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Unified Data Access and Visualization Framework for Photon Science

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Modern photon science facilities such as European XFEL [1], PETRA III [2], BESSY II [3], ESRF-EBS [4], FLASH [5] and FELBE [6] generate data volumes that pose significant challenges for external users, particularly at universities with limited storage and network capabilities. Traditional data access models based on bulk data transfer are increasingly impractical and hinder efficient scientific workflows. In this work, we present the initial design and prototype implementation of a service that enables scalable, selective access to large-scale experimental data. Our approach is based on the Bluesky / Tiled [7] [8] ecosystem and focuses on server-side data slicing and transformation, allowing users to retrieve only the subsets of data required for their analysis. In addition, the system supports on-the-fly data conversion, translating facility-specific data formats into representations optimized for visualization or downstream analysis pipelines at the client side. This reduces bandwidth requirements and eliminates the need for local replication of large datasets while improving interoperability across heterogeneous environments. We describe the system architecture and first proof-of-concept results using representative datasets from photon science beamlines. Initial evaluations demonstrate the feasibility of authenticated and anonymous access, selective data transfer, dynamic data transformation, and integration with common client environments. The presented work lays the foundation for a three-year project funded by the German Federal Ministry, aiming to provide efficient, FAIR-aligned data access for a broad scientific community and to bridge the gap between large-scale research infrastructures and resource-constrained users.

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1. Introduction

1.1 Motivation

Modern photon science facilities such as European XFEL [1], PETRA III [2], BESSY II [3], ESRF-EBS [4], FLASH [5], and FELBE [6] generate rapidly growing data volumes that are increasingly difficult to access and process outside dedicated infrastructure environments. This challenge is expected to intensify further with upcoming facility upgrades such as PETRA IV, BESSY III, and DALI. In particular, universities and smaller research groups often lack the storage and network capacity required for traditional bulk data transfer approaches.

Within the evolving German and European research data landscape, initiatives such as DAPHNE4NFDI [9][10], the Helmholtz Digital Services for Science (HIFIS) [11], and the European Open Science Cloud (EOSC) [12] are establishing frameworks for FAIR (Findable, Accessible, Interoperable, Reusable) and federated data access. However, efficient mechanisms for selective, scalable interaction with large experimental datasets remain a key challenge.

PHOTONIC [13] (Photon Science - Harmonized Online Tools for Open, Navigable, Interactive Computing Framework) addresses this gap by enabling on-demand, selective access to data based on the Bluesky / Tiled [7] [8] ecosystem. Through server-side data slicing and on-the-fly data conversion into client-optimized formats, the approach minimizes data movement while supporting heterogeneous analysis environments. Positioned between ongoing national initiatives and emerging European infrastructures, PHOTONIC contributes to bridging the gap between large-scale facilities and resource-constrained users, thereby supporting interoperable and FAIR-aligned scientific workflows.

1.2 The German and European scientific data Landscape

The PHOTONIC project is positioned at a particularly opportune moment within the German and European research data ecosystem. In Germany, it is closely aligned with the activities of the NFDI consortium DAPHNE4NFDI, which focuses on photon and neutron research at large-scale facilities. These experimental techniques enable detailed insights into the structure and dynamics of matter across a wide range of scientific domains, from materials science to structural biology. PHOTONIC is situated between the first and second funding phases of DAPHNE4NFDI, providing a timely opportunity to complement and extend existing efforts, particularly in the area of efficient and scalable data access.

At the national level, PHOTONIC can be integrated into the HIFIS platform, which enables the provision of its services through the Helmholtz Cloud infrastructure and their inclusion in the HIFIS service catalogue, thereby making them readily accessible to Helmholtz centres and their scientific collaborators. This integration ensures a broad adoption within one of Europe's largest research organizations.

At the European level, PHOTONIC contributes to the ongoing development of EOSC. In particular, it can support two emerging EOSC Nodes: the German NFDI EOSC Node, where DAPHNE4NFDI is a contributing consortium, and the Photon and Neutron Open Science Cluster (PaNOSC) Node - a thematic node dedicated to photon and neutron sciences. Through these connections, PHOTONIC is well positioned to act as a bridging component between national and

PoS(ISGC2026)029

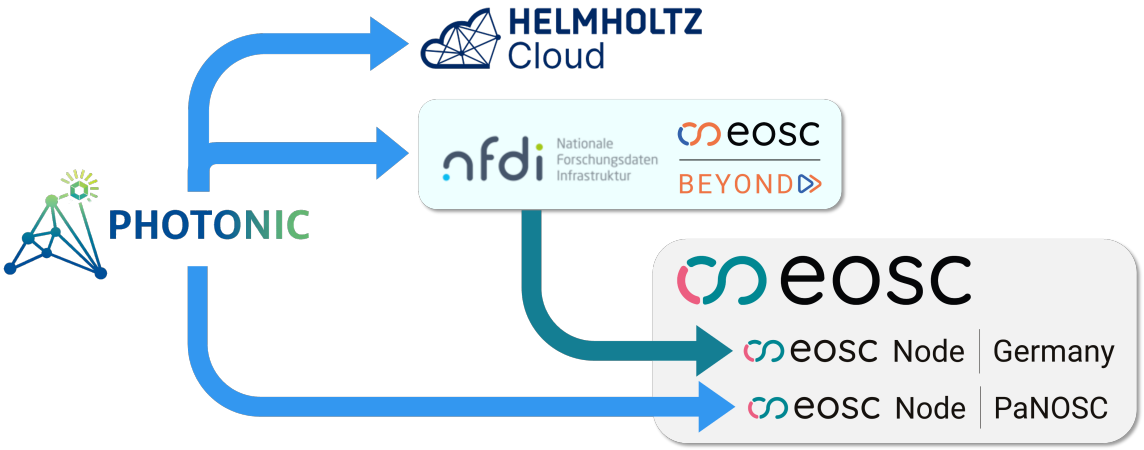

Figure 1: German Photon and Neutron Scientific data landscape

European infrastructures, enabling interoperable, FAIR-aligned access to large-scale scientific data across institutional and geographic boundaries.

1.3 Sustainability considerations

Direct project funding through the German Federal Ministry (BMFTR) is scheduled to conclude in October 2028. By this stage, the project aims to have delivered a production-ready system that meets the defined use cases, provides the required performance, and offers sufficient horizontal scalability to support the anticipated number of concurrent users. To ensure the sustainability of the system beyond the initial funding period, several measures have been put in place. A key aspect is the close collaboration with the core Bluesky / Tiled development teams. This alignment ensures that core components remain actively maintained, benefit from ongoing international development efforts, and continuously incorporate widely adopted new features. In addition, the project is designed for integration into established national and international infrastructures. At the national level, the service will be offered through platforms such as the HIFIS and, in the photon and neutron domain, via the DAPHNE4NFDI consortium. At the European level, integration into nodes of the EOSC Federation is foreseen, either thematically through the PaNOSC node or via the German national EOSC node within NFDI, as illustrated in Fig. 1. While these measures do not in themselves guarantee long-term funding, they are expected to foster broad adoption and establish PHOTONIC as a valuable component within existing research data infrastructures. A growing user base and integration into established platforms will increase the likelihood that project partners, and potentially additional stakeholders, will assume responsibility for continued operation, further development, and long-term deployment beyond the initial funding phase.

2. Use cases and client tools

To cover a broad range of relevant requirements for the first year of the project, we have selected two representative use cases that reflect typical photon science workflows with different characteristics: **X-ray photon correlation spectroscopy (XPCS)**, using the MID instrument at the European XFEL as well as the P10 beamline at PETRA III, and **X-ray reflectivity (XRR)**

PoS(ISGC2026)029

measurements at the P08 beamline at PETRA III (see section 2.1 and 2.2 for details on the underlying physics).

The overall objective is to design, provide, and evaluate user-friendly interfaces both at the beamline and throughout subsequent stages of the data processing chain, with a particular focus on client side tools such as visualization and analysis pipelines. Interface development is co-designed with beamline scientists and university partners. Within this iterative process, an initial set of client side tools will be identified, prioritised, and integrated into the system.

2.1 X-ray reflectivity

X-ray reflectivity (XRR)[14] [15] [16] [17] is a non-destructive technique used to probe thin films and layered surfaces by measuring the intensity of X-rays reflected at grazing incidence angles. The resulting reflectivity curve exhibits a plateau of near-total reflection at small angles, followed by a sharp drop at the critical angle and characteristic oscillations, whose frequency is directly related to the layer thickness. From these measurements, additional properties such as electron density and interface roughness can be inferred, often with near-atomic resolution.

To support XRR workflows effectively, we identify several key data access requirements. The relevant signal is concentrated in a narrow specular region on the detector, such that only a small region of interest (ROI) contains useful information, while the remainder primarily represents background. At the same time, users require access to full detector images for inspection with familiar tools. As access patterns are predominantly interactive rather than streaming-based, optimisations for bulk data throughput are of secondary importance.

A typical workflow involves inspection of full 2D detector images, identification of one or more ROIs, and integration of the signal within these regions as a function of incident angle. In addition, users frequently revisit previously recorded datasets to refine ROI definitions, adjust background subtraction, and recompute reflectivity curves.

Finally, the resulting data products can be linked to *SciCat* [18] to enable cross-experiment comparison and can support the ORSO (Open Reflectometry Standards Organisation) ASCII standard [19], including the conversion of legacy datasets into ORSO-compliant formats.

2.2 X-ray photon correlation spectroscopy

X-ray photon correlation spectroscopy (XPCS) [20] [21][22][23][24][25] probes sample dynamics using coherent X-rays. A coherent beam incident on a disordered sample produces a speckle pattern, whose temporal evolution reflects the underlying dynamics. By correlating detector frames over time, one obtains the relaxation time τ as a function of the scattering vector magnitude q, thereby resolving dynamics across different length scales. XPCS experiments are performed both at free-electron lasers such as the European XFEL, enabling access to sub-μs dynamics via split- or sequential-pulse techniques, and at synchrotron sources such as PETRA III, covering slower dynamics in the millisecond to second range.

Data from XPCS experiments at both facilities are already converted into a common representation, namely the NXxpcs application definition within NeXus [26, 27]. This enables researchers to load, compare, and analyse datasets from different sources without requiring custom data conversion.

PoS(ISGC2026)029

XPCS analysis is inherently parameter-driven, for example with respect to ROI selection or the choice of correlation algorithms. Dedicated tools such as DAMNIT (Data And Metadata iNspection Interactive Thing) [28, 29] and EXtra-speckle [30] encapsulate these workflows and provide interactive user interfaces. Whereas the computation of correlation functions previously required on the order of weeks of offline processing, these tools now enable near real-time feedback during beamtime. This allows users to iteratively adjust analysis parameters and assess data quality within minutes.

3. System concept

3.1 The architecture

Figure 2 illustrates the overall architecture of the envisioned system. The design follows a client-server paradigm, where the server-side components are deployed at large-scale research facilities with direct access to extensive data repositories, such as synchrotron light sources and X-ray free-electron lasers.

On the client side, existing user applications, primarily data analysis pipelines and visualization tools, are executed at universities and laboratories, which typically operate under constrained storage capacity and limited network bandwidth.

The technical roadmap, together with relevant information about the project structure and source code, is maintained in a publicly available GitLab repository [31], using issues and milestones. This approach enables asynchronous collaboration while providing continuous transparency via the issue board.

To identify potential shortcomings in both the codebase and the deployment architecture at an early stage, we agreed on the development of a minimum viable product (MVP) within the first project year. The primary objective of this MVP is to evaluate critical aspects that may require further investigation or architectural adjustments. To support this effort, an initial *Tiled* deployment has already been established for demonstration and testing purposes. It comprises:

- a *Kubernetes* [32] cluster deployed within the DESY core infrastructure,
- an initial, *Tiled* deployment on this cluster,
- representative scientific datasets in commonly used formats, accessible from within the cluster.

As next steps, we have identified a set of key topics that require thorough investigation, as they may affect the overall feasibility of the approach:

- **Access to scientific data from *Kubernetes* .** The datasets to be served by the system reside on mass storage systems within the DESY and PETRA III infrastructures, rather than on storage local to the *Kubernetes* cluster. Therefore, robust and high-performance mechanisms must be evaluated to provide efficient access from the cluster to these data sources.

PoS(ISGC2026)029

- **AAI infrastructure.** As outlined above, the system is intended to become part of a broader German and European research ecosystem. This necessitates integration with existing Authentication and Authorization Infrastructures (AAI), such as those provided by HIFIS and the EOSC, requiring careful evaluation of interoperability.

- **Security.** Providing access to data that is not yet publicly available introduces significant risks. Early engagement with all stakeholders is required, alongside the identification of robust technical solutions. Initial experimentation will be conducted using open data, followed by staged progression to synthetic private data and eventually embargoed datasets.

3.2 Access to live beamline data

While the MVP phase focuses on providing access to data that has already been archived and catalogued within the mass storage infrastructure, we plan to extend the system in the second project year to support access to live data streams. This introduces additional complexity, in particular due to the heterogeneity of data acquisition systems across different beamlines. Nevertheless, all aspects evaluated during the initial phase remain directly relevant for this extended mode of operation.

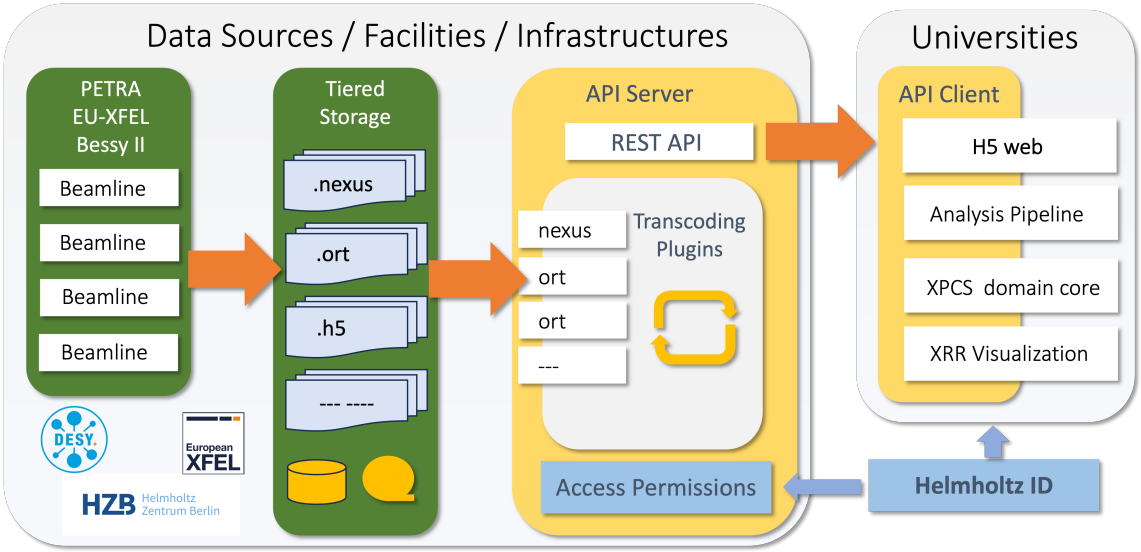

Figure 2: High level PHOTONIC Architecture.

3.3 Data formats and transcoding

Data-driven scientific investigation requires access both to the underlying observations (data) and to sufficient contextual information describing how these observations were obtained (metadata). This information is typically recorded in files that adhere to specific file formats and metadata conventions in order to enable interoperability and software reuse. The landscape of file formats and metadata standards is not static; multiple solutions coexist. These differences may arise from the need to support distinct scientific use cases, or they may reflect the evolution of formats and standards as newer approaches address limitations of earlier ones.

PoS(ISGC2026)029

Analysis and visualization software cannot support all existing file formats. As a result, researchers may encounter situations in which the most suitable analysis tools do not support the data format provided by a given beamline. This creates a trade-off: either manually convert the data—introducing delays and additional effort—or rely on less capable software.

Within the PHOTONIC project, we are systematically cataloguing the file formats and metadata approaches used across the target beamlines, together with the corresponding scientific use cases and the software ecosystems that support them. This analysis enables us to identify scenarios in which it is beneficial to convert data between formats or to transform metadata into alternative schemas.

As no single universally optimal solution is expected, we investigate the concept of a common intermediate representation into which requested data can be transformed, and from which it can be converted into the formats required by specific applications.

Such an approach may also have applicability beyond the PHOTONIC project. For example, the data transformation component could evolve into a general-purpose translation tool for scientific data formats. In addition, it could be used to validate whether files conform to expected format specifications and provide sufficient metadata to support the intended analyses.

We will align our work with previous and ongoing activities, including the consolidation efforts carried out within the OSCARS project [33, 34], as well as standardization work conducted by the NFDI FAIRmat consortium [35].

Most importantly, we will engage with domain experts and organize meetings with beamline scientists.

4. Early Stage implementation

The *Tiled* service was successfully deployed on a *Kubernetes* (K8s) cluster using a GitOps workflow managed through ArgoCD [36], as part of an infrastructure setup. Persistent storage was provisioned via Ceph-backed [37] Persistent Volume Claims (PVCs) within the photonics-dev namespace, making data available across pod restarts. The storage volume was further tested by attaching a second independent PVC. As data volume grows, it can have independent modular storage. We explored the *Tiled* client to interact with the *Tiled* server, and access specific data slices such as a small 100x100 region of a larger image directly on demand, eliminating the need to load or download the entire dataset. A dedicated PVC was additionally created and populated with 26.5 GB of P02.1 [38] (DESY) sample data to serve as an example dataset through the *Tiled* service. Additionally, to identify the most suitable storage back-end for *Tiled* on K8s, we are comparing Ceph, GPFS [39]/IBM Spectrum Scale CSI driver [40], and NFS-CSI [41]; we are actively exploring layered benchmark possibilities. The result will isolate the contribution of each component, and will separate *Tiled* 's intrinsic performance from issues caused by the K8s stack and by the storage back-end itself. Initial results show that *Tiled* itself is not a limiting factor at the scale of interest.

PoS(ISGC2026)029

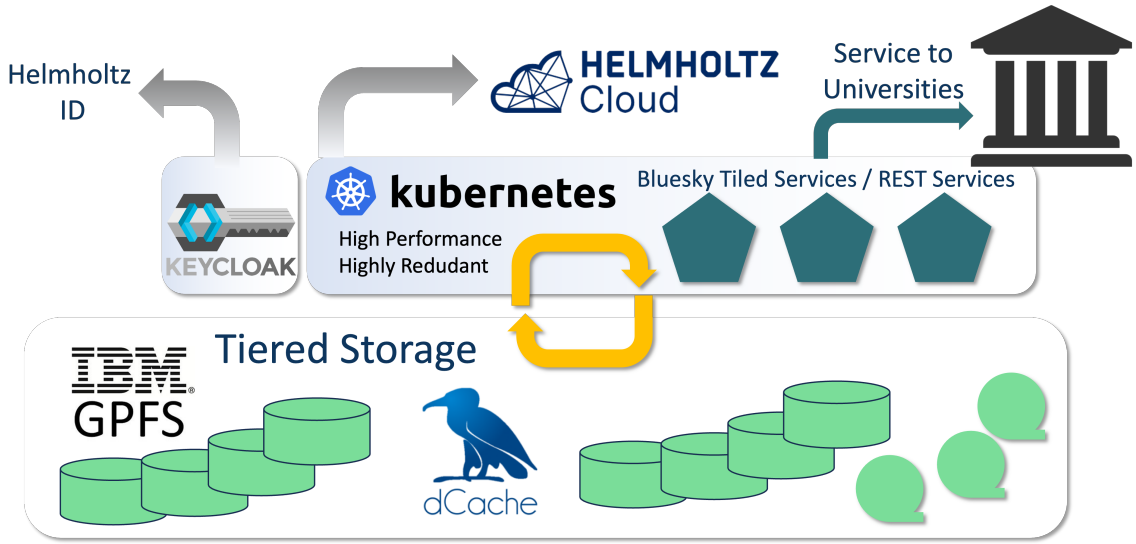

Figure 3: Proof of concept deployment.

5. Discussion

The results demonstrate the feasibility of a server-centric approach to data access in photon science, where selective retrieval and on-the-fly transformation replace traditional bulk data transfer. The prototype based on the *Tiled* ecosystem shows that fine-grained access to data subsets can significantly reduce data movement while supporting common scientific workflows.

The selected use cases, XRR and XPCS, illustrate complementary access patterns, ranging from interactive exploration of detector images to parameter-driven analysis of time-resolved data. This highlights the need for a flexible system capable of supporting heterogeneous workflows without enforcing a single access paradigm.

Several challenges remain. System performance depends on the interaction between storage backends, the *Kubernetes* layer, and the data access service. While initial results indicate that *Tiled* is not a limiting factor, further benchmarking is required to identify bottlenecks and optimise the overall system. In addition, integration with federated Authentication and Authorization Infrastructures (AAI) introduces both technical and organisational complexity.

The investigation of data formats and transcoding strategies underscores the importance of interoperability. While standards such as NeXus provide a strong foundation, intermediate representations and dynamic format conversion remain necessary, particularly when integrating legacy data and diverse software ecosystems.

Overall, the presented work provides a solid foundation for scalable, FAIR-aligned data access in photon science. Future work will focus on extending the system to live data streams, improving performance, and strengthening integration with national and European research infrastructures.

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PoS(ISGC2026)029