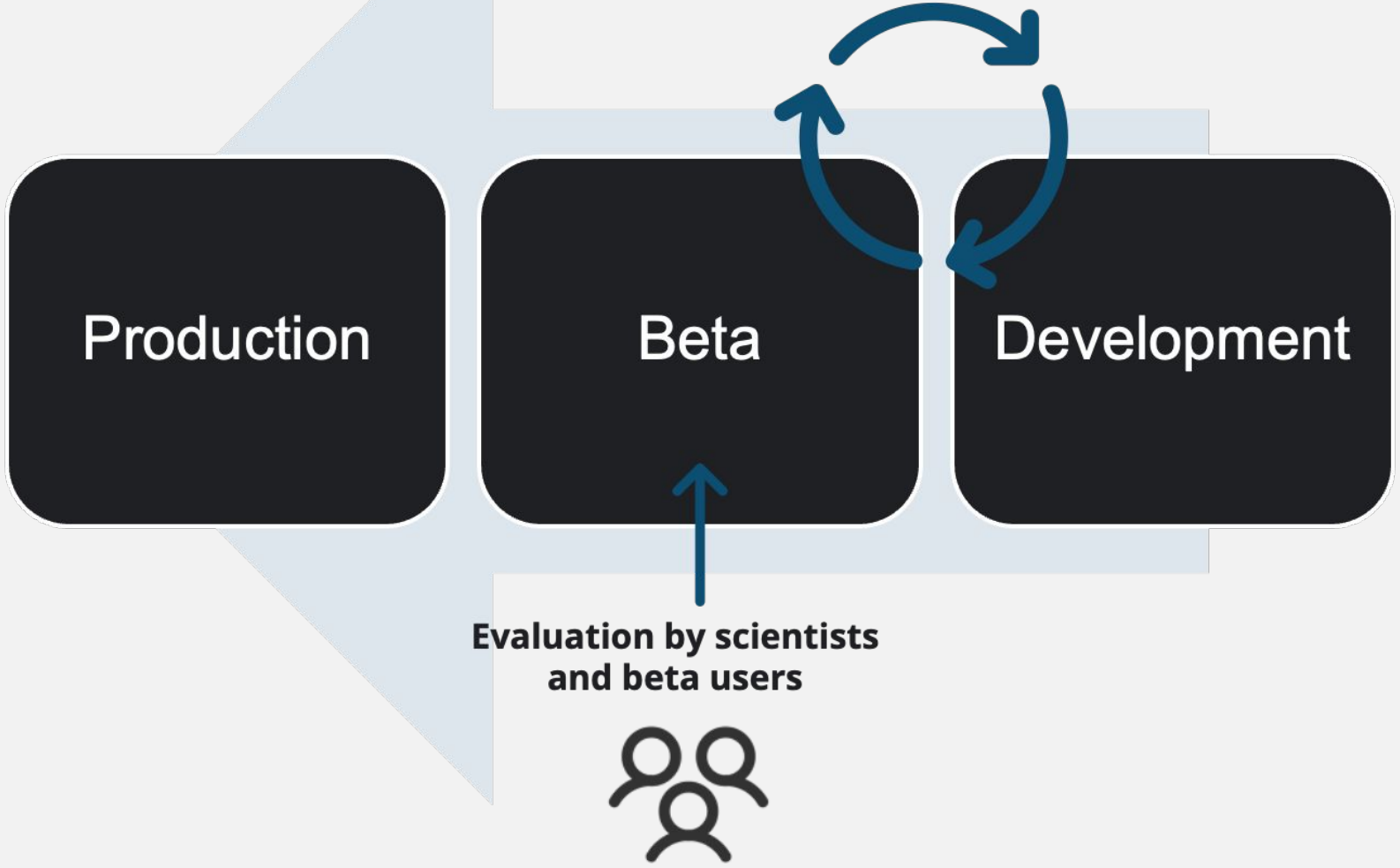


- Each region provides triple geo-redundancy for data storage
- Load balancing per availability zone to ensure data throughput
- Each AZ provides >2.7 TBit of data access BW

Total Global Bandwidth:

3 Regions **x** 3 Availability Zones **x** 2.7 TBit **=** >20 TBits

Deployment schedule



Scientist Interaction with Containers

Container-Based Compute

developers

facilities

institutions

Default & Custom Environments

interactive sessions

container

Python

Automated Processing Jobs

UI Managed

API Endpoint

Explorative Analysis Tools

virtual machines

notebooks

Scalable Global Compute Cluster

- Up to 32 dedicated nodes (64 CPUs) **per beamline**
- Newest CPU Architectures: 4th Gen. AMD & Intel & NVIDIA GPUs
- Running on >99% renewable energy saving up to 70% CO2eq compared to on premise

Sharing and collaboration

Direct Sharing:

- Experiment Data
- Processing Job
- Software Environment
- Analysis Tools

Collaborators

Make data & software reusable for everyone

Publish Data & Tools:

Data & Software Repository

Collaborators

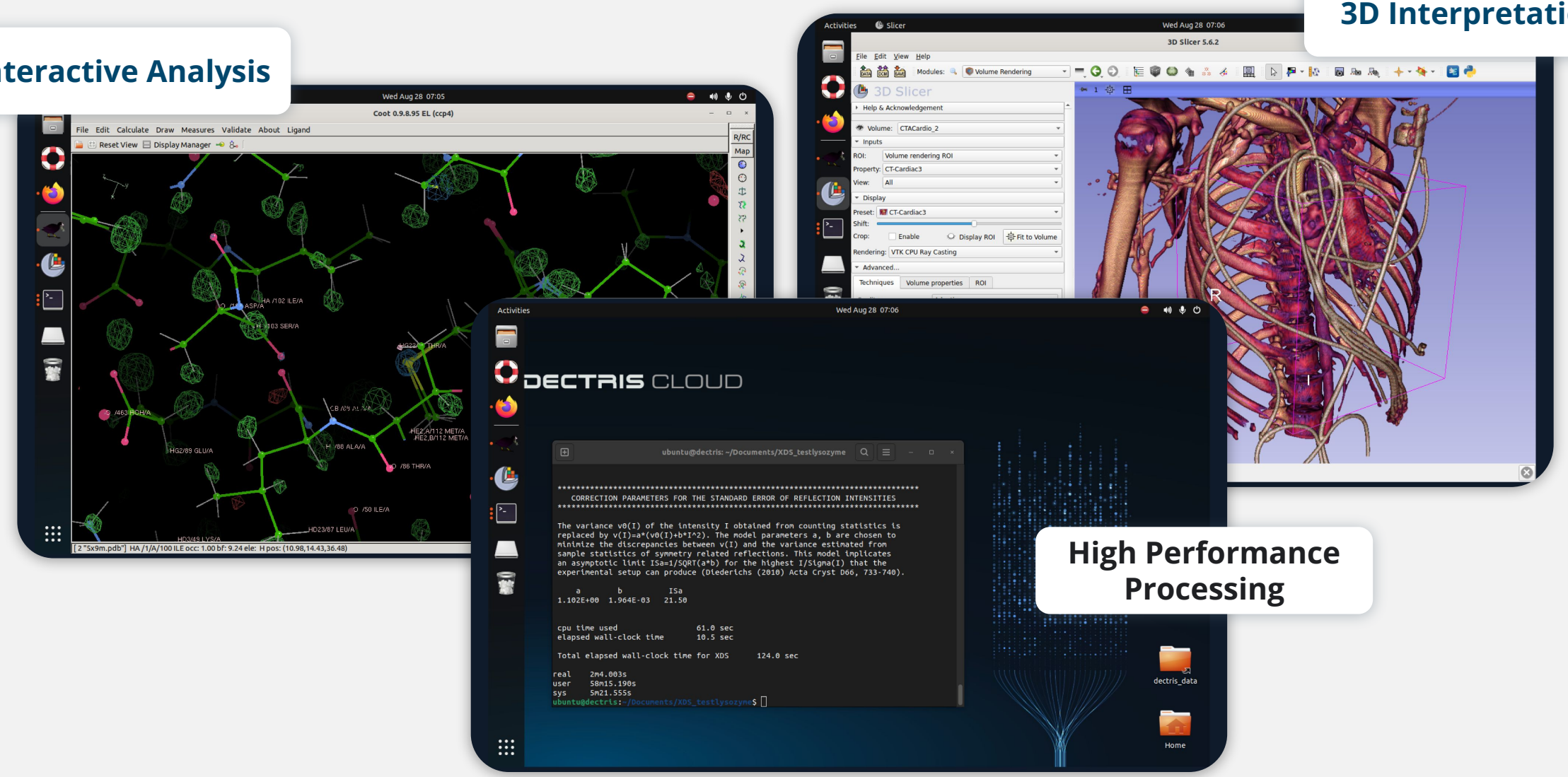
User Benefits:

+ **Sharing of data & software:**
+ **No data transfer**
+ **No software reinstallation**

Sessions: Run Virtual Machine in Cloud

Interactive Analysis

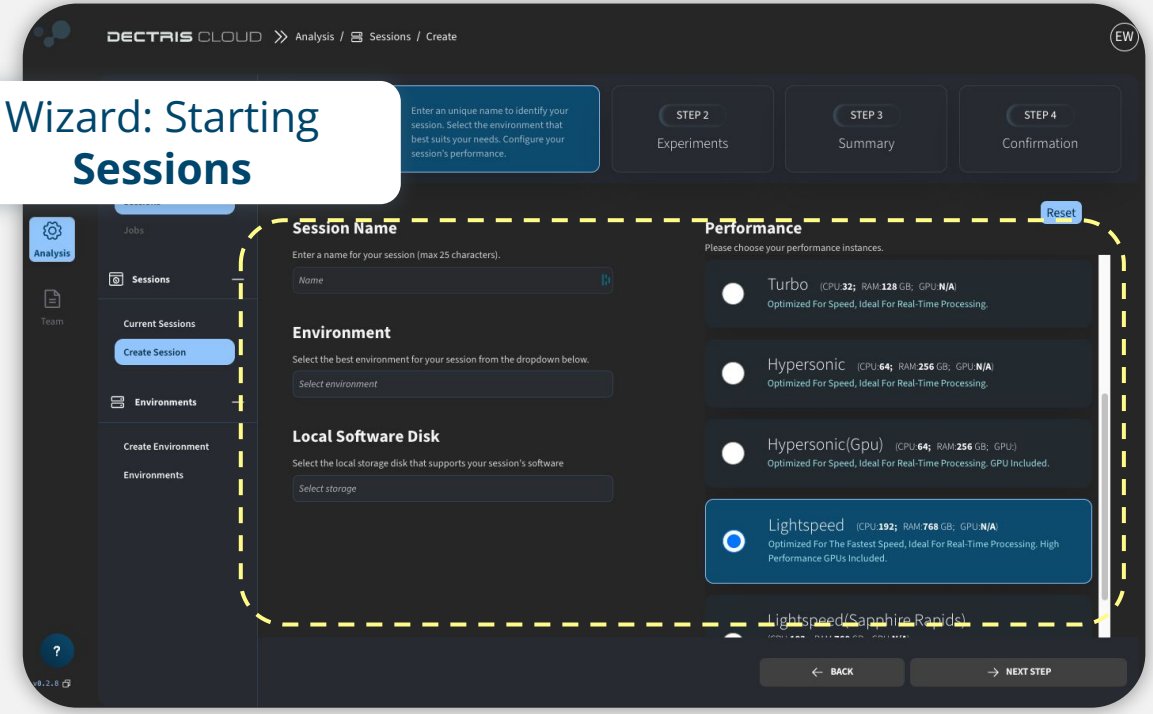
3D Interpretation



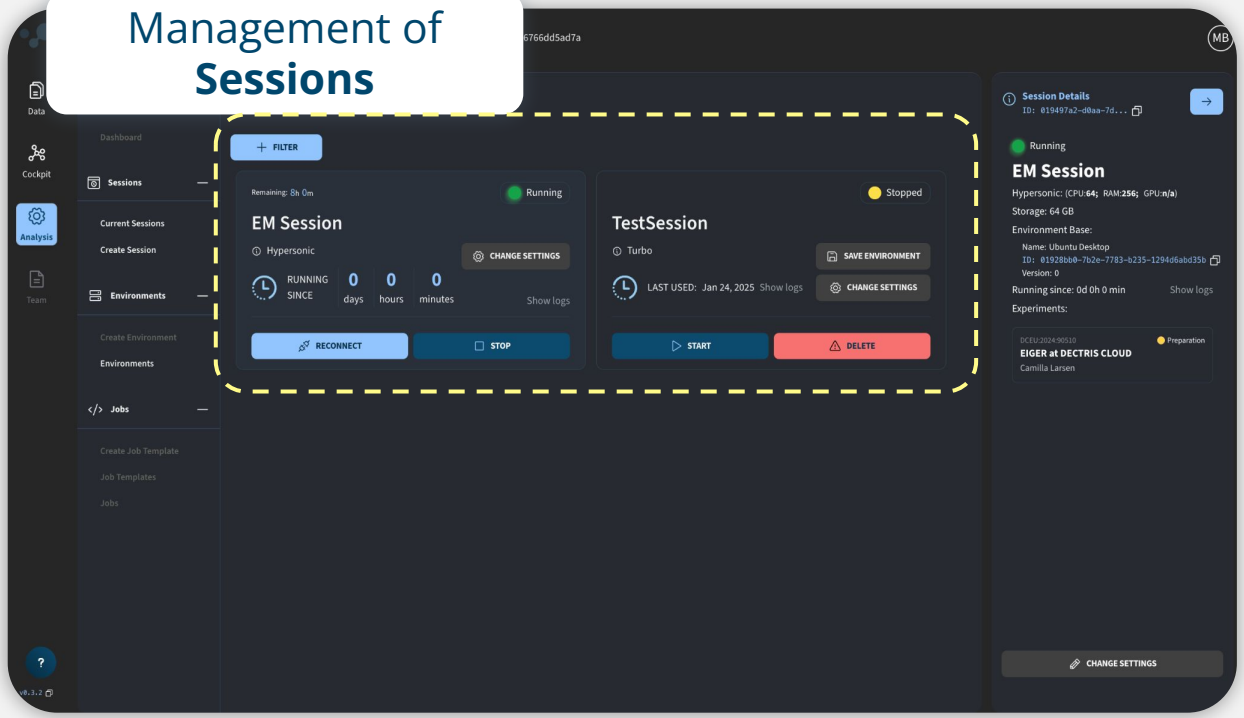
High Performance Processing

Sessions: Run Virtual Machine in Cloud

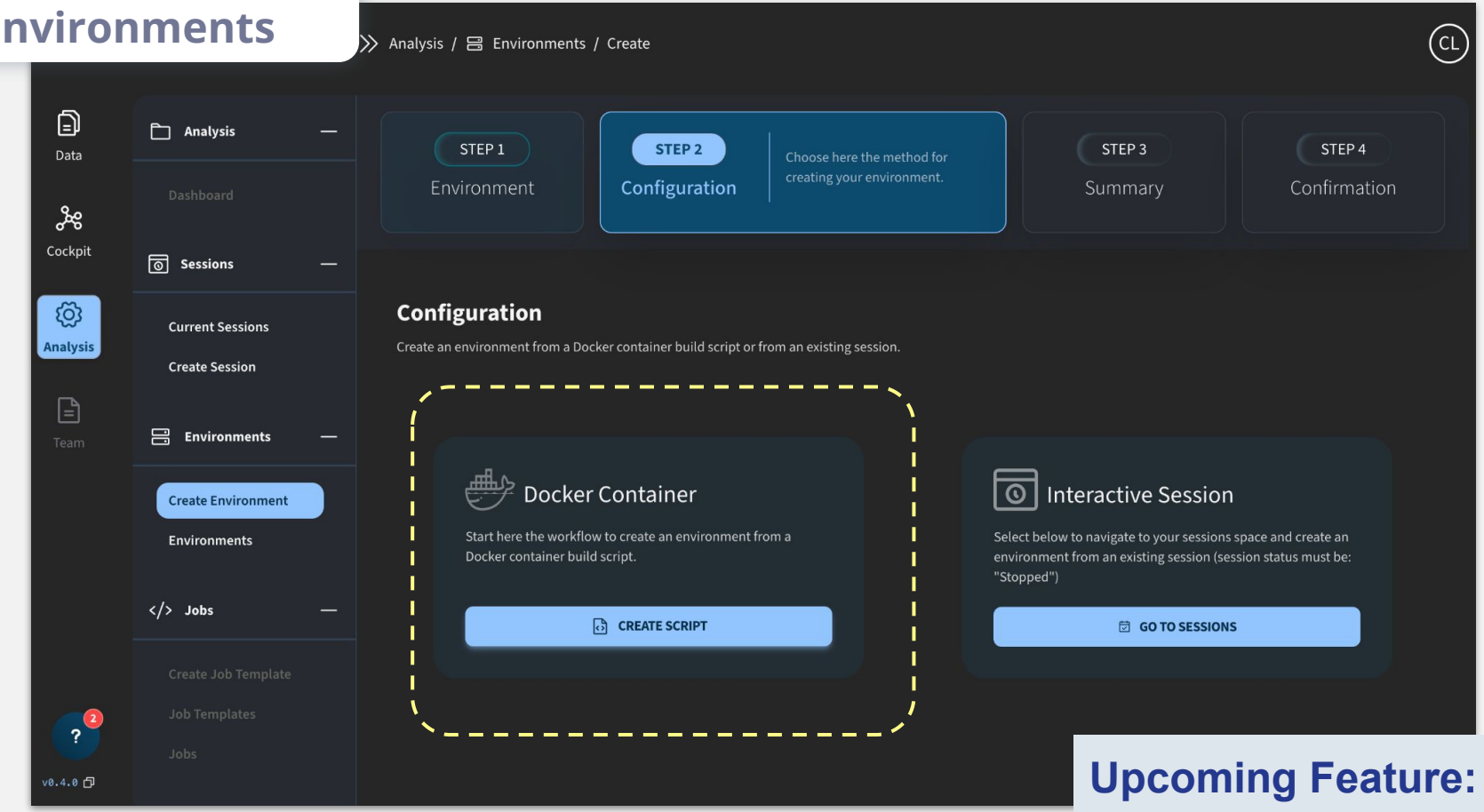
Wizard: Starting **Sessions**



Management of **Sessions**



Custom **Environments**



Upcoming Feature:
Define environment from session

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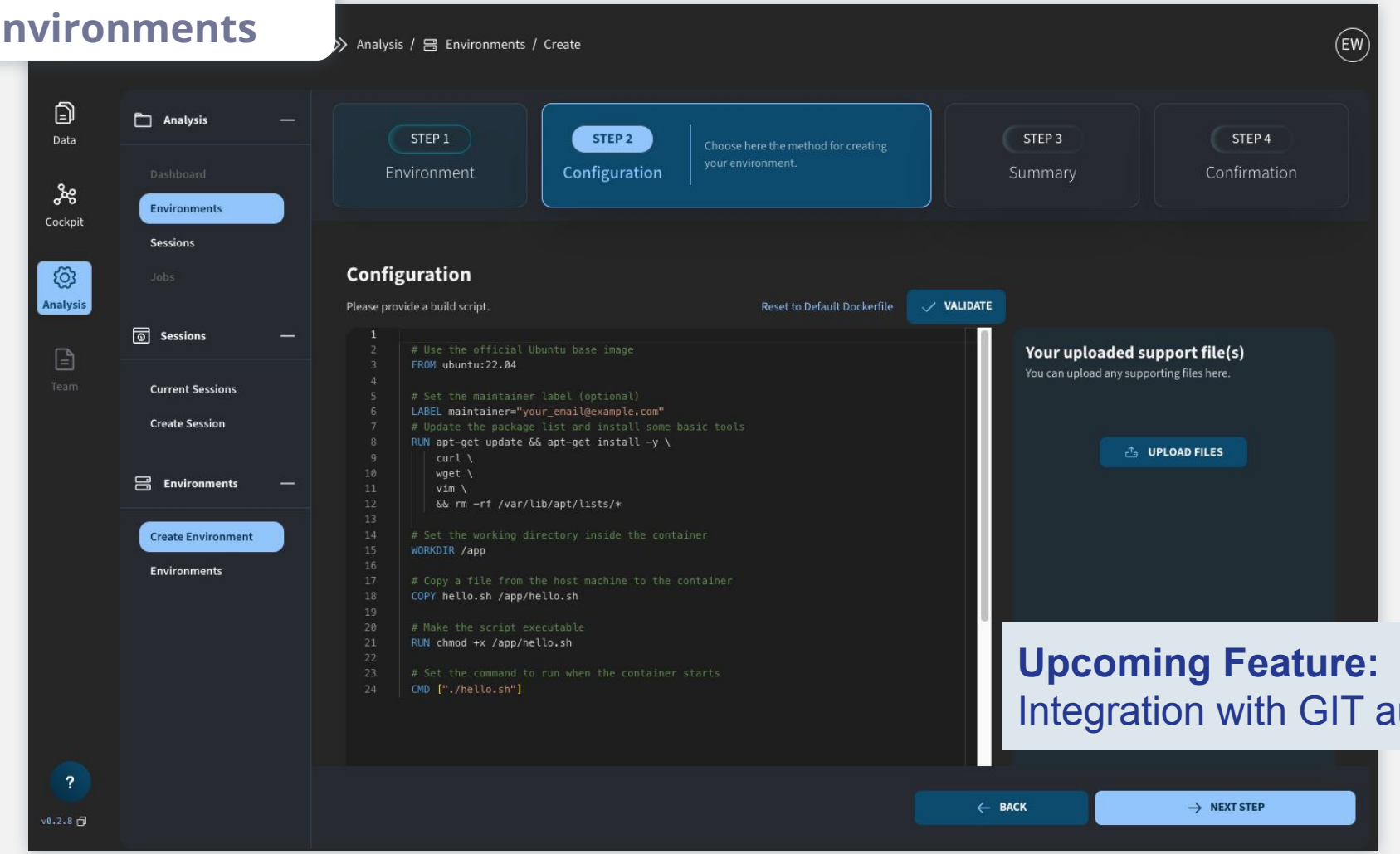
Custom **Environments**



Upcoming Feature:
Integration with GIT automation

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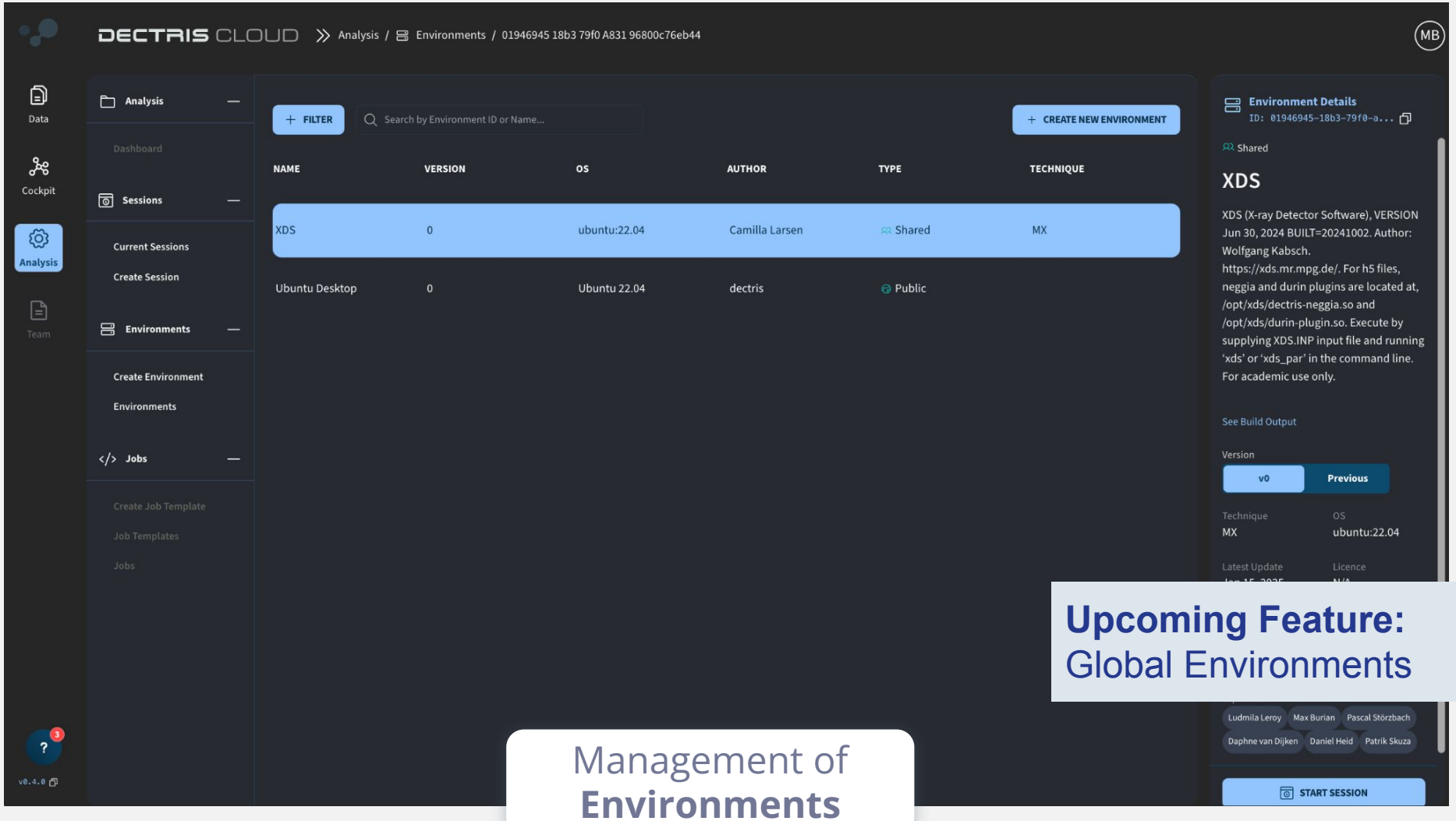
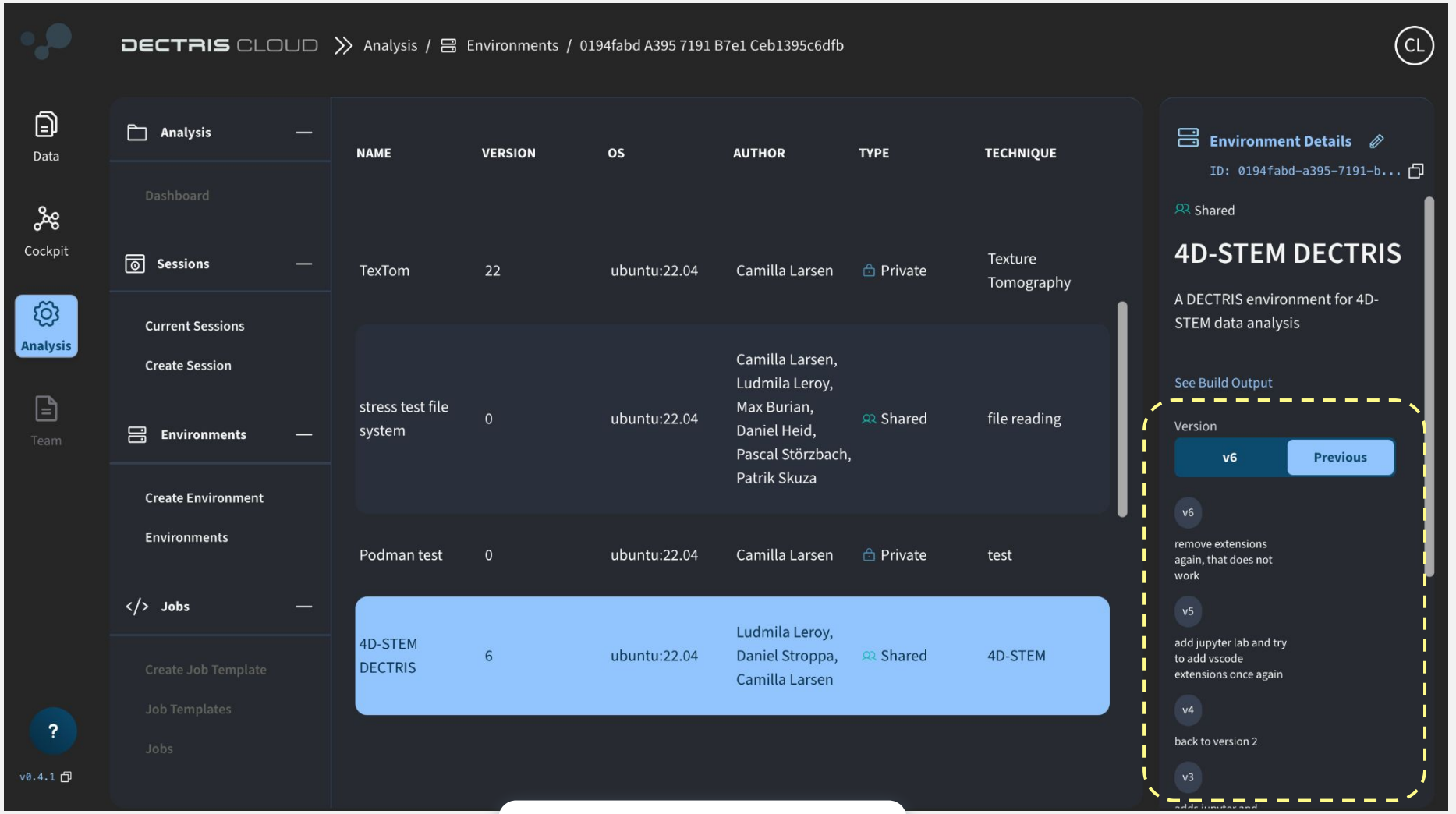


Upcoming Feature:
Global Environments

Management of
Environments

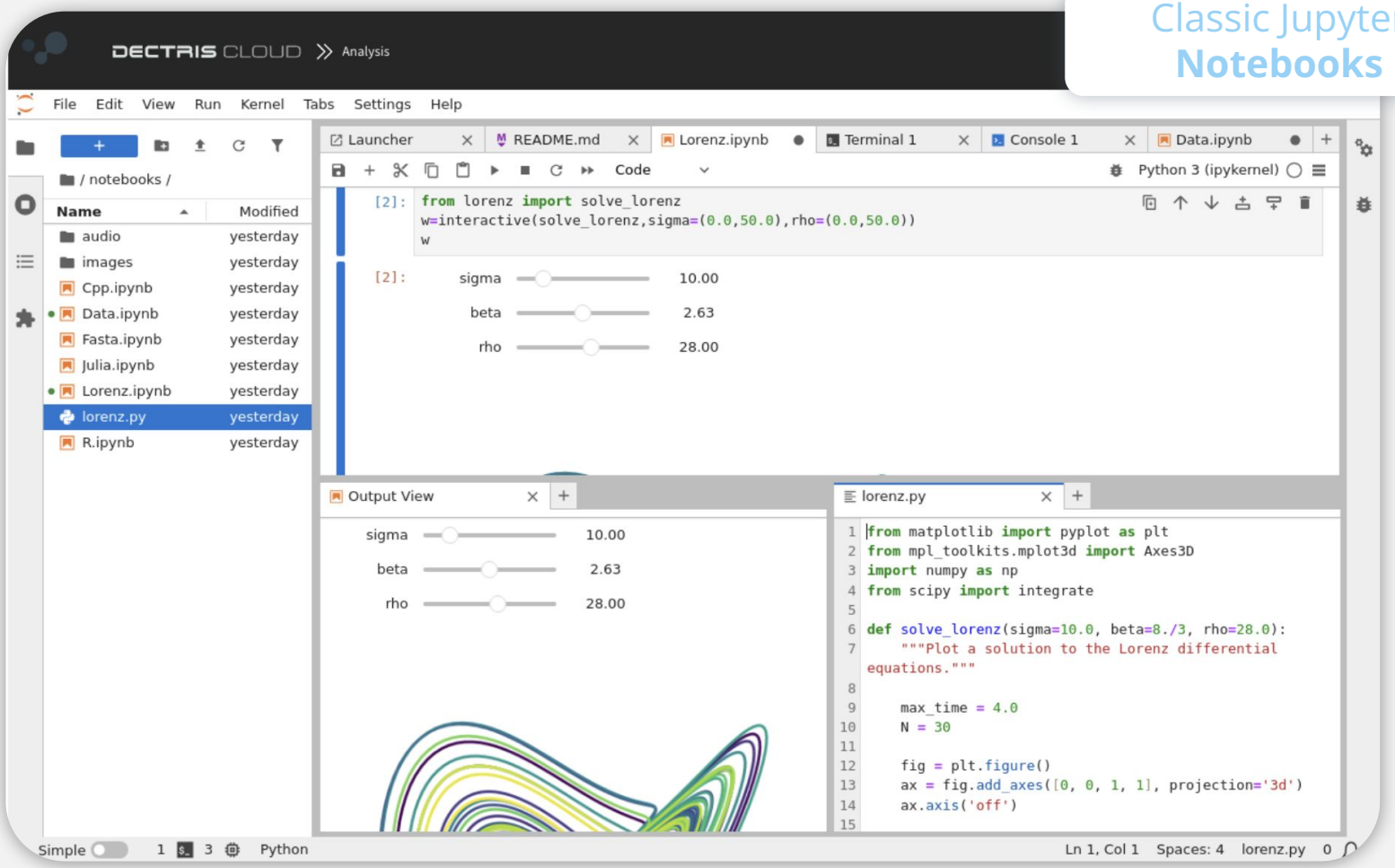


Version history of
Environments

Notebooks: Jupyter Lab

Ready in April ‘25

Classic Jupyter
Notebooks



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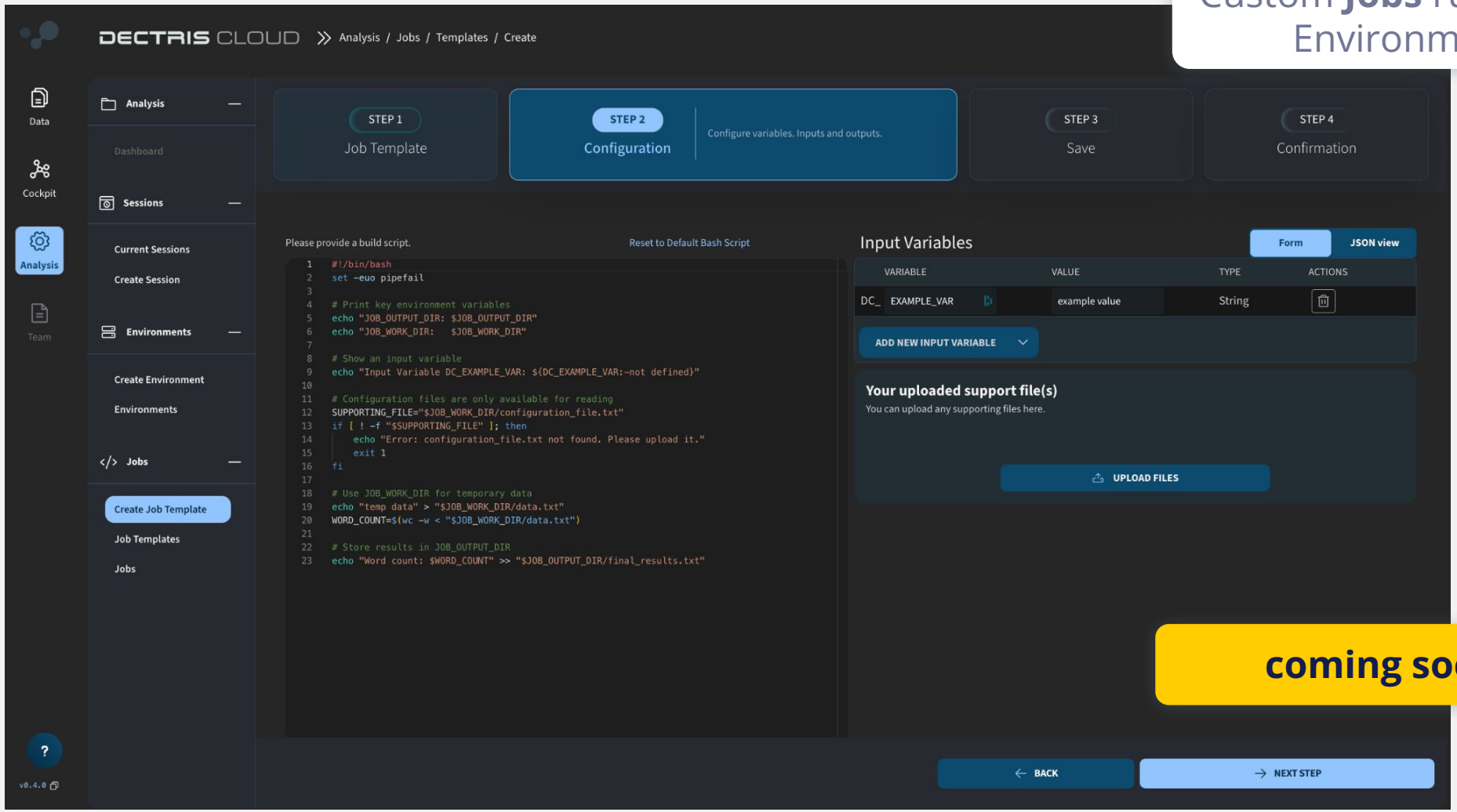
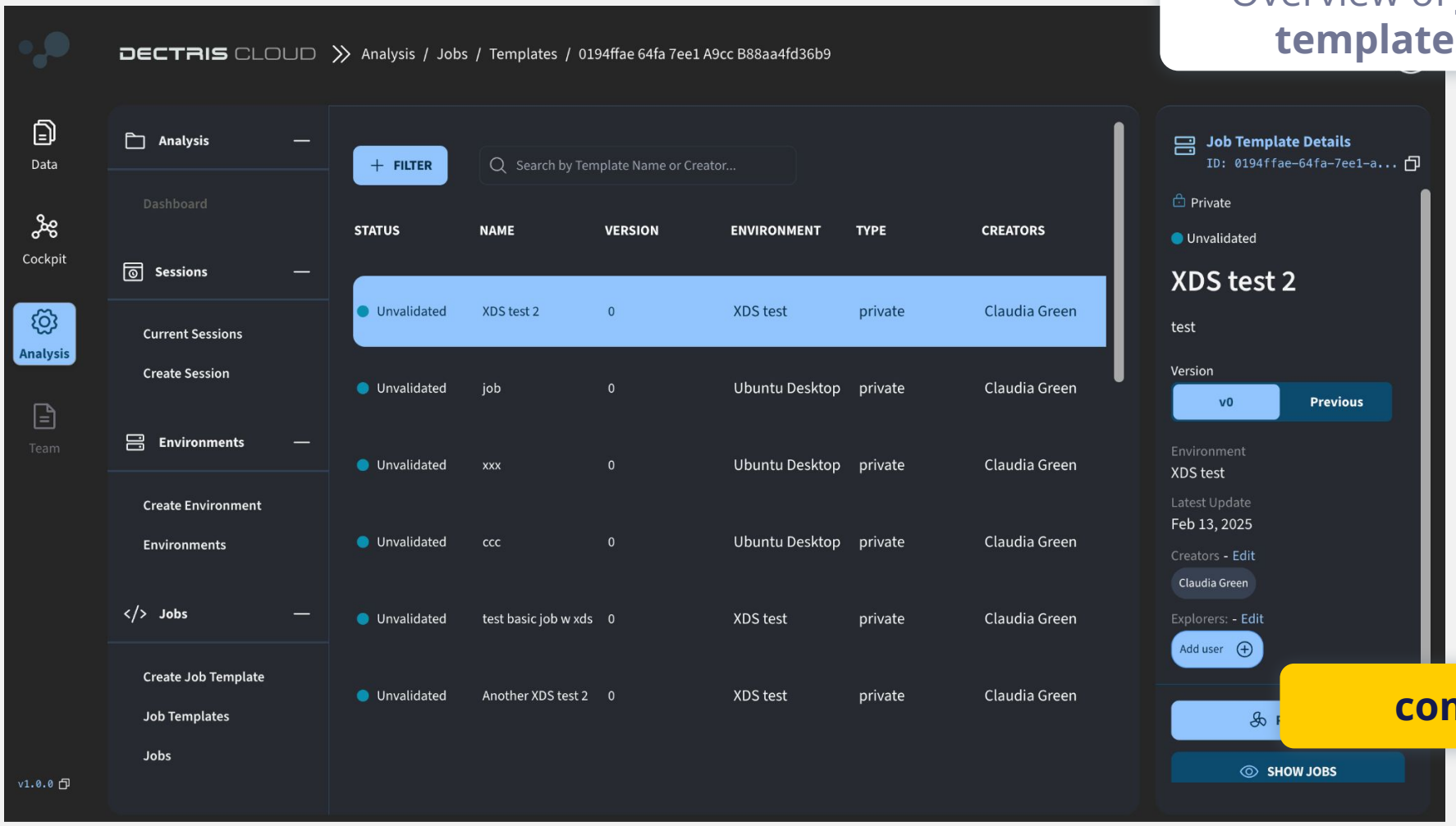
Custom **Jobs** running in Environment



coming soon!

DECTRIS CLOUD

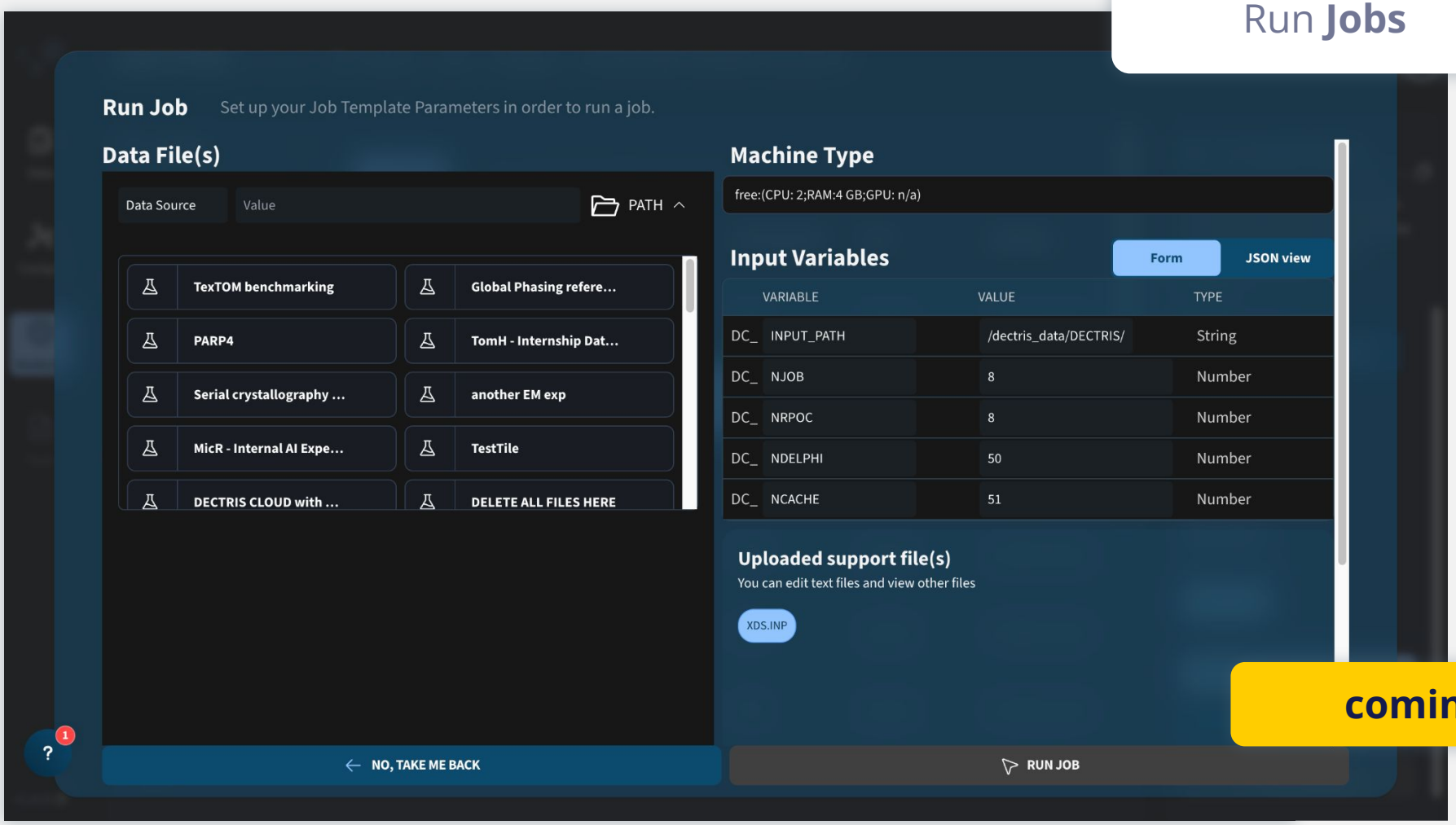
Overview of **job templates**



coming soon!

DECTRIS CLOUD

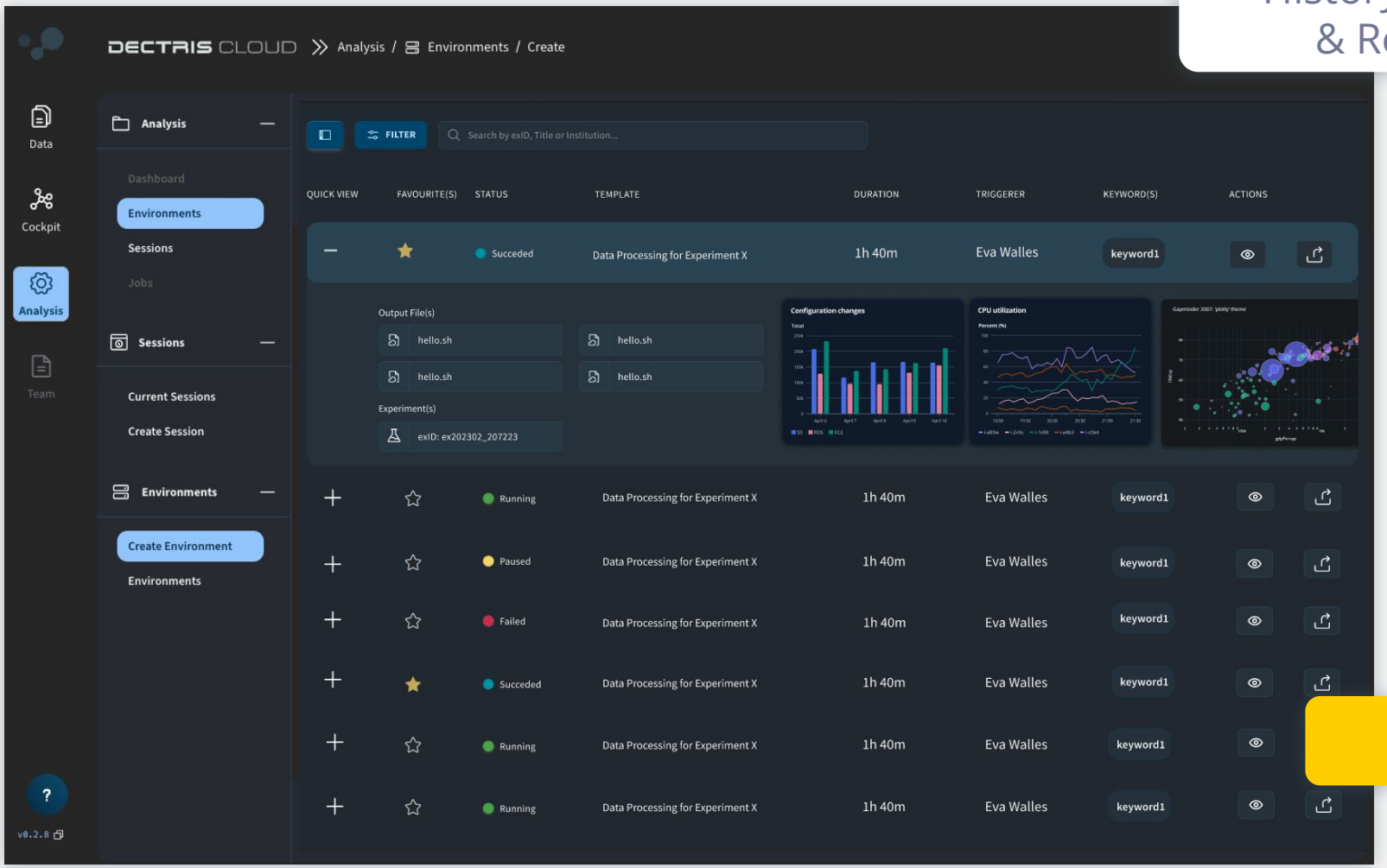
Run **Jobs**



coming soon!

DECTRIS CLOUD

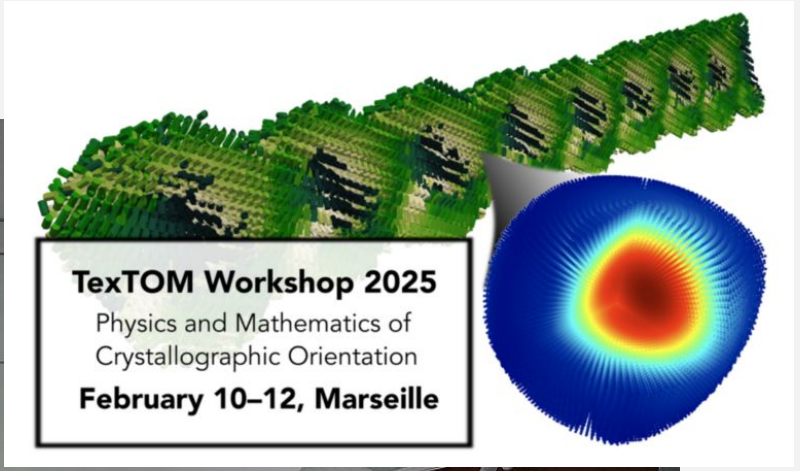
History of **Jobs** & Results

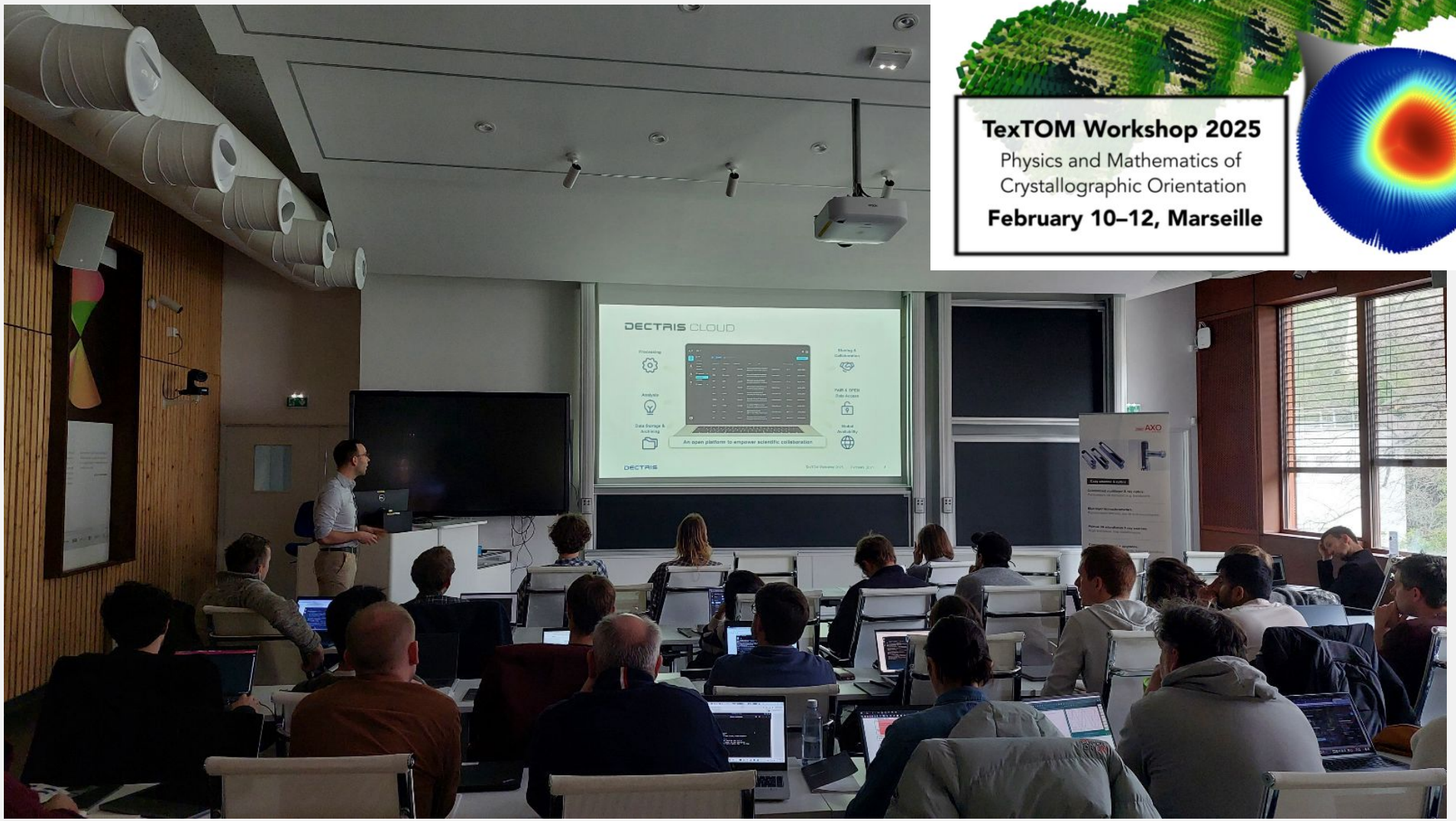


coming soon!

Examples

TexTOM workshop 2025



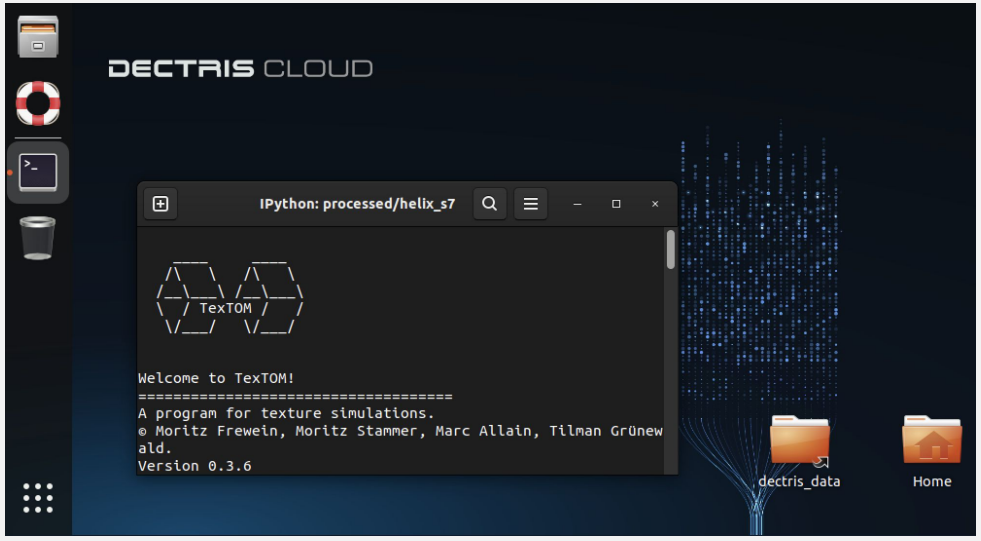


TexTOM workshop 2025

- 44 participants
- DECTRIS CLOUD Supported tutorial session:
  - Simultaneous access to a 150 GB synchrotron data set on the cloud
  - Each participant should be able to independently experience the full scientific pipeline

⇒ Scalable compute power (2500 simultaneous CPUs)

⇒ Easy access to scientific software (containers)



PX1 - Data Processing Pipeline

EIGER X 16M
@ 100 Hz

6-7 GBits

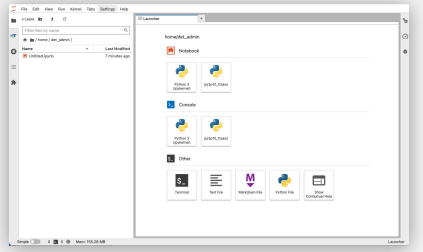
DECTRIS CLOUD

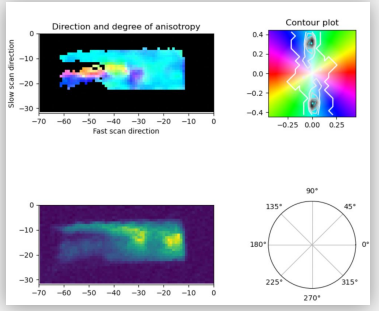
CLOUD STORAGE

Virtual Machine
Masking, Calibration, Image Analysis, Alignment, ...

Real-Time Processing
Azimuthal integration with >100 img/sec on single node

2D Analysis
Interactive plotting and analysis of reconstructions





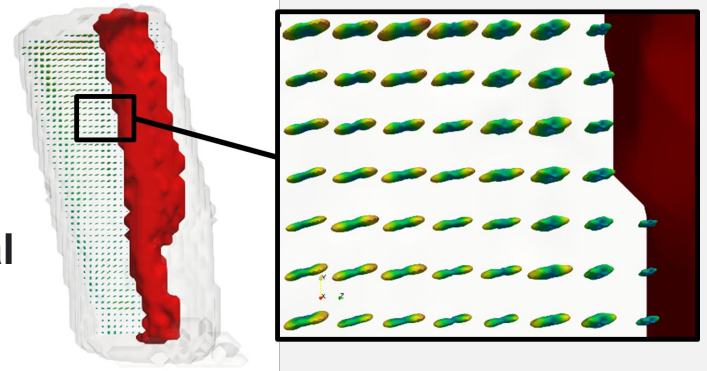
Results:

- Handled >50 TB of real experiment data within 4 days
- Full data processing and analysis done via cloud

- Reconstruction of reciprocal space map in each voxel

Extraction of main **structural orientation**

Results



Torne Tänzer, Tatiana Kochetkova, Mathieu Simon, Christian Appel, Filip Leonarski, Ezequiel Panepucci, Meitian Wang, Philippe Zysset, Marianne Liebi

microMAX - Massive Data Upload

JUNGFRAU 4M
@ 2 kHz

25 GBits

DECTRIS CLOUD

Virtual Machine
MX pipeline, spot integration, Hyper-parameter optimization

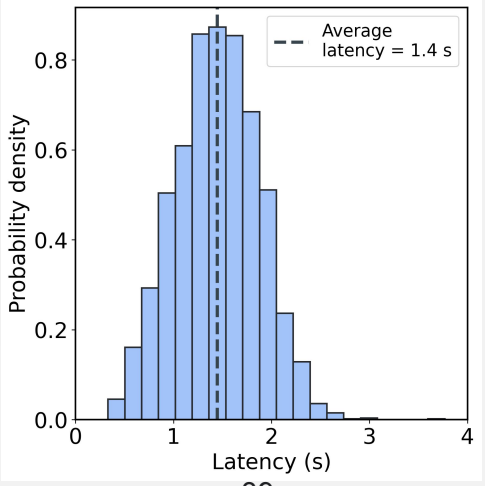
BL 8.3.1 - MX pipelines

Pilatus3 S 6M
@ 100 Hz

1 GBits

DECTRIS CLOUD

Virtual Machine
MX pipelines



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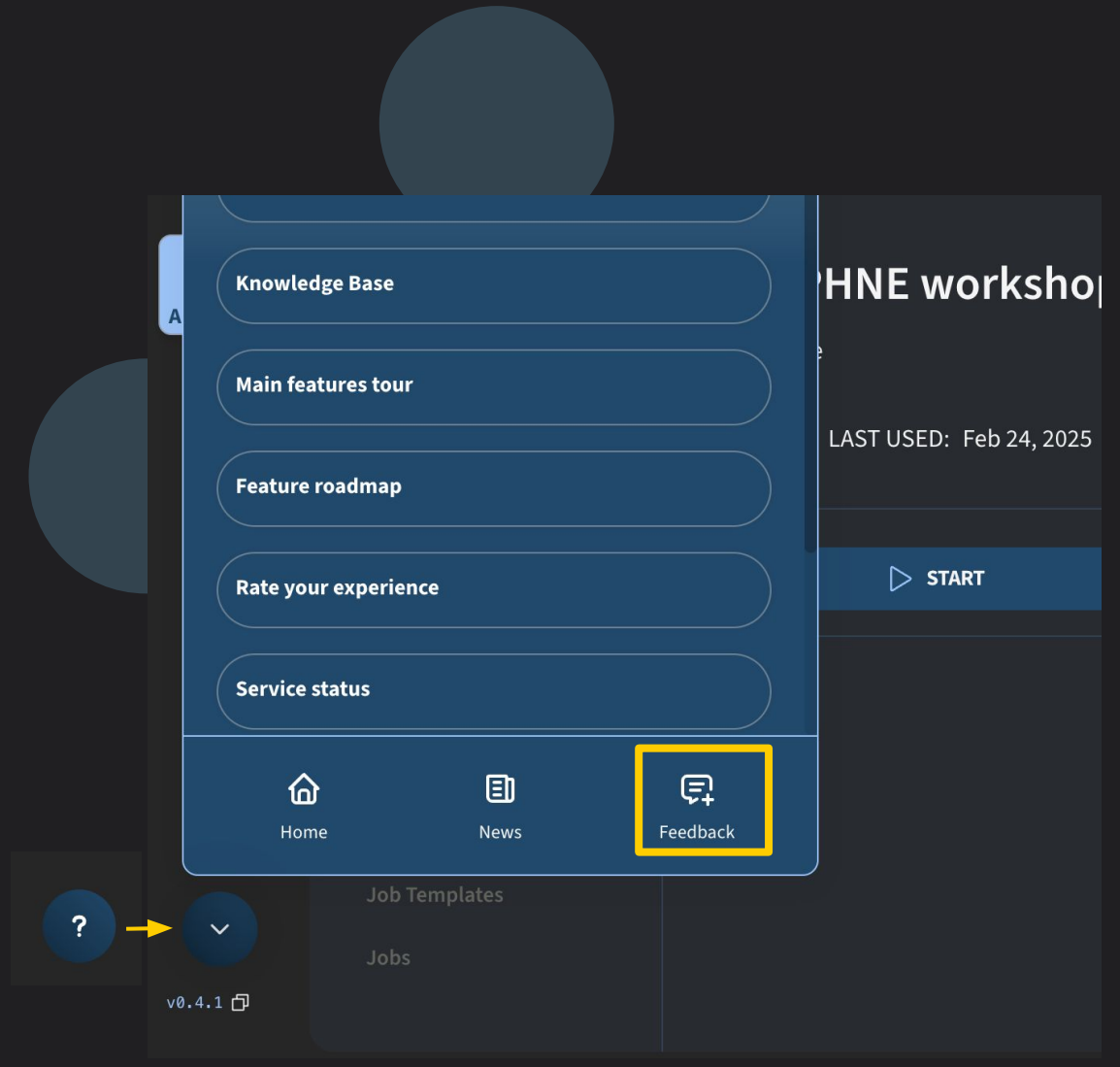
CLOUD

Thank You!

Reach out via
camilla.larsen@dectris.com

or



dectris.cloud