



# 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



**EIGER2**



**PILATUS4**

**New!**



**MYTHEN2**



**SELUN**

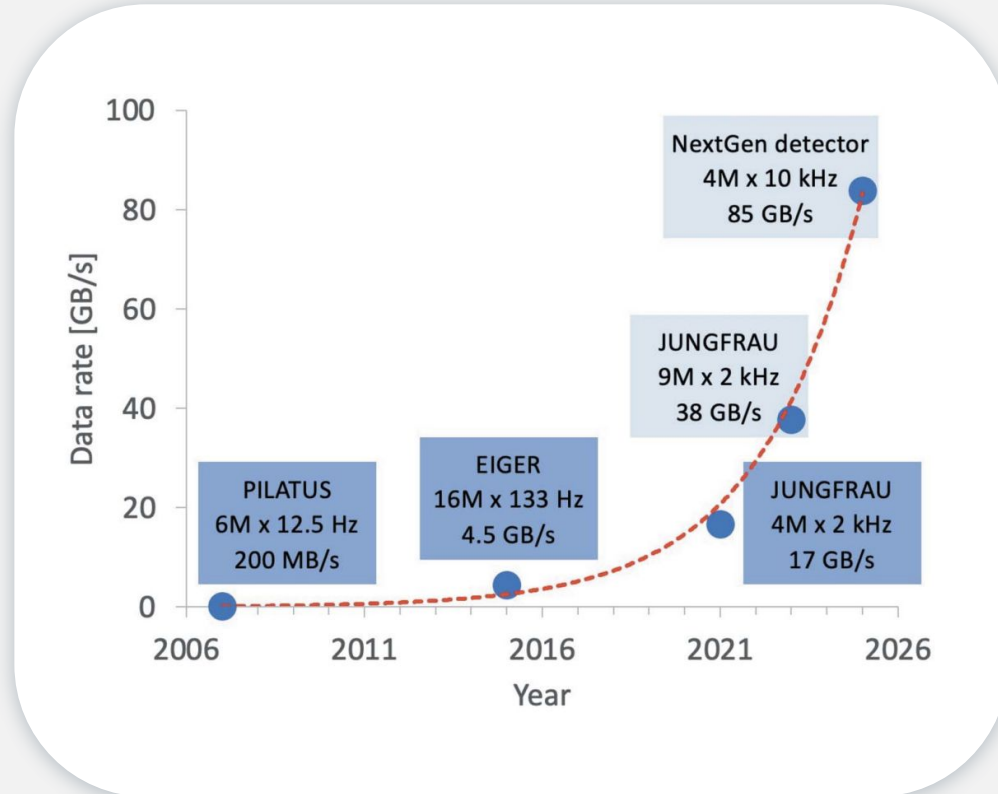
**New!**

**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

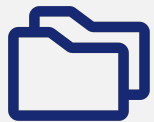
Processing



Analysis



Data Storage & Archiving



Sharing & Collaboration



FAIR & OPEN  
Data Access



Global  
Availability

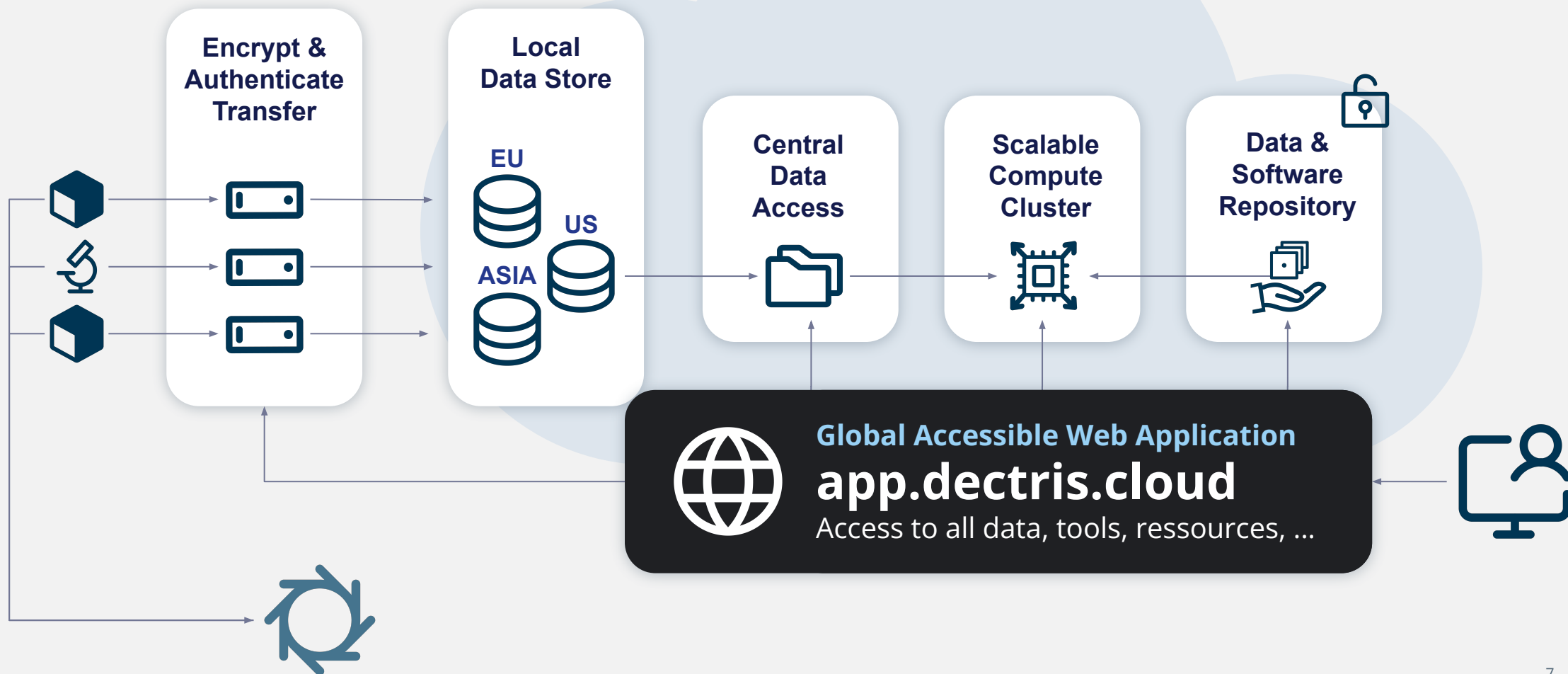


An open platform to empower scientific collaboration

The screenshot shows the Dectris Cloud interface with a sidebar on the left containing 'Data', 'Experiments', 'Collaboration', and 'Projects'. The main area displays a table of experiments with columns for Experiment ID, Institution, Laboratory, Date, Title, Principal Investigator, and Status. The table contains 10 rows of data.

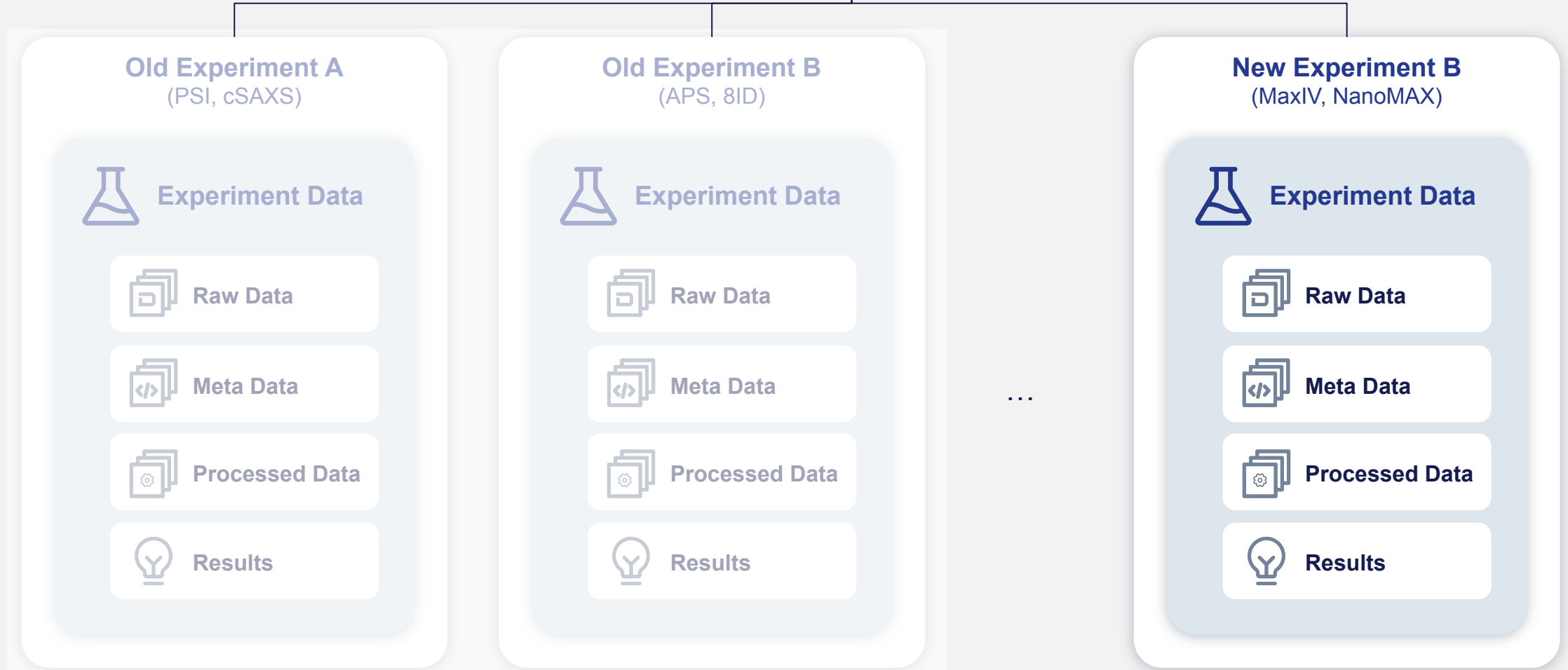
EXPERIMENT ID	INSTITUTION	LABORATORY	DATE	TITLE	PRINCIPAL INVESTIGATOR	STATUS
ESRF	ID02A	Feb. 2022	SAXS investigation of local interactions of hydrogen atoms in NaCl+ soluted ri...	Charles Brown	Done	ex2202_02895
ASLS	Ptychprobe	Dec. 2021	Rare earth precepitation mapping at nanoscale in Manganite samples fro...	David Hunter	Done	ex2112_00422
ESRF	ID15B	July 2021	Total scattering study of CsPbBr3 perovskite nanocrystals in hexafluori...	Christina Franke	Done	ex2107_09221
ESRF	BM18	May 2021	XRD-CT study on myelin formation in frontal lobe sections of rat brain	Charles Brown	Done	ex2105_03342
MaxiV	ForMAX	June 2023	Nanoscale characterization of calcinated pine wood using TTSAXS	Markus Olensson	Done	ex2306_22311
PETRAIII	P06	Oct. 2023	Naonscale 3D X-Ray CT of calcinated femur bone vicinit to titanium impla...	Markus Olensson	Running	ex2310_03321
MaxiV	ForMAX	Oct. 2023	Investigation of high temperature treated pine wood calcinated sample...	Markus Olensson	Running	ex2310_45221
ALBA	XALOC	Dec. 2023	High resolution structure determination of the photoactive yell...	Andrea Gonzalez	Preparation	ex2312_00312
SLS	PXIII	Mar. 24	Pump probe serial crystallography investigation of the transient state of...	Ravin Tahendra	Preparation	ex2403_02382

# DECTRIS CLOUD Web Service





# A New Experiment





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


MB


DECTRIS  
CLOUD


9




# DECTRIS CLOUD

  
Data

  
Cockpit


  
Analysis

  
Team

DECTRIS CLOUD >> Cockpit

MB


### BL 8.3.1



ALS


Lab Managers

Ludmila Leroy

**MAINTENANCE MODE**  
Upload temporarily paused

GO TO COCKPIT


### XALOC



ALBA


Lab Managers

Pascal Störzbach Ludmila Leroy

Initial DECTRIS Cloud Comissioning  
Pascal Störzbach

GO TO COCKPIT


### EIGER



DECTRIS


Lab Managers

Ludmila Leroy

ANAXAM Imaging test  
Ludmila Leroy

GO TO COCKPIT


### PILATUS



DECTRIS


Lab Managers

Ludmila Leroy

PILATUS at DECTRIS CLOUD  
Ludmila Leroy

GO TO COCKPIT


### DEMO



The Pequod Synchrotron


Lab Managers

Ishmael

The White Whale Experiment  
Captain Ahab

GO TO COCKPIT


### VPD



Northwestern


Lab Managers

Daniel Heid Ludmila Leroy

**MAINTENANCE MODE**  
Upload temporarily paused

GO TO COCKPIT


### MicroMAX




MAX IV

Lab Managers

Ludmila Leroy

**MAINTENANCE MODE**  
Upload temporarily paused

GO TO COCKPIT

  
?

1

v0.2.8

Overview of Active Experiments

# Experiment Starts: Activate!

The screenshot displays the DECTRIS Cloud Cockpit interface for the EIGER experiment. The interface is divided into several sections:

- Header:** DECTRIS CLOUD >> Cockpit / EIGER
- Left Sidebar:** Data, Cockpit (selected), Analysis, Team.
- Main Content Area:**
  - EIGER DECTRIS:** A dashed box containing four status cards:
    - Detector:** Health: ok, Status: idle
    - HUB:** Health: ok, Status: configured
    - Cloud:** Health: ok, Status: running
    - Processing:** Health: None, Status: None (coming soon)
  - Files:** A list of files including upload\_test/series\_10\_data\_000016.h5, upload\_test/series\_10\_data\_000002.h5, upload\_test/series\_8\_data\_000042.h5, upload\_test/series\_5\_data\_000027.h5, upload\_test/series\_7\_master.h5, upload\_test/series\_10\_data\_000040.h5, upload\_test/series\_8\_data\_000039.h5, upload\_test/series\_11\_data\_000015.h5, and upload\_test/series\_11\_data\_000060.h5.
  - Experiment:** A section with buttons: SWITCH EXPERIMENT, CREATE NEW EXPERIMENT, and TOKEN.

- Right Sidebar:**
- Experiment ID:** t
- Status:** Running
- Experiment Name:** ANAXAM Imaging test
- testing Sessions at DC:**
  - Facility: DECTRIS
  - Laboratory: EIGER Lab
  - Expected Starting Date: 2024-11-12
  - Expected End Date: 2024-11-14
  - Type: Proprietary
  - Keywords: anaxam, imaging, Add keyword...
- Principal Investigator - Edit:** Ludmila Leroy
- Experiment Collaborators - Edit:** Add user
- Buttons:** GO TO ROOT FOLDER, GO TO LOGBOOK, EDIT EXPERIMENT

Live Experiment Status

# Experiment Data Management

The screenshot displays the DECTRIS Cloud web interface. The left sidebar contains navigation links for Data, Cockpit, Analysis, Team, and Projects. The main content area shows the 'EIGER at DECTRIS CLOUD' experiment details, including its ID (DECTRIS:2024:14828), location (EIGER Lab), date (2024/06), and PI (Ludmila Leroy). Below this, there are sections for FOLDERS and FILES. The FILES section lists a file named 'Lysozyme-Lyz8\_1\_master.h5' (350 files). A dashed white box highlights the 'Download' and 'Upload' buttons, and a yellow box highlights the 'Archive Data', 'Retrieve Data', 'Restore Version', and 'Restore Deleted' buttons. A 'Ready in March '25' badge is also present. On the right, a 'File Browser' section shows a list of available experiments with their IDs, titles, and status (Running, Preparation, Done, Maintenance). At the bottom right, there are buttons for 'GO TO ROOT FOLDER' and 'GO TO LOGBOOK'.

**Ready in March '25**

**File Browser**

**Download** **Upload**

**Archive Data**

**Retrieve Data**

**Restore Version**

**Restore Deleted**

**DECTRIS CLOUD** >> Data / Dectris Data / 2024/DECTRIS:2024:14828/Raw\_data

**EIGER at DECTRIS CLOUD**  
ID: DECTRIS:2024:14828

DECTRIS EIGER Lab 2024/06 PI Ludmila Leroy

**FOLDERS**  
No folders in current directory

**FILES**  
✓ Lysozyme-Lyz8\_1\_master.h5 (350 files)

**Quick Navigate Experiment Data**  
ID: DECTRIS:2024:14828

**Available Experiments**  
Search by Experiment ID, Title, PI or Institution...

Experiment ID	Experiment Title	Status
MAXIV:2024:18037	DECTRIS CLOUD is now at MicroMAX	Done
DECTRIS:2024:35389	Generated by API	Done
XALOC:2024:11205	Initial DECTRIS Cloud Commissioning	Running
MAXIV:2024:60875	This is an example title	Preparation
DECTRIS:2024:42046	PILATUS at DECTRIS CLOUD	Running
DECTRIS:2024:14828	EIGER at DECTRIS CLOUD	Running
SRI:2024:00001	Skyline Research Innovators (SRI)	Running
PEQUOD:2025:00002	Whale Song Analysis Experiment	Preparation
PEQUOD:2025:00001	The White Whale Experiment	Running
MAXIV:2024:79877	Serial crystallography with Lysozyme	Maintenance

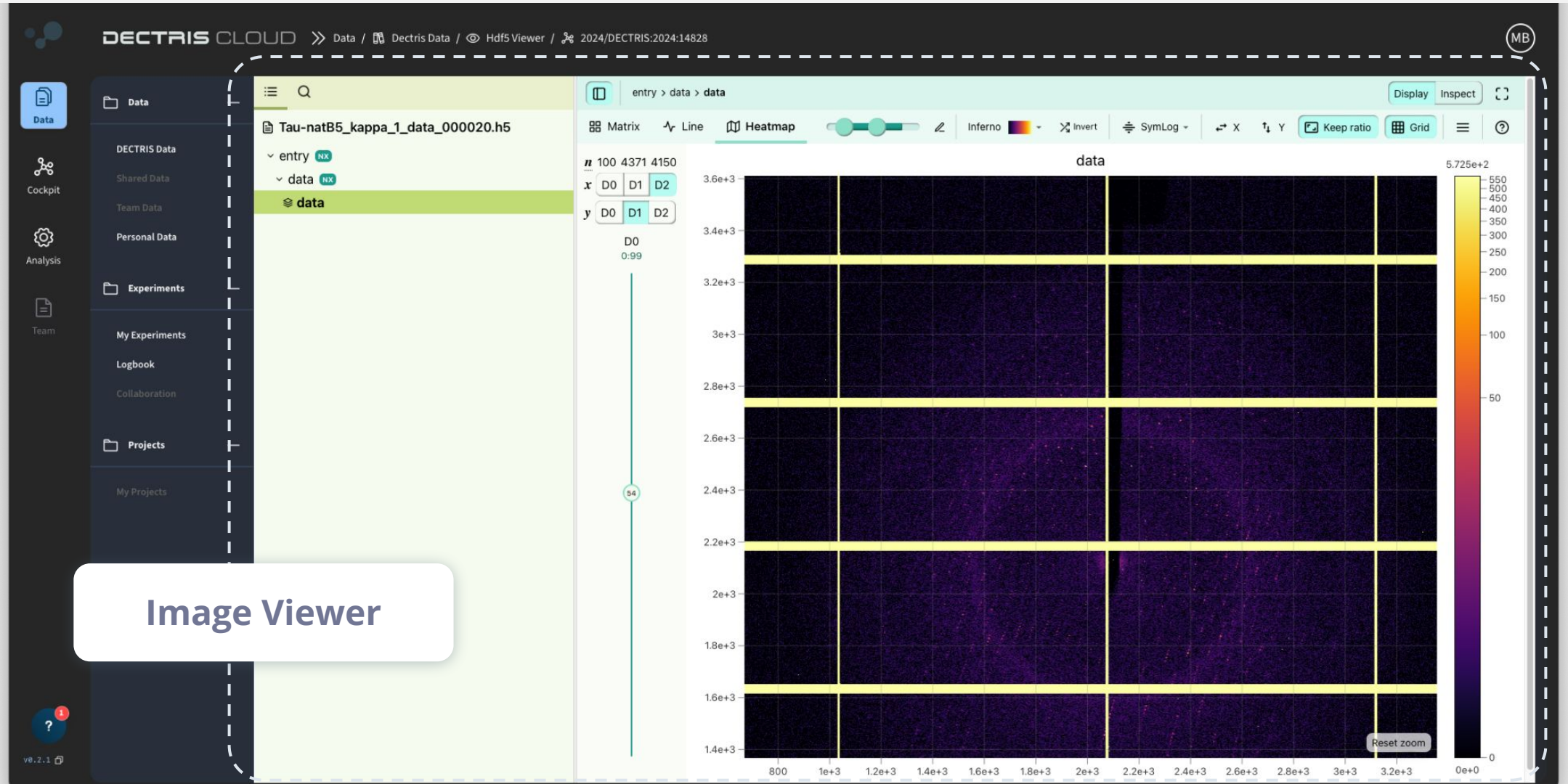
**GO TO ROOT FOLDER**

**GO TO LOGBOOK**

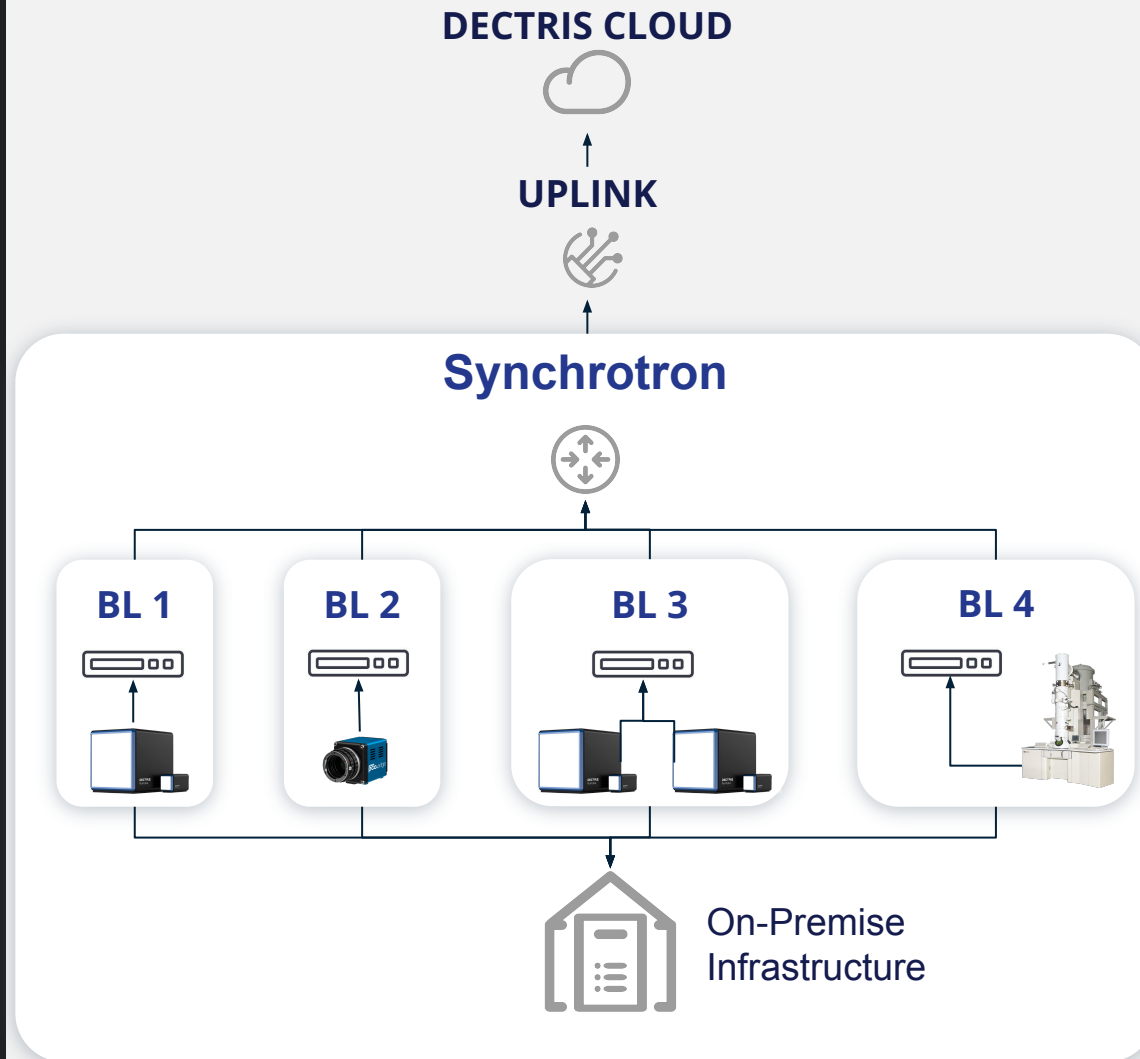




# DECTRIS CLOUD

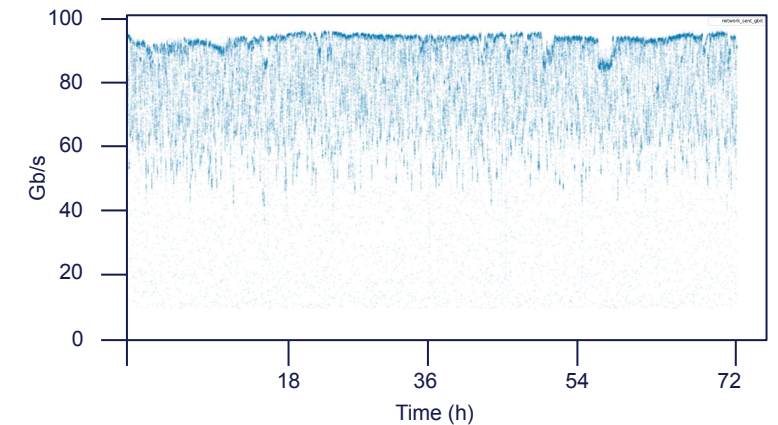


# Getting Data into the Cloud



DATA STREAM

## Upload Performance

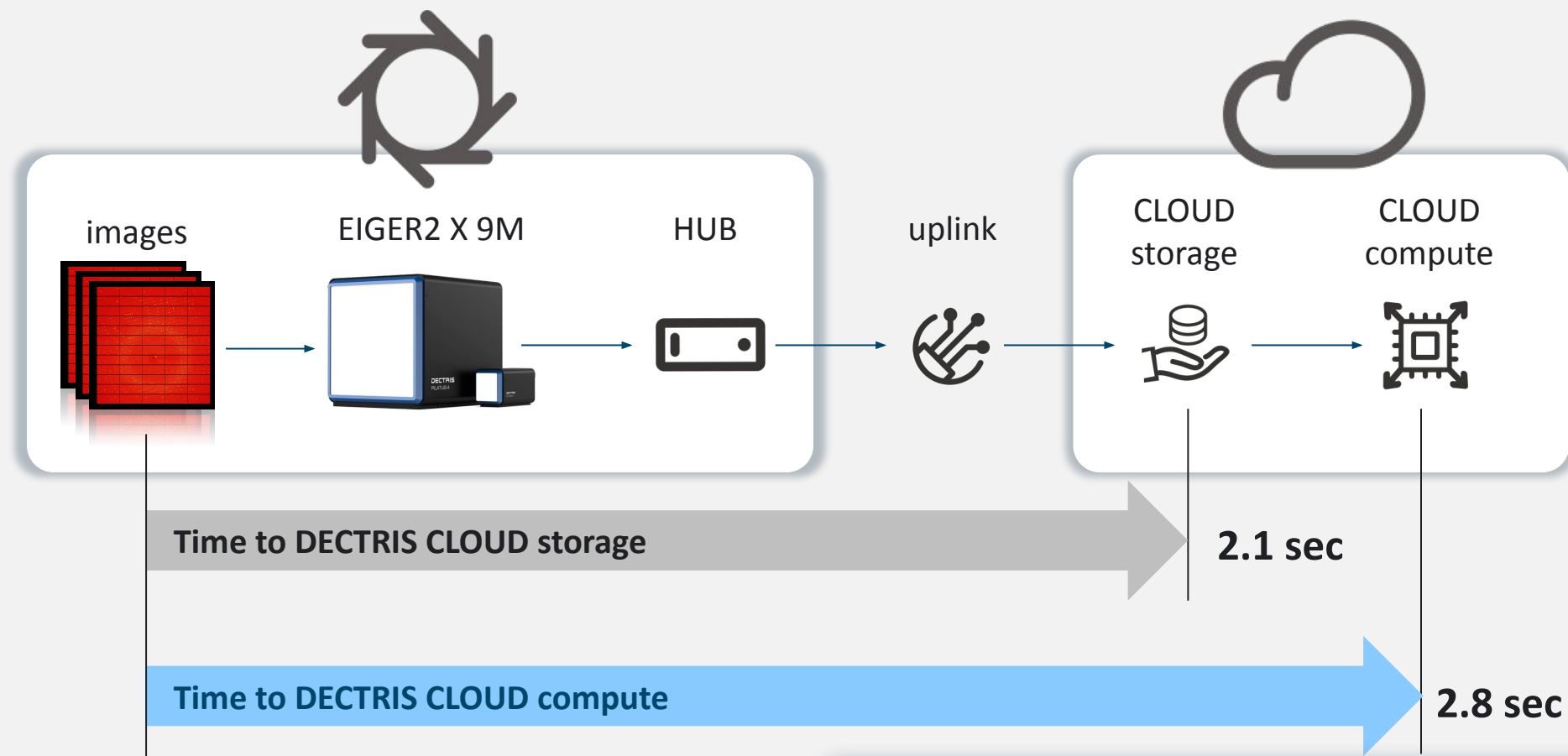


Uninterrupted upload of 1.2 PetaBytes in 72h

Average bandwidth of 92 GBits

2023, ALBA (ESP), XAIRA Beamline

# Performance Results: Upload Latency

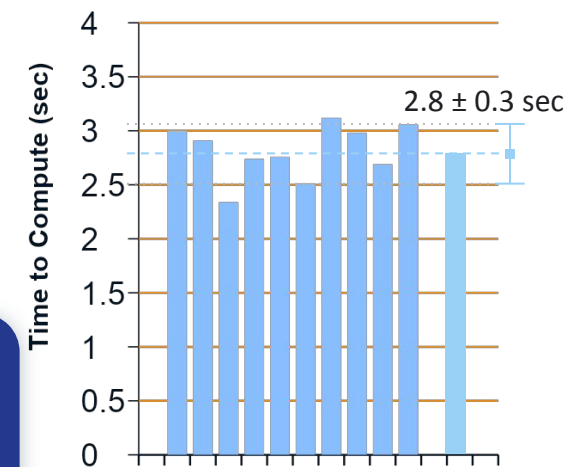
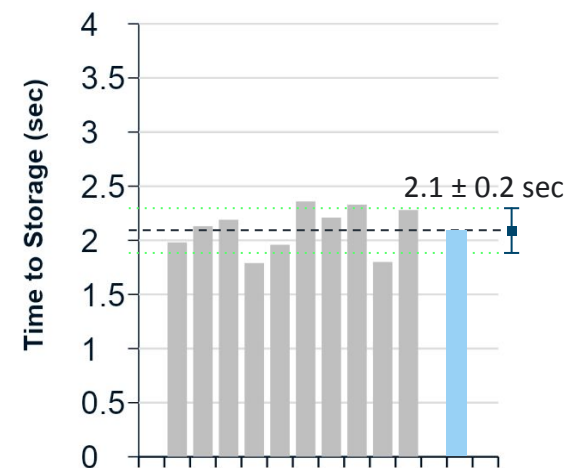


Data becomes available in < 3 sec

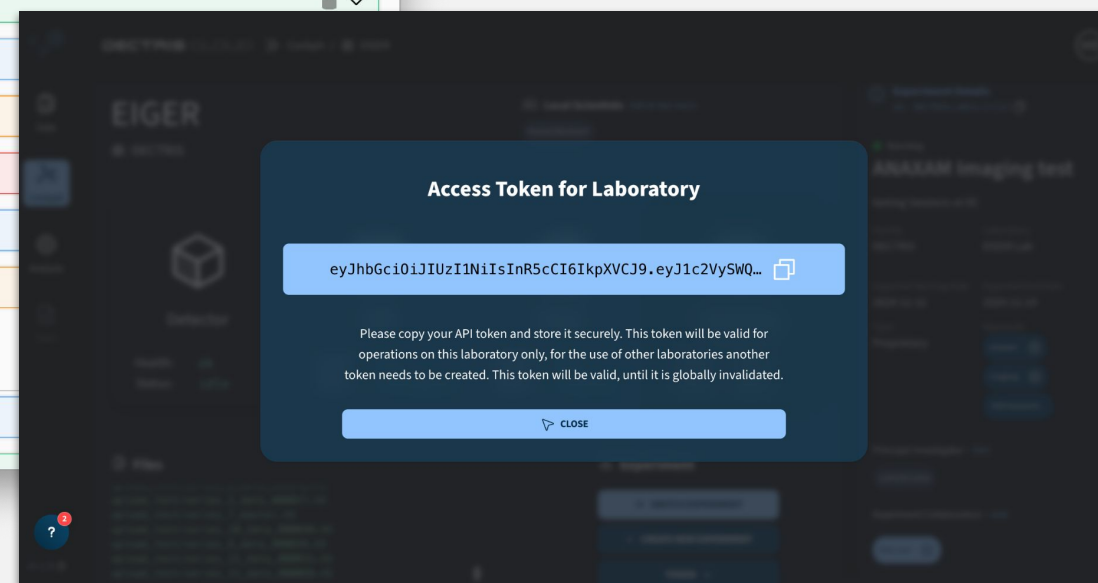
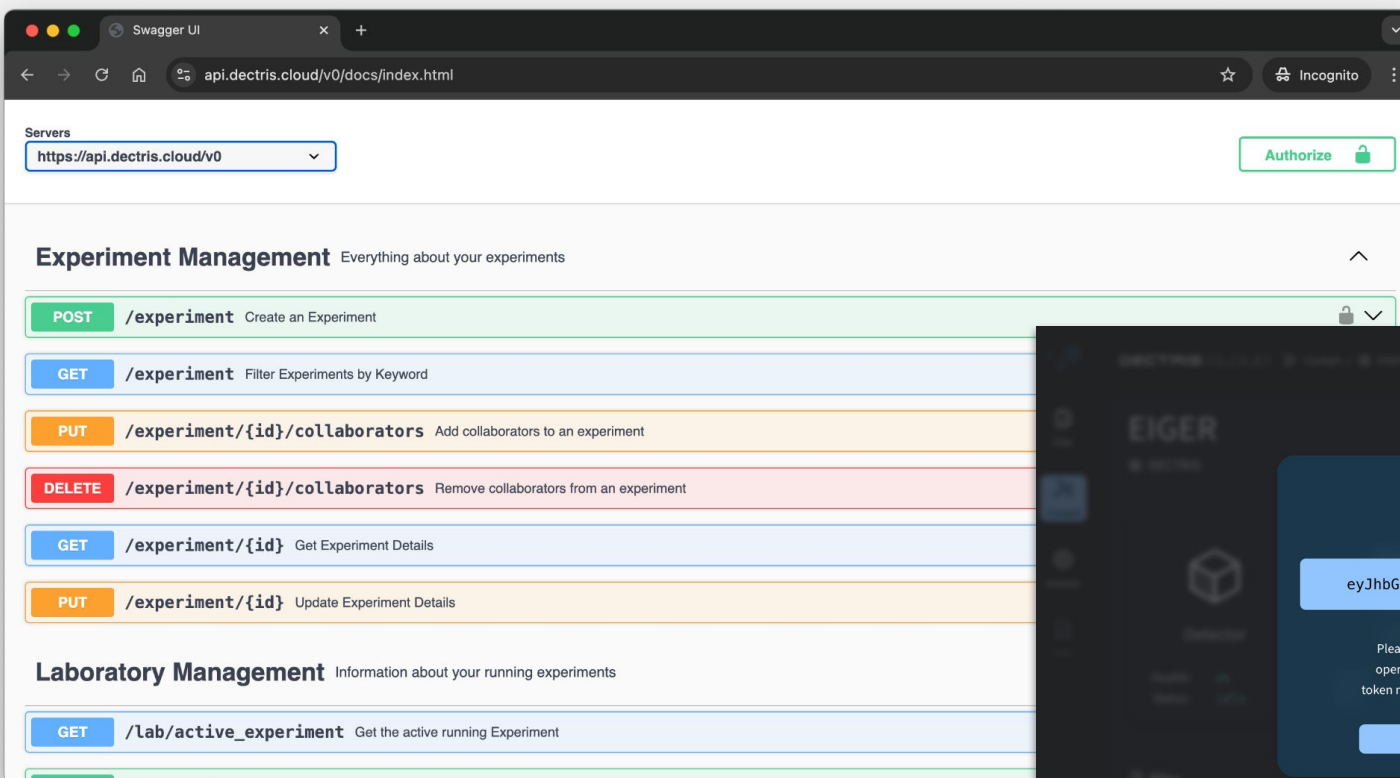
User Benefit:

- + Instant access to data in cloud
- + No manual data copy

## Latency Measurements



# DECTRIS CLOUD





# Implementation Overview



# DECTRIS CLOUD Implementation

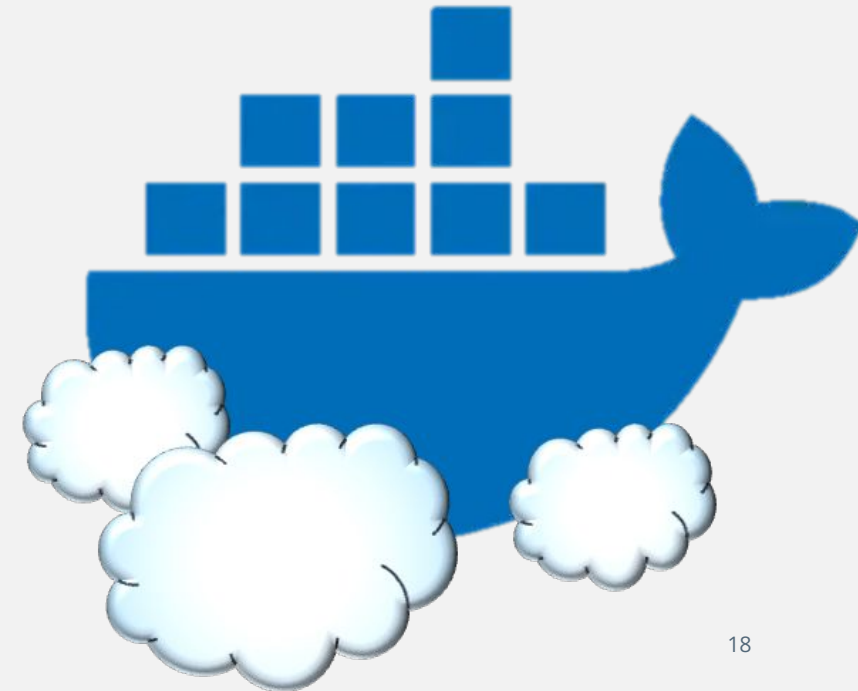


## Multi-cloud

- Redundancy
- Optimization
- Scalability

## Containerization

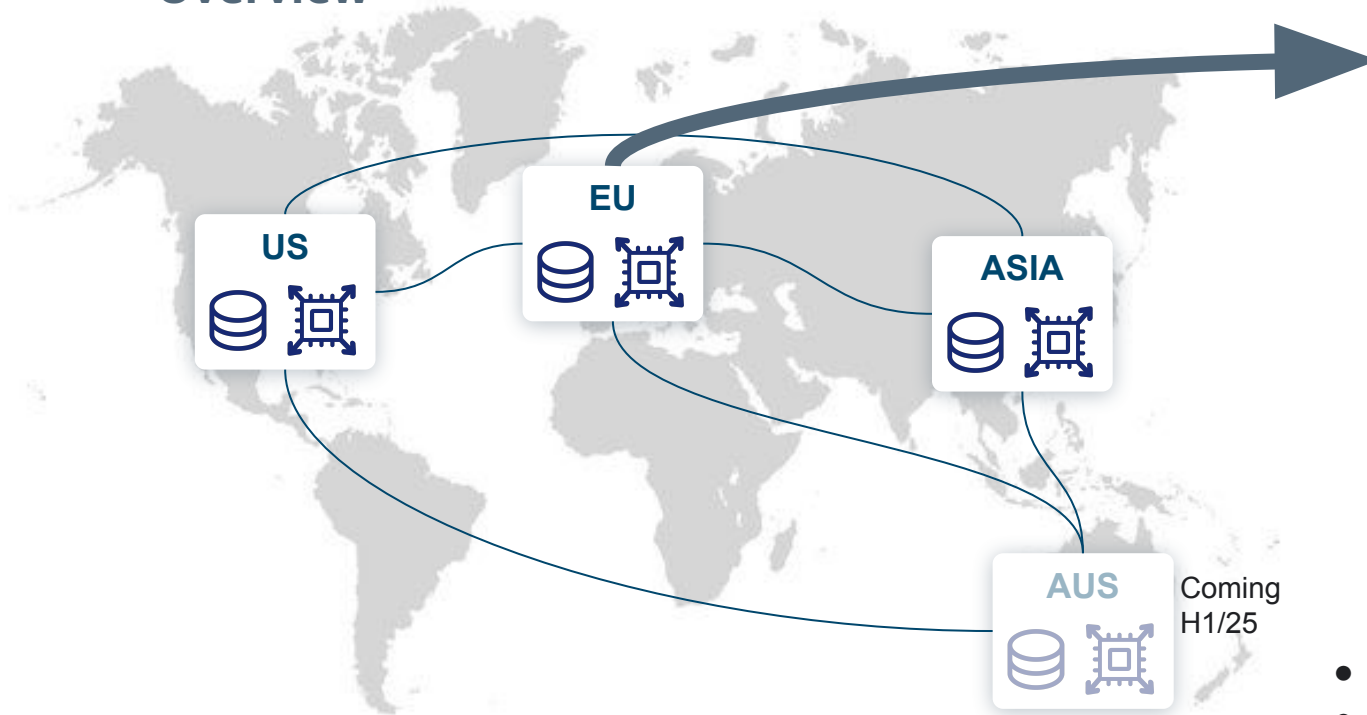
- Uniformity
- Collaboration
- Reproducible workflows





# Global Data Bandwidth Capacity

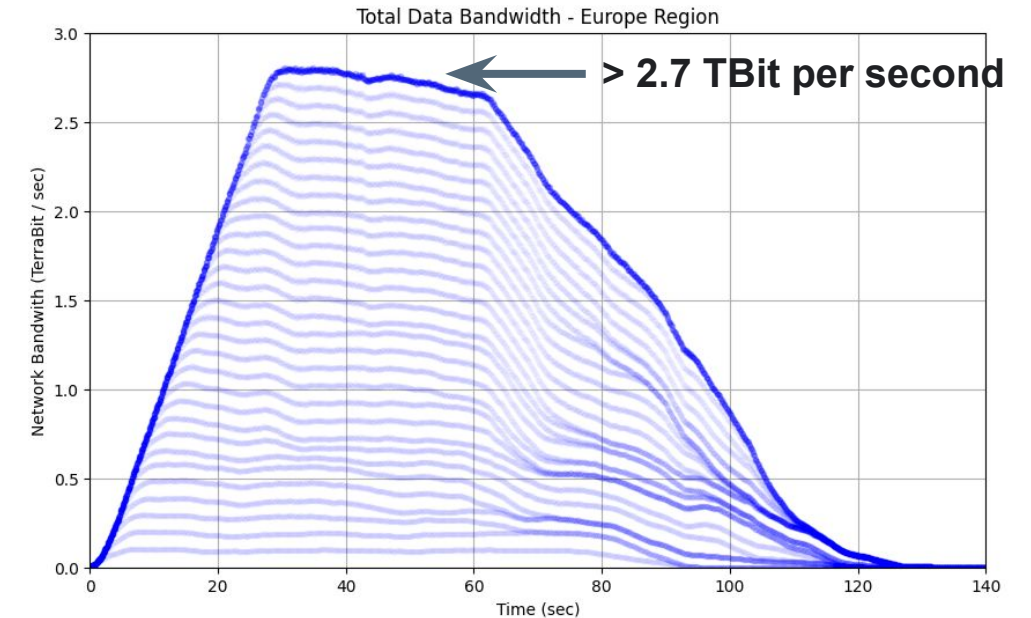
## Cloud Architecture Overview



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



## 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

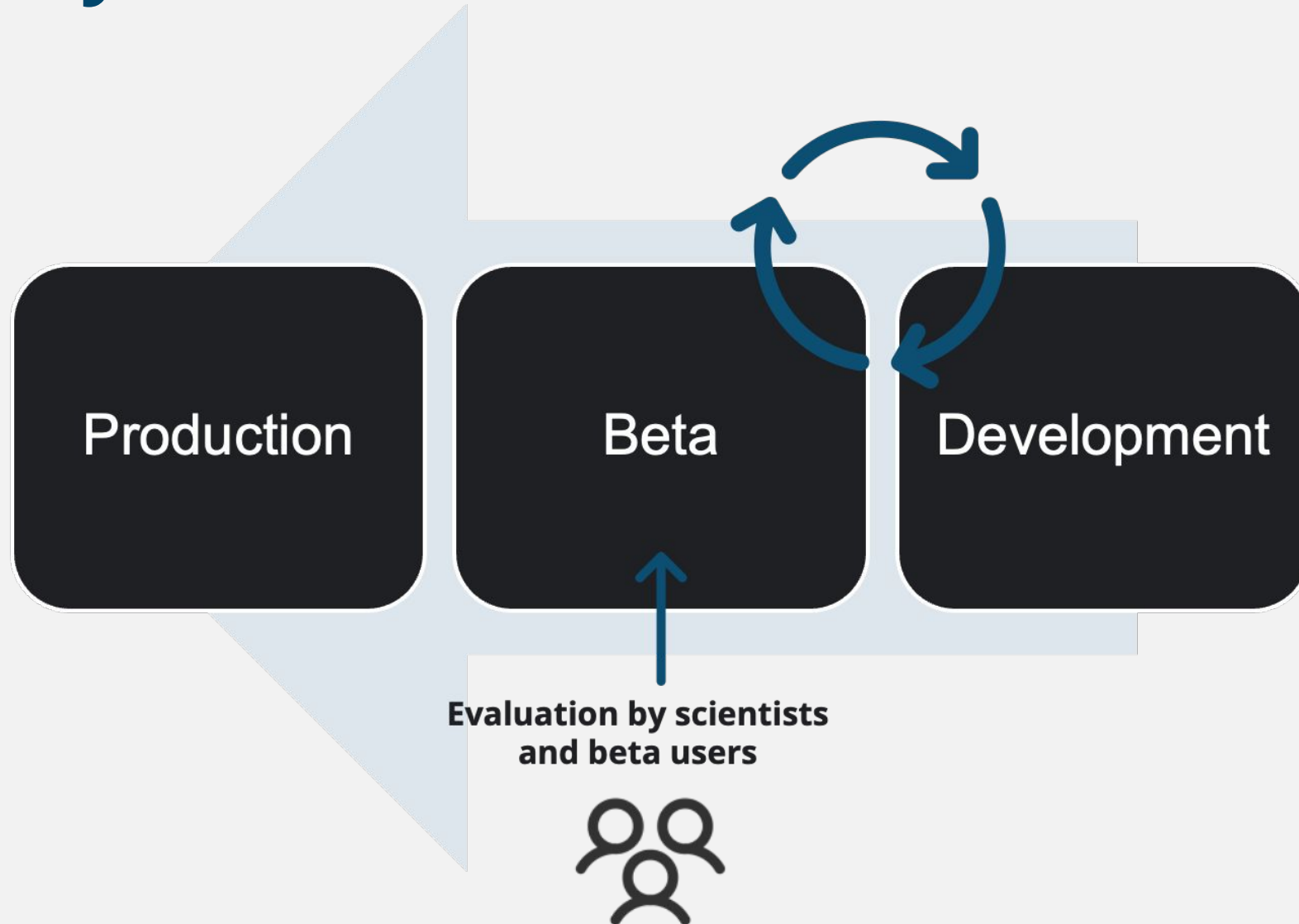
**Total Global Bandwidth:**

3 Regions x 3 Availability Zones x 2.7 Tbit = >20 TBits

19



# Deployment schedule

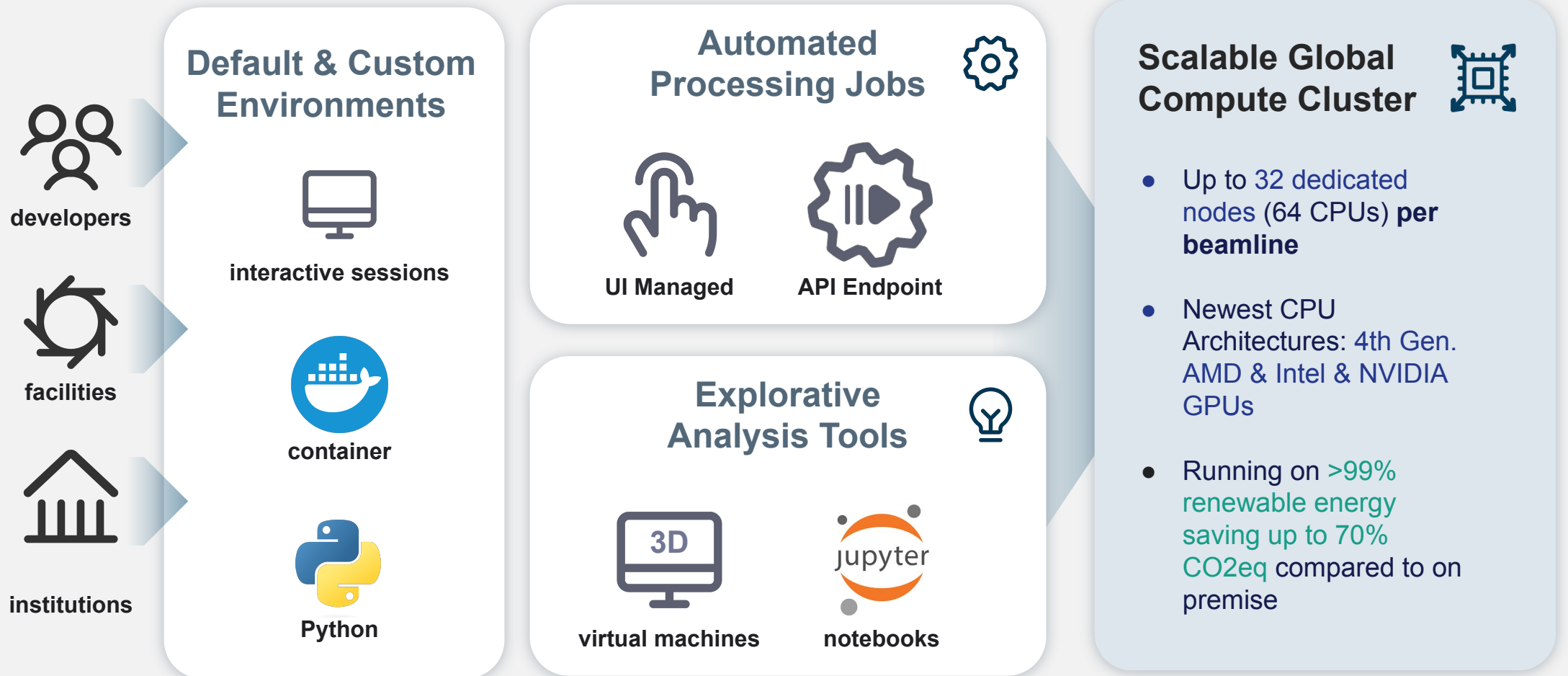






# Scientist Interaction with Containers

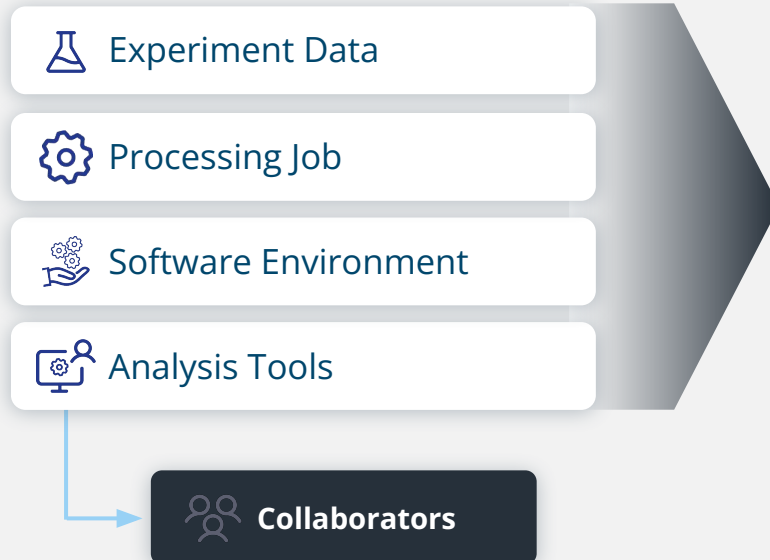
# Container-Based Compute





# Sharing and collaboration

Direct Sharing:



Make data & software reusable for everyone

Publish Data & Tools:

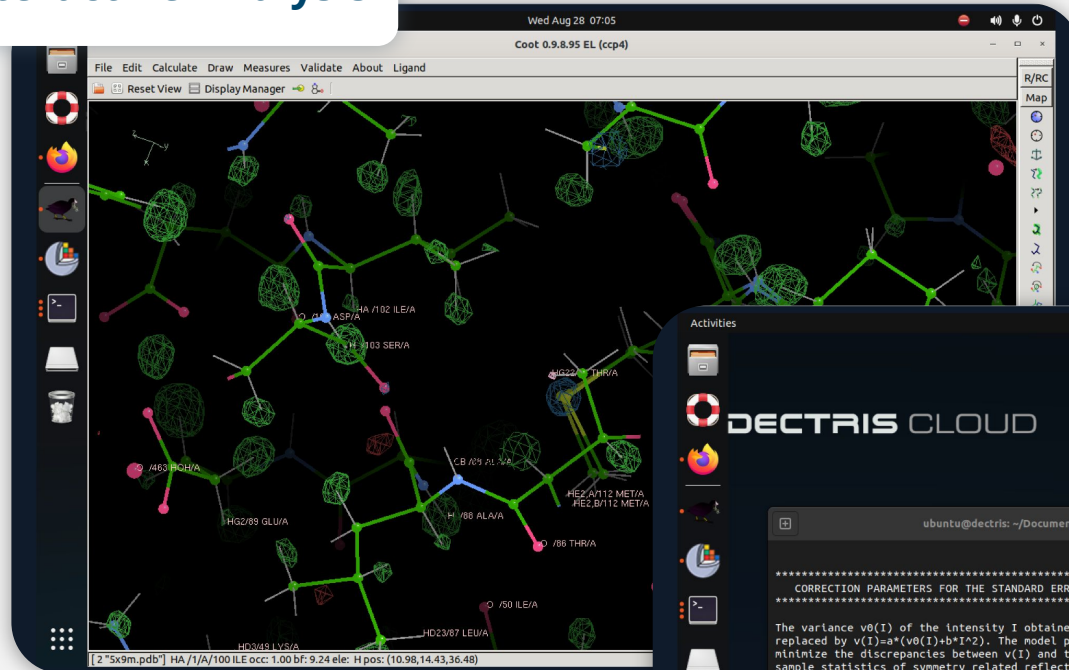


User Benefits:

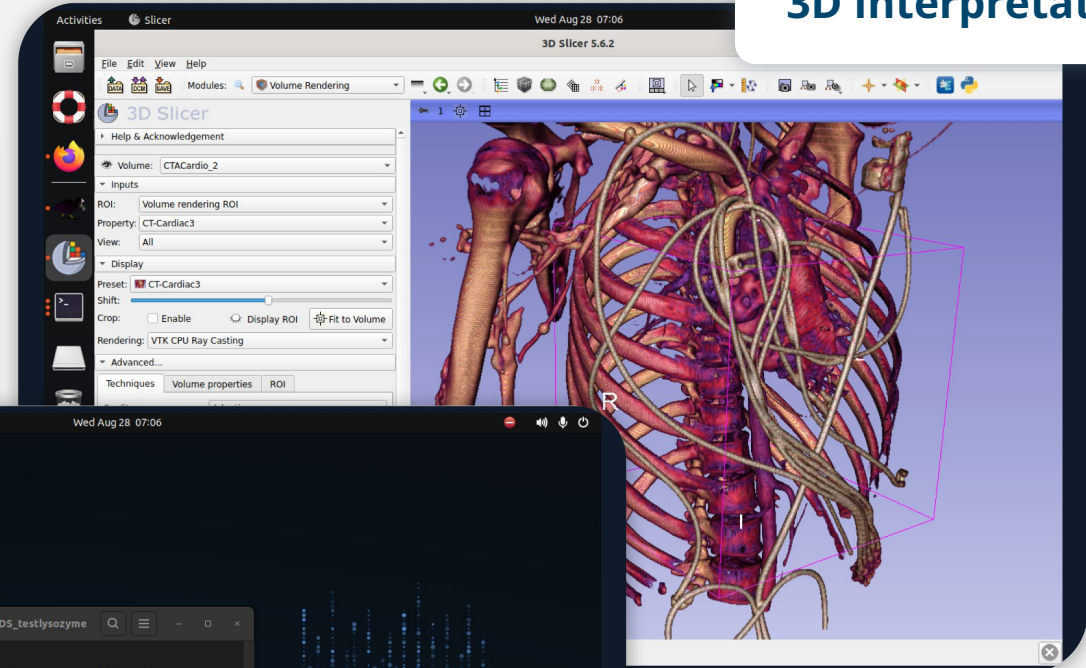
- + Sharing of data & software:
- + No data transfer
- + No software reinstallation

# Sessions: Run Virtual Machine in Cloud

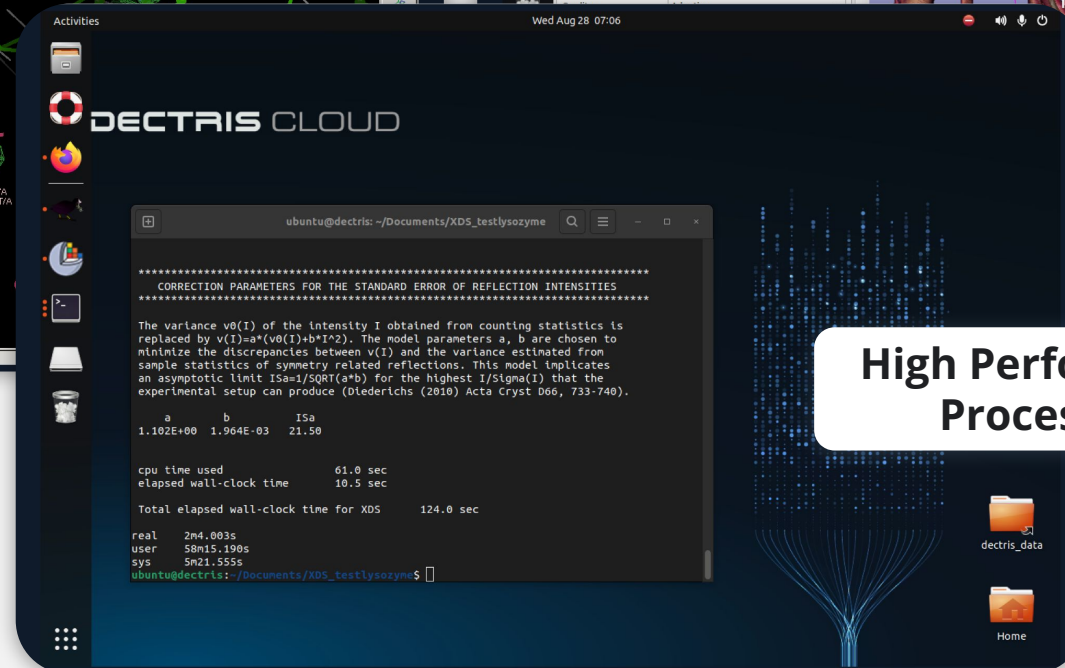
Interactive Analysis



3D Interpretation



High Performance Processing



Activities DECTRIS CLOUD Wed Aug 28 07:06

```
ubuntu@dectris: ~/Documents/XDS_testlysozyme
CORRECTION PARAMETERS FOR THE STANDARD ERROR OF REFLECTION INTENSITIES

The variance v0(I) of the intensity I obtained from counting statistics is
replaced by v(I)=a*(v0(I)+b*I^2). The model parameters a, b are chosen to
minimize the discrepancies between v(I) and the variance estimated from
sample statistics of symmetry related reflections. This model implicates
an asymptotic limit Isa=1/SQRT(a*b) for the highest 1/Sigma(I) that the
experimental setup can produce (Diederichs (2010) Acta Cryst D66, 733-740).

a      b      Isa
1.102E+00 1.964E-03 21.50

cpu time used      61.0 sec
elapsed wall-clock time 10.5 sec

Total elapsed wall-clock time for XDS      124.0 sec

real    2m4.003s
user    58m15.190s
sys     5m21.555s
ubuntu@dectris:~/Documents/XDS_testlysozyme$
```

# Sessions: Run Virtual Machine in Cloud

## Wizard: Starting Sessions

DECTRIS CLOUD >> Analysis / Sessions / Create

STEP 1: Create Session (Current) | STEP 2: Experiments | STEP 3: Summary | STEP 4: Confirmation

Enter an unique name to identify your session. Select the environment that best suits your needs. Configure your session's performance.

**Session Name**  
Enter a name for your session (max 25 characters).  
Name:

**Environment**  
Select the best environment for your session from the dropdown below.  
Select environment:

**Local Software Disk**  
Select the local storage disk that supports your session's software.  
Select storage:

**Performance**  
Please choose your performance instances.

- ☐ Turbo (CPU:32; RAM:128 GB; GPU:N/A)  
Optimized For Speed, Ideal For Real-Time Processing.
- ☐ Hypersonic (CPU:64; RAM:256 GB; GPU:N/A)  
Optimized For Speed, Ideal For Real-Time Processing.
- ☐ Hypersonic(Gpu) (CPU:64; RAM:256 GB; GPU:J)  
Optimized For Speed, Ideal For Real-Time Processing. GPU Included.
- ☒ Lightspeed (CPU:192; RAM:768 GB; GPU:N/A)  
Optimized For The Fastest Speed, Ideal For Real-Time Processing. High Performance GPUs Included.
- ☐ Lightspeed(Sapphire Rapids) (CPU:192; RAM:768 GB; GPU:N/A)  
Optimized For The Fastest Speed, Ideal For Real-Time Processing. High Performance GPUs Included.

Reset

← BACK | → NEXT STEP

## Management of Sessions

Dashboard | Sessions | Cockpit | Analysis | Team

**EM Session**  
Remaining: 8h 0m  
Running  
RUNNING SINCE: 0 days 0 hours 0 minutes  
Show logs  
RECONNECT | STOP

**TestSession**  
Stopped  
LAST USED: Jan 24, 2025  
Show logs  
START | DELETE

**Session Details**  
ID: 019497a2-d8aa-7d...  
Running  
**EM Session**  
Hypersonic; (CPU:64; RAM:256; GPU:n/a)  
Storage: 64 GB  
Environment Base:  
Name: Ubuntu Desktop  
ID: 019288a8-762e-7783-6235-1294d6abd35e  
Version: 0  
Running since: 0d 0h 0 min  
Show logs  
Experiments:  
EIGER at DECTRIS CLOUD  
Camilla Larsen  
Preparation  
CHANGE SETTINGS

## Custom Environments

The screenshot displays the DECTAIS Cloud user interface for creating a custom environment. The breadcrumb navigation at the top reads 'Analysis / Environments / Create'. The left sidebar contains navigation links for Data, Cockpit, Analysis (highlighted), and Team. The 'Analysis' section is expanded, showing 'Current Sessions', 'Create Session', 'Environments', and 'Jobs'. The 'Environments' section includes a 'Create Environment' button and a list of 'Environments'. The main content area shows a four-step process: STEP 1 Environment, STEP 2 Configuration (active), STEP 3 Summary, and STEP 4 Confirmation. The 'Configuration' step is titled 'Configuration' and includes the instruction 'Create an environment from a Docker container build script or from an existing session.' Below this, there are two options: 'Docker Container' (with a 'CREATE SCRIPT' button) and 'Interactive Session' (with a 'GO TO SESSIONS' button). A dashed yellow box highlights the 'Docker Container' option.

**Upcoming Feature:**  
Define environment from session

## Custom Environments

The screenshot shows the 'Create Environment' wizard in DECTAIS CLOUD, specifically Step 2: Configuration. The interface is dark-themed. On the left is a sidebar with navigation icons for Data, Cockpit, Analysis (active), and Team. The main area has a top navigation bar with 'Analysis / Environments / Create' and a user profile icon 'EW'. Below this is a progress bar with four steps: STEP 1 Environment, STEP 2 Configuration (active), STEP 3 Summary, and STEP 4 Confirmation. The 'Configuration' step is highlighted in blue. The main content area is titled 'Configuration' and includes the instruction 'Please provide a build script.' and a 'Reset to Default Dockerfile' link. A 'VALIDATE' button with a checkmark is present. A code editor displays a Dockerfile script: 

```
1
2 # Use the official Ubuntu base image
3 FROM ubuntu:22.04
4
5 # Set the maintainer label (optional)
6 LABEL maintainer="your_email@example.com"
7 # Update the package list and install some basic tools
8 RUN apt-get update && apt-get install -y \
9     curl \
10    wget \
11    vim \
12    && rm -rf /var/lib/apt/lists/*
13
14 # Set the working directory inside the container
15 WORKDIR /app
16
17 # Copy a file from the host machine to the container
18 COPY hello.sh /app/hello.sh
19
20 # Make the script executable
21 RUN chmod +x /app/hello.sh
22
23 # Set the command to run when the container starts
24 CMD ["/hello.sh"]
```

 To the right of the code editor is a section titled 'Your uploaded support file(s)' with the text 'You can upload any supporting files here.' and an 'UPLOAD FILES' button. At the bottom of the wizard are 'BACK' and 'NEXT STEP' buttons. A version indicator 'v0.2.8' is in the bottom left corner.

Configuration

Please provide a build script. [Reset to Default Dockerfile](#) [VALIDATE](#)

```
1
2 # Use the official Ubuntu base image
3 FROM ubuntu:22.04
4
5 # Set the maintainer label (optional)
6 LABEL maintainer="your_email@example.com"
7 # Update the package list and install some basic tools
8 RUN apt-get update && apt-get install -y \
9     curl \
10    wget \
11    vim \
12    && rm -rf /var/lib/apt/lists/*
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14 # Set the working directory inside the container
15 WORKDIR /app
16
17 # Copy a file from the host machine to the container
18 COPY hello.sh /app/hello.sh
19
20 # Make the script executable
21 RUN chmod +x /app/hello.sh
22
23 # Set the command to run when the container starts
24 CMD ["/hello.sh"]
```

Your uploaded support file(s)  
You can upload any supporting files here.

[UPLOAD FILES](#)

[← BACK](#) [→ NEXT STEP](#)

**Upcoming Feature:**  
Integration with GIT automation

# DECTAIS CLOUD

DECTAIS CLOUD >> Analysis / Environments / 01946945 18b3 79f0 A831 96800c76eb44

Analysis

Dashboard

Sessions

Current Sessions

Create Session

Environments

Create Environment

Environments

Jobs

Create Job Template

Job Templates

Jobs

+ FILTER

Search by Environment ID or Name...

+ CREATE NEW ENVIRONMENT

NAME	VERSION	OS	AUTHOR	TYPE	TECHNIQUE
XDS	0	ubuntu:22.04	Camilla Larsen	Shared	MX
Ubuntu Desktop	0	Ubuntu 22.04	dectris	Public	

Environment Details

ID: 01946945-18b3-79f0-a...

Shared

### XDS

XDS (X-ray Detector Software), VERSION Jun 30, 2024 BUILT=20241002. Author: Wolfgang Kabsch.  
<https://xds.mr.mpg.de/>. For h5 files, neggia and durin plugins are located at /opt/xds/dectris-neggia.so and /opt/xds/durin-plugin.so. Execute by supplying XDS.INP input file and running 'xds' or 'xds\_par' in the command line. For academic use only.

See Build Output

Version

v0 Previous

Technique OS

MX ubuntu:22.04

Latest Update Licence

Jun 15, 2025 N/A

START SESSION

Ludmila Leroy Max Burian Pascal Störzbach

Daphne van Dijken Daniel Heid Patrik Skuza

v0.4.0

Management of  
Environments

Upcoming Feature:  
Global Environments





Data

Cockpit

Analysis

Team

v0.4.1

Analysis

Dashboard

Sessions

Current Sessions

Create Session

Environments

Create Environment

Environments

Jobs

Create Job Template

Job Templates

Jobs

NAME

VERSION

OS

AUTHOR

TYPE

TECHNIQUE

TexTom

22

ubuntu:22.04

Camilla Larsen

Private

Texture Tomography

stress test file system

0

ubuntu:22.04

Camilla Larsen, Ludmila Leroy, Max Burian, Daniel Heid, Pascal Störzbach, Patrik Skuza

Shared

file reading

Podman test

0

ubuntu:22.04

Camilla Larsen

Private

test

4D-STEM DECTRIS

6

ubuntu:22.04

Ludmila Leroy, Daniel Stroppa, Camilla Larsen

Shared

4D-STEM

Environment Details

ID: 0194fabd-a395-7191-b...

Shared

4D-STEM DECTRIS

A DECTRIS environment for 4D-STEM data analysis

See Build Output

Version

v6

Previous

v6

remove extensions again, that does not work

v5

add jupyter lab and try to add vscode extensions once again

v4

back to version 2

v3

add vscode

## Version history of Environments

# Notebooks: Jupyter Lab

Ready in April '25

Classic Jupyter  
Notebooks

The screenshot displays the DECTRIS CLOUD Jupyter Lab interface. The top bar shows the DECTRIS CLOUD logo and the 'Analysis' tab. The left sidebar contains a file explorer with a list of files and folders: 'audio', 'images', 'Cpp.ipynb', 'Data.ipynb', 'Fasta.ipynb', 'Julia.ipynb', 'Lorenz.ipynb' (selected), 'lorenz.py' (selected), and 'R.ipynb'. The main area is divided into three panes. The top pane shows the code editor for 'Lorenz.ipynb' with the following code:

```
[2]: from lorenz import solve_lorenz
w=interactive(solve_lorenz,sigma=(0.0,50.0),rho=(0.0,50.0))
w
```

The middle pane shows the 'Output View' with interactive sliders for 'sigma' (10.00), 'beta' (2.63), and 'rho' (28.00). The bottom pane shows the 'lorenz.py' file with the following code:

```
1 from matplotlib import pyplot as plt
2 from mpl_toolkits.mplot3d import Axes3D
3 import numpy as np
4 from scipy import integrate
5
6 def solve_lorenz(sigma=10.0, beta=8./3, rho=28.0):
7     """Plot a solution to the Lorenz differential
8     equations."""
9
10     max_time = 4.0
11     N = 30
12
13     fig = plt.figure()
14     ax = fig.add_axes([0, 0, 1, 1], projection='3d')
15     ax.axis('off')
```

The bottom status bar shows 'Simple' mode, '1' tab, '3' files, 'Python' kernel, and 'Ln 1, Col 1 Spaces: 4 lorenz.py 0'.

Custom **Jobs** running in Environment

The screenshot displays the DECTRAIS CLOUD web interface. On the left is a sidebar with navigation icons for Data, Cockpit, Analysis (selected), and Team. The main header shows the breadcrumb 'Analysis / Jobs / Templates / Create'. Below this is a progress bar with four steps: STEP 1 Job Template, STEP 2 Configuration (active), STEP 3 Save, and STEP 4 Confirmation.

The 'Configuration' step is divided into two panels. The left panel, titled 'Please provide a build script.', contains a text editor with a bash script. The right panel, titled 'Input Variables', features a table for defining variables and an upload section for support files.

**Build Script:**

```

1 #!/bin/bash
2 set -euo pipefail
3
4 # Print key environment variables
5 echo "JOB_OUTPUT_DIR: $JOB_OUTPUT_DIR"
6 echo "JOB_WORK_DIR: $JOB_WORK_DIR"
7
8 # Show an input variable
9 echo "Input Variable DC_EXAMPLE_VAR: ${DC_EXAMPLE_VAR:-not defined}"
10
11 # Configuration files are only available for reading
12 SUPPORTING_FILE="$JOB_WORK_DIR/configuration_file.txt"
13 if [ ! -f "$SUPPORTING_FILE" ]; then
14     echo "Error: configuration_file.txt not found. Please upload it."
15     exit 1
16 fi
17
18 # Use JOB_WORK_DIR for temporary data
19 echo "temp data" > "$JOB_WORK_DIR/data.txt"
20 WORD_COUNT=$(wc -w < "$JOB_WORK_DIR/data.txt")
21
22 # Store results in JOB_OUTPUT_DIR
23 echo "Word count: $WORD_COUNT" >> "$JOB_OUTPUT_DIR/final_results.txt"
  
```

**Input Variables Table:**

VARIABLE	VALUE	TYPE	ACTIONS
DC_EXAMPLE_VAR	example value	String	[icon]

Below the table is a button 'ADD NEW INPUT VARIABLE' and a section 'Your uploaded support file(s)' with an 'UPLOAD FILES' button.

At the bottom of the interface are 'BACK' and 'NEXT STEP' buttons.

coming soon!



# DECTRAIS CLOUD

## Overview of job templates

Data

Cockpit

Analysis

Team

Analysis

Dashboard

Sessions

Current Sessions

Create Session

Environments

Create Environment

Environments

Jobs

Create Job Template

Job Templates

Jobs

+ FILTER

Search by Template Name or Creator...

STATUS	NAME	VERSION	ENVIRONMENT	TYPE	CREATORS
Unvalidated	XDS test 2	0	XDS test	private	Claudia Green
Unvalidated	job	0	Ubuntu Desktop	private	Claudia Green
Unvalidated	xxx	0	Ubuntu Desktop	private	Claudia Green
Unvalidated	ccc	0	Ubuntu Desktop	private	Claudia Green
Unvalidated	test basic job w xds	0	XDS test	private	Claudia Green
Unvalidated	Another XDS test 2	0	XDS test	private	Claudia Green

Job Template Details

ID: 0194ffae-64fa-7ee1-a...

Private

Unvalidated

XDS test 2

test

Version

v0Previous

Environment

XDS test

Latest Update

Feb 13, 2025

Creators - Edit

Claudia Green

Explorers: - Edit

Add user +

SHOW JOBS

coming soon!



## Run Jobs

### Run Job

Set up your Job Template Parameters in order to run a job.

#### Data File(s)

Data SourceValue

PATH

	TextTOM benchmarking		Global Phasing refere...
	PARP4		TomH - Internship Dat...
	Serial crystallography ...		another EM exp
	MicR - Internal AI Expe...		TestTile
	DECTRIS CLOUD with ...		DELETE ALL FILES HERE

#### Machine Type

free:(CPU: 2;RAM:4 GB;GPU: n/a)

#### Input Variables

Form

JSON view

VARIABLE	VALUE	TYPE
DC_ INPUT_PATH	/dectris_data/DECTRIS/	String
DC_ NJOB	8	Number
DC_ NRPOC	8	Number
DC_ NDELPHI	50	Number
DC_ NCACHE	51	Number

#### Uploaded support file(s)

You can edit text files and view other files

XDS.INP

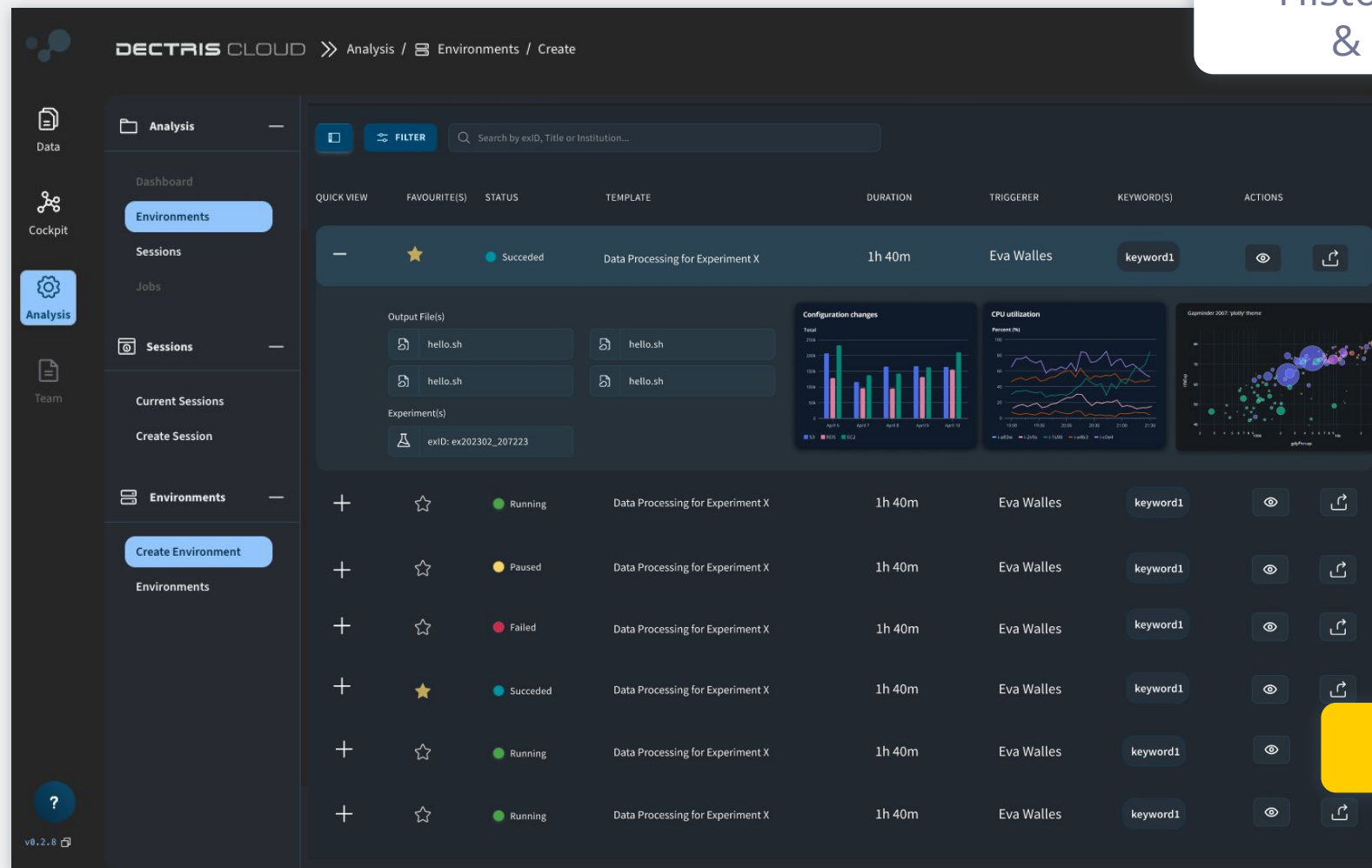
?

← NO, TAKE ME BACK

▶ RUN JOB

coming soon!

## History of Jobs & Results



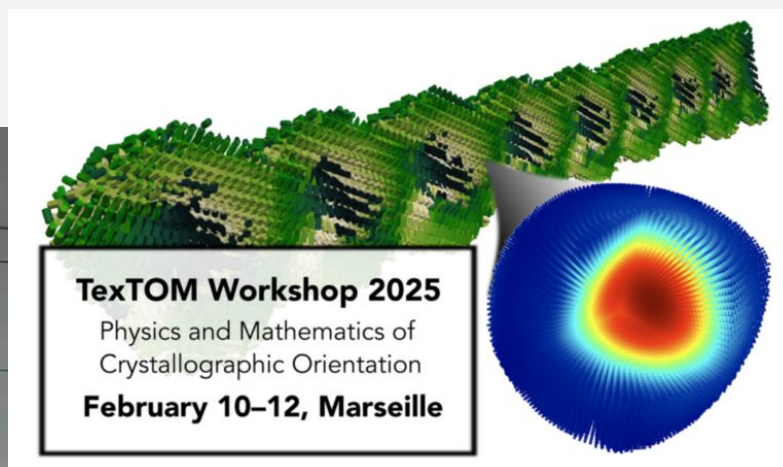
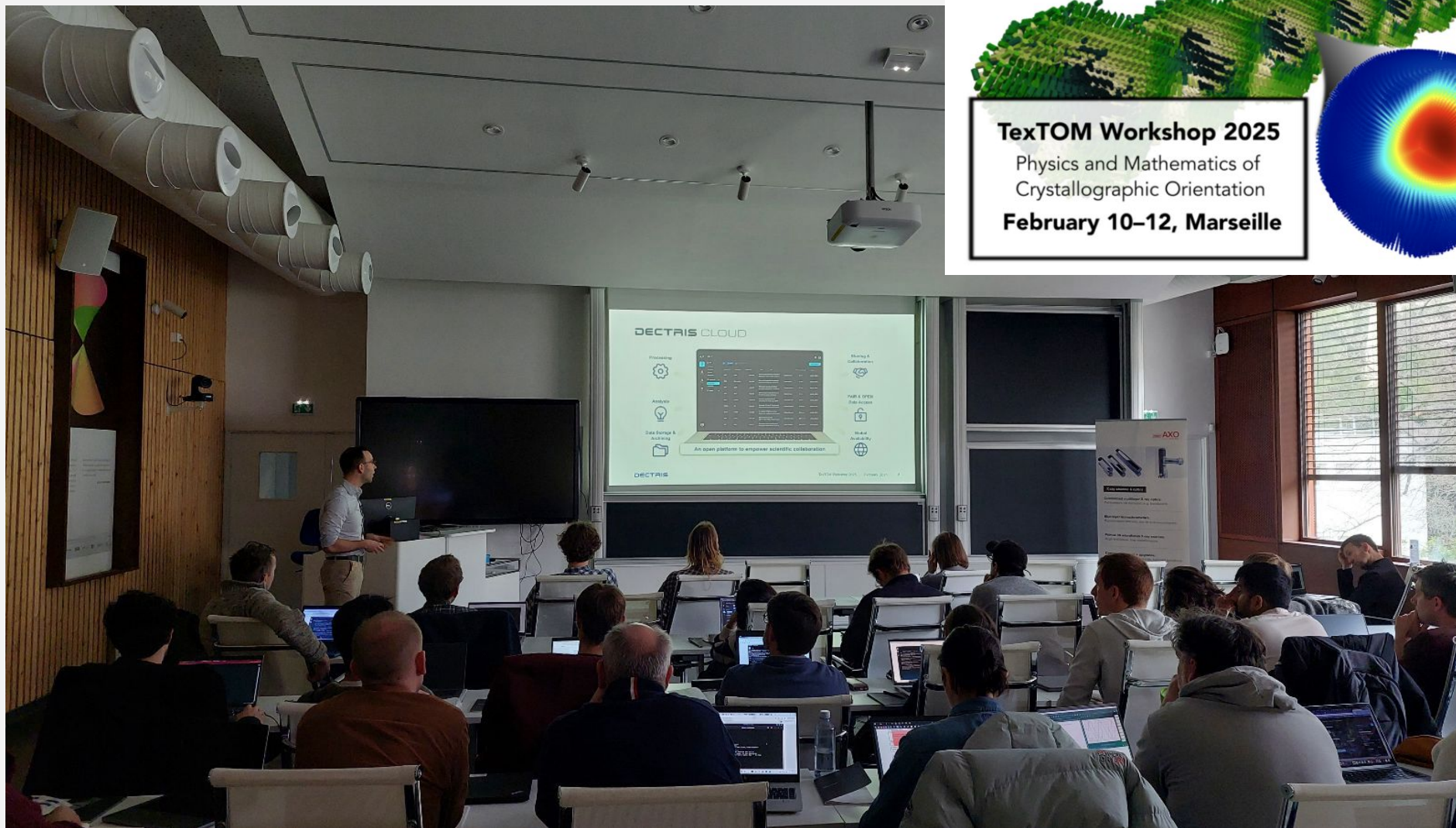
coming soon!



# Examples



# TexTOM workshop 2025





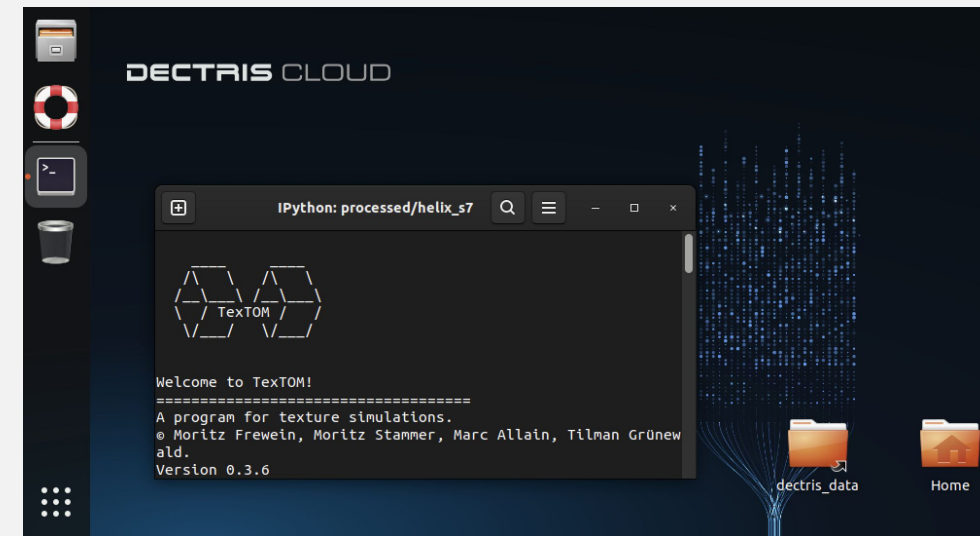


# TexTOM workshop 2025

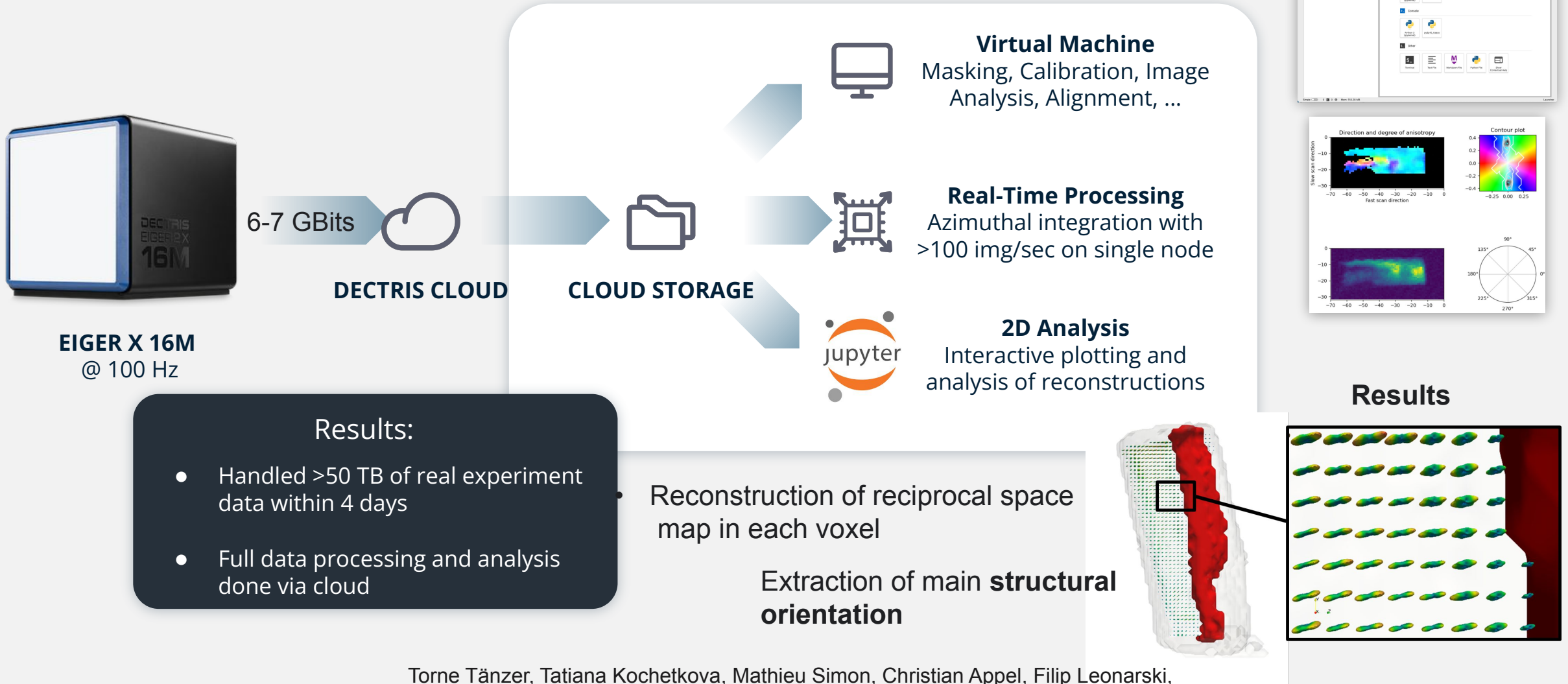
- 44 participants
- DECTRIS CLOUD Supported tutorial session:
  - Simultaneous access to a 150 GB synchrotron data set on the cloud
  - Each participant should be able to independently experience the full scientific pipeline

⇒ Scalable compute power (2500 simultaneous CPUs)

⇒ Easy access to scientific software (containers)



# PX1 - Data Processing Pipeline



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

# microMAX - Massive Data Upload

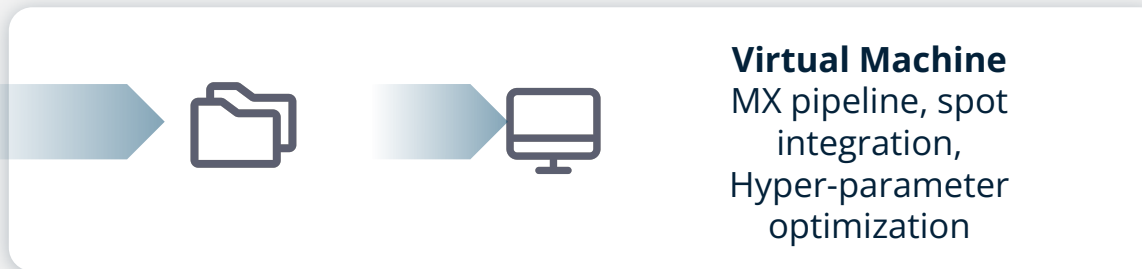


**JUNGFRAU 4M**  
@ 2 kHz

25 GBits



DECTRIS CLOUD



## BL 8.3.1 - MX pipelines

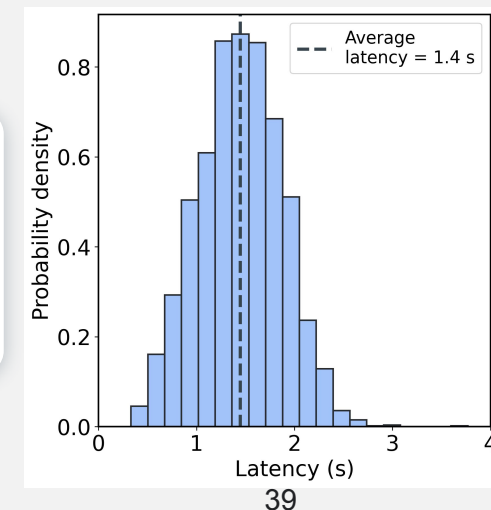
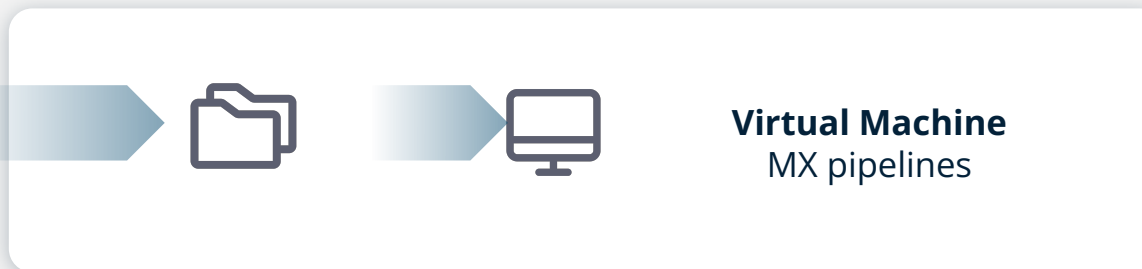


**Pilatus3 S 6M**  
@ 100 Hz

1 GBits



DECTRIS CLOUD



DECTRIS  
CLOUD

# Thank You!

Reach out via  
[camilla.larsen@dectris.com](mailto:camilla.larsen@dectris.com)

[dectris.cloud](https://dectris.cloud)

or

