DECTRIS CLOUD

White paper

DECTRIS CLOUD at Synchrotron Facilities

Three case studies on Integration and Performance

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Section 2 of this white paper describes functionality of the DECTRIS CLOUD platform and the different ways data upload to the cloud can be facilitated. Specific implementation examples are given in section 3, while the appendix in section 4 gives concrete step-by-step instructions for each implementation example.

1. Introduction

The DECTRIS CLOUD platform [1], launched in August 2024 [2], addresses the increasing challenges of managing and extracting insights from the huge data volumes generated by modern synchrotron experiments. Recent advances in hybrid photon-counting (HPC) detectors have driven orders-of-magnitude increases in data rates, straining beamline storage, transfer, and processing pipelines [3], [4], [5], [6], [7], [8]. Next-generation detectors such as JUNGFRAU and SELUN now run at kilohertz to hundreds-of-kilohertz frame rates, producing raw streams in the tens of gigabytes per second. For example, a JUNGFRAU 4-megapixel detector delivers 17 GB/s at 2 kHz [7], while SELUN's full-readout mode (190 × 190 px, 32 bit, 30 kHz) generates a raw stream of about 4 GB/s [9]. As synchrotrons upgrade to diffraction-limited sources and higher-brilliance beams, the associated gains in flux, resolution, and time-resolved acquisition will push data rates well beyond the limits of conventional on-premise storage and compute infrastructure. DECTRIS CLOUD mitigates this bottleneck by streaming data directly to elastic cloud resources, enabling real-time analysis and scalable, cost-controlled storage.

To manage the significant data rates produced by synchrotron and X-ray Free Electron Laser (XFEL) detectors, facilities have begun adopting cloud-based solutions for data handling, analysis, and remote access. Platforms such as VISA (Virtual Infrastructure for Scientific Analysis) provide researchers with virtual desktop environments, facilitating remote data analysis and experiment control [10]. CryoCloud, specifically designed for cryo-electron microscopy, offers cloud-native GPU-accelerated data processing, eliminating the need for local high-performance computing infrastructure [11]. Additionally, initiatives like PaNOSC and ExPaNDS have promoted FAIR (Findable, Accessible, Interoperable, Reusable) data standards across facilities, enhancing collaboration and data sharing in the scientific community [12].

DECTRIS CLOUD proposes a new way of handling scientific data by enabling efficient data streaming for online analysis, automated storage management, and scalable cloud-based processing, ensuring that beamlines can keep pace with the rapidly evolving landscape of high-speed X-ray science. Being accessible through a web application, DECTRIS CLOUD offers an intuitive interface that allows researchers to interact with their data remotely. This significantly reduces the reliance on local computational infrastructure and makes data analysis workflows available to a wider range of users, regardless of their level of expertise in data management or software development.

In this white paper, we (i) detail how DECTRIS CLOUD integrates with synchrotron beamlines to enable rapid data upload and immediate cloud-based analysis; (ii) outline key features available through the web application; and (iii) illustrate the platform's flexibility via three commissioning experiments carried out at distinct macromolecular-crystallography beamlines: microMAX (MAX IV, SE), BL 8.3.1 (ALS, US) and P14 (PETRA III, DE). Our aim is to show that bringing a beamline online is a straightforward, low-risk step toward faster, insight-driven science.

2. DECTRIS CLOUD Integration Approaches

2.1 Upload Configuration

Efficient integration of DECTRIS CLOUD at a beamline involves two key aspects: (i) establishing reliable methods for uploading experimental data to the cloud, and (ii) enabling workflows on the DECTRIS CLOUD platform for managing experiments, curating data, and providing users with tools to visualize, analyze, and interact with data.

For the initial beamline data upload, DECTRIS CLOUD offers two distinct approaches: DECTRIS CLOUD HUB, a high-performance hardware solution facilitating direct and efficient data transfers, and DECTRIS CLOUD SYNC, a flexible software-based solution suitable for simpler integration requirements.

2.1.1 Upload via DECTRIS CLOUD HUB

The DECTRIS CLOUD HUB (DC-HUB) is a dedicated server equipped with substantial RAM and specialized software for securely handling high-speed synchrotron detector data. Acting as both a data orchestrator and local buffer, the DC-HUB facilitates continuous and secure transfers to DECTRIS CLOUD storage. The DC-HUB efficiently manages sustained, gigabyte-scale data streams, providing minimal latency and uninterrupted uploads via internal RAM-based buffering, even during network disruptions.

2.1.2 Upload via DECTRIS CLOUD SYNC

DECTRIS CLOUD SYNC is standalone software designed to automate data uploads from local storage to DECTRIS CLOUD. Running quietly in the background as a daemon (background service), SYNC monitors specified directories on the local computer or server and uploads new data files as they arrive. It ensures data integrity through real-time encryption and authentication, securely assigning data to the active experiment configured via a license file.

By default, DECTRIS CLOUD SYNC monitors directories such as /opt/dectris/cloud_sync/raw and /opt/dectris/cloud_sync/work, which can be customized or extended in its configuration file located at /etc/dectris/dectris_sync.conf. Laboratory staff can conveniently activate or deactivate SYNC via the DECTRIS CLOUD web application or API, offering straightforward data management adaptable to various laboratory infrastructures and operational contexts.

Technical requirements for DECTRIS CLOUD SYNC are minimal. The local facility must ensure a dedicated user account with sufficient permissions to run the daemon and access the specified directories. Running DC-SYNC involves simply executing the provided binary, requiring no additional installations or dependencies on the beamline computer.

2.2 Web Application Functionality

2.2.1 Experiment Management and Data Curation

Once the data upload has been configured on the facility side, the destination of the data must also be set up within the DECTRIS CLOUD platform. Integrated beamlines each have a dedicated cockpit in DECTRIS CLOUD, which is a space offering an overview of ongoing experiments, data uploads, detectors, HUBs, cloud storage, and computational resources (Fig. 1). Each connected beamline can at any given time have one active experiment, which defines the destination of data uploaded either via the DECTRIS CLOUD HUB or SYNC software. From the cockpit area, beamline scientists manage active experiments, initiate new experiments, and define access permissions for users. Alternatively, API tokens can be generated for integrating experiment management directly into beamline control systems [13].

The DECTRIS CLOUD platform organizes experiment data in structured directories, containing folders such as raw data, processed results, and auxiliary files, alongside a logbook for recording experimental details. Laboratory scientists can grant experiment-specific access to external users, enabling collaborative data review and analysis.

For installation, the DC-HUB is physically positioned at the beamline or in a server room, and connected to the local network to receive data from the local data storage. DC-HUB is designed to receive data with no need for communication back to the local network such that all incoming traffic from the DC-HUB can be blocked, for secure integration.

Data upload from the DC-HUB to the cloud can occur either through a dedicated high-bandwidth uplink managed by DECTRIS to ensure latency as low as <3s, or via the facility's existing local infrastructure. If the facility chooses to use its own infrastructure, the facility must assign the DC-HUB a suitable IP address to ensure it has external network access required for data uploads.

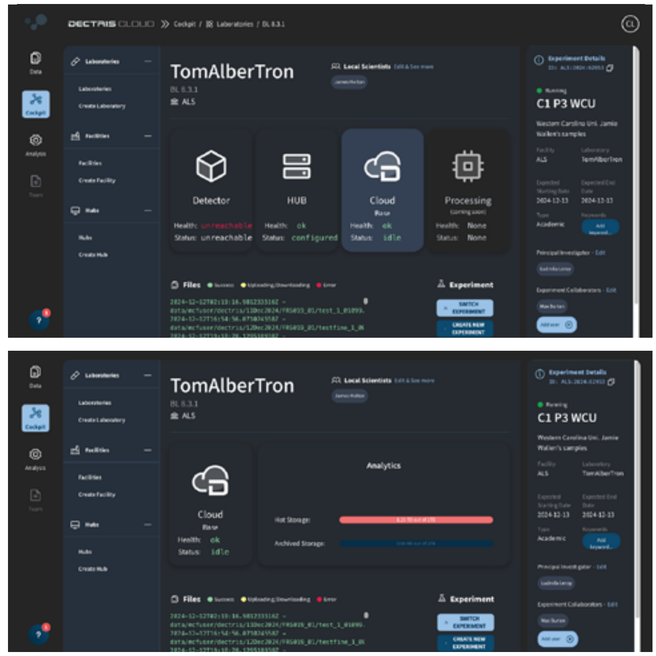

Figure 1: The cockpit page of a beamline, providing a status overview of various services and recently uploaded files for the current or last active experiment. Local beamline scientists can create or switch experiments directly from this interface. Expandable panels, such as the cloud panel, offer quick insights into current usage of hot and archive storage.

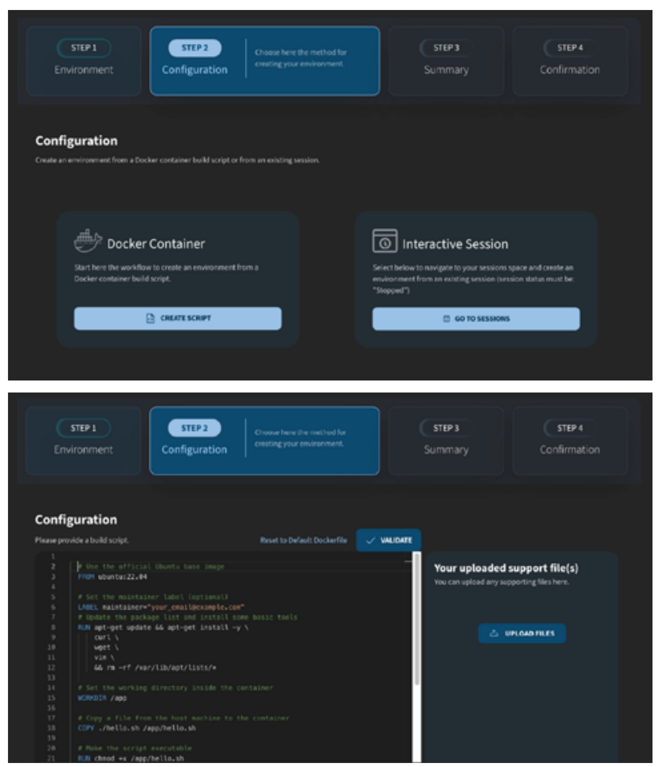

Figure 2: Examples of the environment creation pages, showing the initial configuration page (top) as well as the Docker-based environment configuration page (bottom).

2.2.2 Shareable Analysis Tools

DECTRIS CLOUD includes comprehensive analytical tools accessible through its web application, offering users flexible options for data processing and analysis. Users can launch virtual machine environments ("Sessions") or execute predefined analysis workflows ("Job Templates") seamlessly within the platform. Analysis environments consist of versioned containers ("Environments") with pre-installed scientific software and can be created either by defining a Dockerfile (see Fig. 2) or by configuring software within a session and saving the session as a reusable environment.

Environments and Job Templates can be shared among users, providing ready-to-use analytical tools specific to each beamline's datasets. While sessions offer private computational spaces granting users complete autonomy over resource usage, Jobs offer simple, point-and-click workflows launched directly from the web application. Results from Jobs, including curated plots and output files, are conveniently accessible via a job overview table and stored in the "processed" directory within the experiment folder, visible to all experiment collaborators. Examples of session and job workflows are shown in Fig. 3.

3 Commissioning Case Studies

3.1 MicroMAX at MAX IV

3.1.1 Beamline specification

The MicroMAX beamline at the MAX IV Laboratory in Sweden is a high-brilliance macromolecular crystallography (MX) beamline dedicated to collecting diffraction data from challenging protein crystals with micrometer dimensions. Designed specifically for structural biology applications, MicroMAX employs focused, highly coherent X-ray beams that facilitate high-resolution, rapid data collection from microcrystals [14].

During the commissioning of DECTRIS CLOUD at MicroMAX, the beamline was equipped with a JUNGFRAU 9M detector [15]. The JUNGFRAU detector is a hybrid photon-counting detector known for its exceptional sensitivity, dynamic range, and low-noise performance. It is particularly suited for high-speed experiments requiring accurate photon counting and high frame rates. The 9M variant of the JUNGFRAU detector comprises nine individual detector modules, collectively offering an active area suitable for capturing diffraction data efficiently at high temporal resolution.

3.1.2 Data upload from the JUNGFRAU Detector

Before the commissioning experiment at MicroMAX, a dedicated 100 Gbit/s DECTRIS CLOUD internet uplink was installed at the beamline, ensuring sufficient bandwidth to handle the high data rates of the JUNGFRAU detector. A DECTRIS CLOUD HUB was shipped and installed onsite, where it was connected directly to the provided uplink and also had a local one-way connection to MAX IV's internal data server.

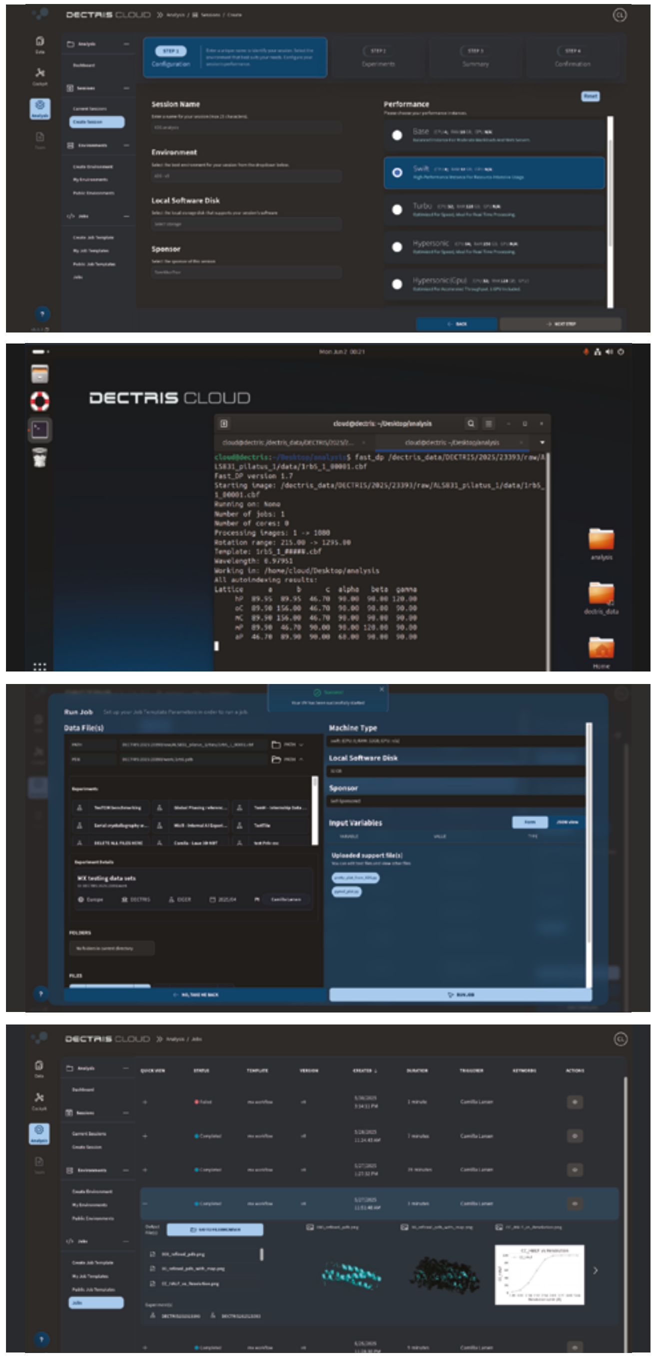

Figure 3: Examples of analysis workflows available on the platform, showing (first): configuring a session and choosing its performance type before starting, (second) a running session, (third) the menu for launching a job, and (fourth) the output of a Job.

Data acquisition and streaming from the detector were handled by JUNGFRAUJOCH, a modular software platform developed by PSI specifically for JUNGFRAU detectors [7]. JUNGFRAUJOCH acquires detector frames, performs real-time corrections and compression, and streams data using ZeroMQ sockets. For the DECTRIS CLOUD commissioning at MicroMAX, JUNGFRAUJOCH's built-in capability to daisy-chain data streams was leveraged by using two file writers in series: the primary writer captured and stored data locally at high speed, while a secondary writer simultaneously received the data stream and wrote files directly to the DECTRIS CLOUD HUB for rapid upload to the cloud. This integrated configuration enabled simultaneous local backup and near-real-time cloud-based analysis, significantly streamlining remote data access and processing workflows.

3.2 BL 8.3.1 at ALS

3.2.1 Beamline specification

Beamline 8.3.1 at the Advanced Light Source (ALS), located in the United States, is dedicated to macromolecular crystallography experiments requiring high-resolution structural determination [16]. Data collection at this beamline typically occurs over just a few minutes, enabling high-throughput workflows and efficient data generation. The beamline is optimized for rapid and automated data acquisition, supported by robotic sample-changing systems and remote experiment monitoring capabilities. BL 8.3.1 is equipped with a DECTRIS Pilatus3 S 6M detector, which provides a maximum frame rate of up to 100 Hz.

3.2.2 Data upload from the local file system

The primary objective of the ALS commissioning experiment was to demonstrate that DECTRIS CLOUD could be seamlessly integrated at an existing beamline, offering users the flexibility to easily enable or disable cloud-based workflows as required.

Unlike the MicroMAX experiment, a dedicated internet uplink provided by DECTRIS was not installed at ALS, as sufficient bandwidth for the experiment was already provided locally by the ESnet [17]. However, a DECTRIS CLOUD HUB and accompanying router were installed onsite at the beamline. Rather than directly interfacing with the detector control unit, data was transferred from the beamline's existing local data server to the CLOUD HUB using an rsync-based bridge. This integration approach required no physical adjustments to the beamline's detector or cabling infrastructure, and allowed uploads to DECTRIS CLOUD to be easily toggled via the DECTRIS CLOUD cockpit web interface or locally by pausing the rsync process.

During the commissioning period, several protein crystallography datasets were collected at frame rates of 50–100 Hz, achieving consistent data transfer rates of approximately 1 Gbit/s, comfortably handled by the CLOUD HUB. Additionally, the latency between local data acquisition and cloud availability for analysis was systematically measured (see Fig. 4), revealing a typical latency under 3 seconds per dataset and an average latency of just 1.4 seconds.

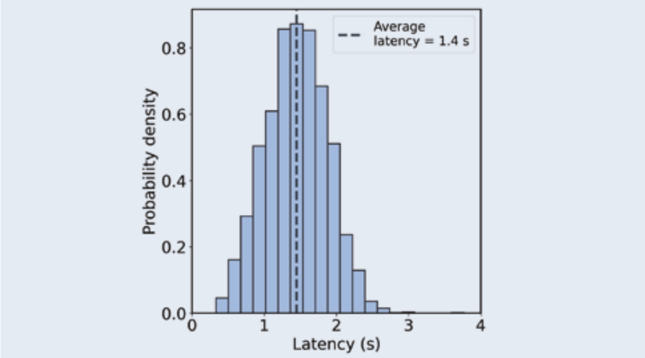

Figure 4: Histogram of file latencies measured at beamline 8.3.1, estimated from the time difference between the creation time stamp of each file and the time they were first viewable in a virtual machine mounted to the experiment.

3.3 P14 at EMBL

3.3.1 Beamline specifications

Beamline P14 at EMBL Hamburg, located at the PETRA III synchrotron at DESY in Hamburg, Germany, is dedicated to high-resolution macromolecular crystallography [18]. It provides interchangeable beam conditions, from a 2 × 6 μm² micro-beam to a collimated beam up to 300 μm, and is tunable 7–20 keV (26.7 keV on request). The station is equipped with a DECTRIS EIGER2 CdTe 16M detector, delivering 133 Hz full-frame or 750 Hz in 4M ROI (16/32-bit), with optional 8-bit modes of 280 Hz and 1120 Hz, enabling high-speed data collection for demanding structural-biology experiments.

3.3.2 Data upload from the local filesystem

A DECTRIS CLOUD HUB was installed at beamline P14 without a dedicated internet uplink, as the existing shared bandwidth at the facility was anticipated to sufficiently handle the data rates generated by the EIGER2 detector. Similar to the ALS commissioning, data was initially stored on the local filesystem before being copied to the DECTRIS CLOUD HUB, which then transferred the data directly to the cloud. During a remote measurement campaign, standard rotational crystallography datasets from more than 25 samples were successfully uploaded to DECTRIS CLOUD. Simultaneous data analysis was performed remotely using the exploratory sessions, employing predominantly ADXV, XDS and autoPROC software. The observed data rates remained below 1 Gbit/s, allowing reliable and efficient uploads via the facility's shared network connection.

4. Appendix: Step-by-Step Instructions

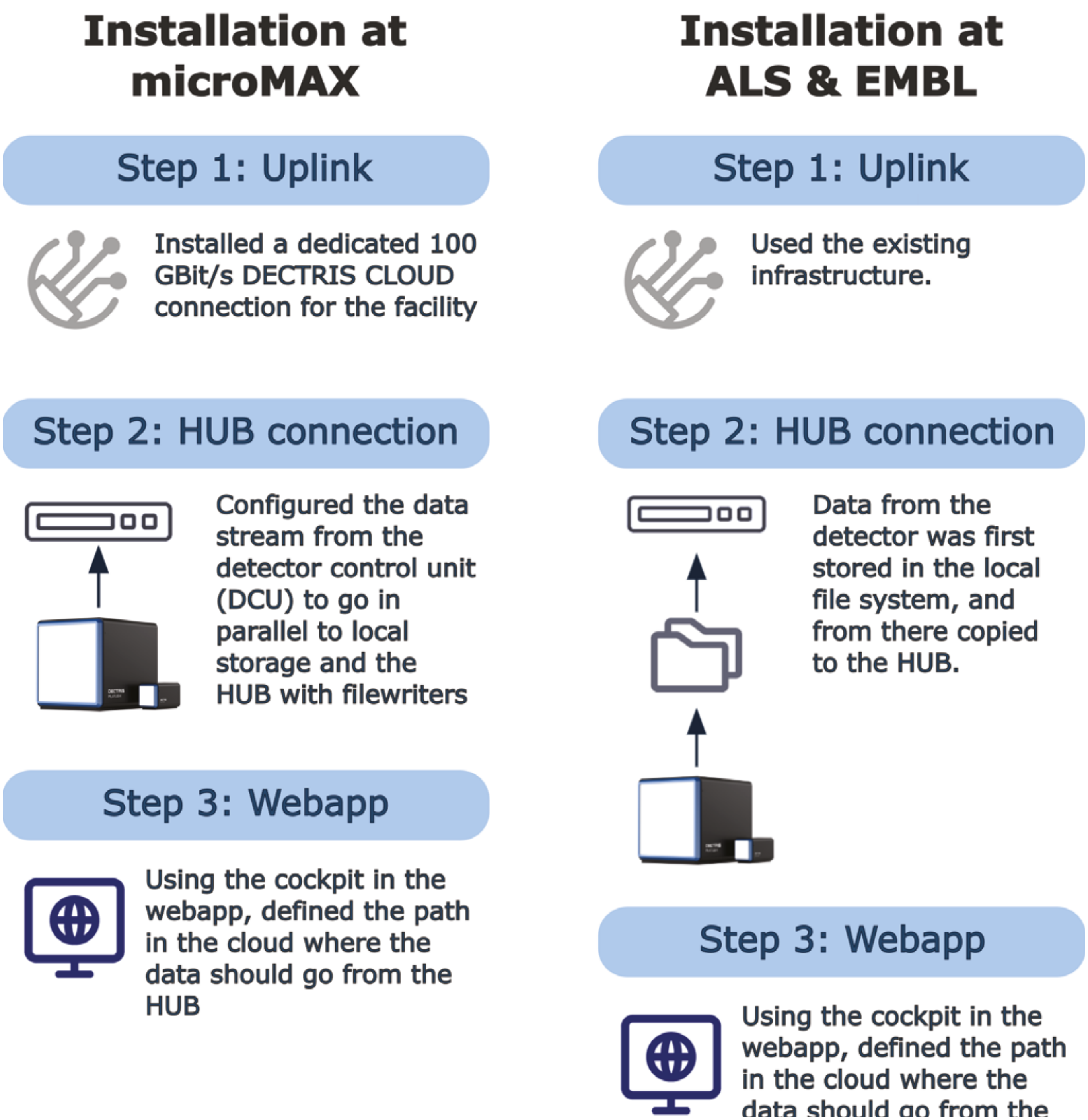

Figure 5: Schematic overview of how DECTRIS CLOUD was enabled at the different test beamlines. In all cases, the integration was performed by (i) ensuring enough bandwidth, (ii) installing and configuring the HUB, and (iii) configuring a path in the cloud, either through the cockpit or via an API call, where the data should go from the HUB. With the newer DECTRIS SYNC feature, the HUB hardware installation can be skipped in favor of a software installation of a program that facilitates the upload.

5. Conclusions

As demonstrated by the commissioning experiments conducted across different beamlines, integrating DECTRIS CLOUD into synchrotron facilities is straightforward, involving minimal configuration steps: ensuring adequate bandwidth, connecting the DECTRIS CLOUD HUB, and specifying file destinations within the cloud platform. Uploading data from local file systems not only provides facilities with the flexibility of retaining local data copies but also underscores the detector-agnostic nature of DECTRIS CLOUD, as it seamlessly integrates data from both DECTRIS and non-DECTRIS detectors. This latter workflow can also be enabled by the DECTRIS CLOUD SYNC software uploader, requiring no hardware to be shipped or installed.

The ease with which cloud uploads can be activated or deactivated, highlights the versatility of DECTRIS CLOUD as an optional, user-driven service. Consequently, DECTRIS CLOUD represents an accessible, easily deployable solution that empowers researchers to remotely access experimental data and leverage streamlined, cloud-based analysis workflows from anywhere in the world.

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