Handling Petabyte Data Sets at European XFEL: Updates on Policy and Implementation

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European XFEL

User Meeting 2023

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European XFEL

[in]Valuable Scientific Data

■ We continue to generate increasingly massive amounts of scientific data

■ The approach of storing all generated data long-term is becoming unsustainable

■ We have an obligation to increase the value of the data by adhering to the FAIR principles

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Handling Petabyte Data Sets at European XFEL: Updates on Policy and Implementation   Steve Aplin, Data Department European XFEL
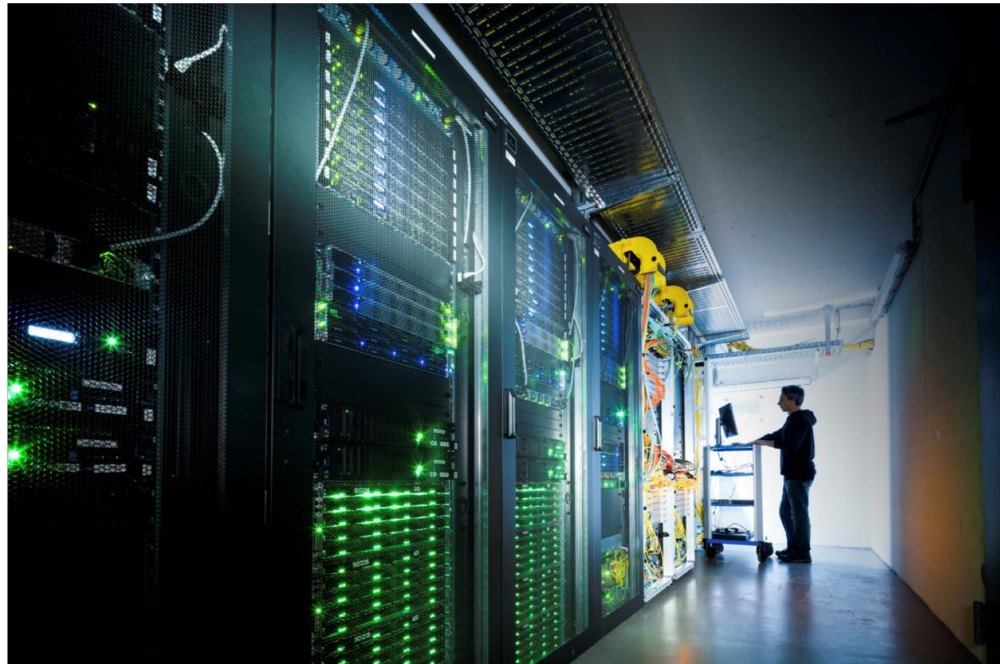
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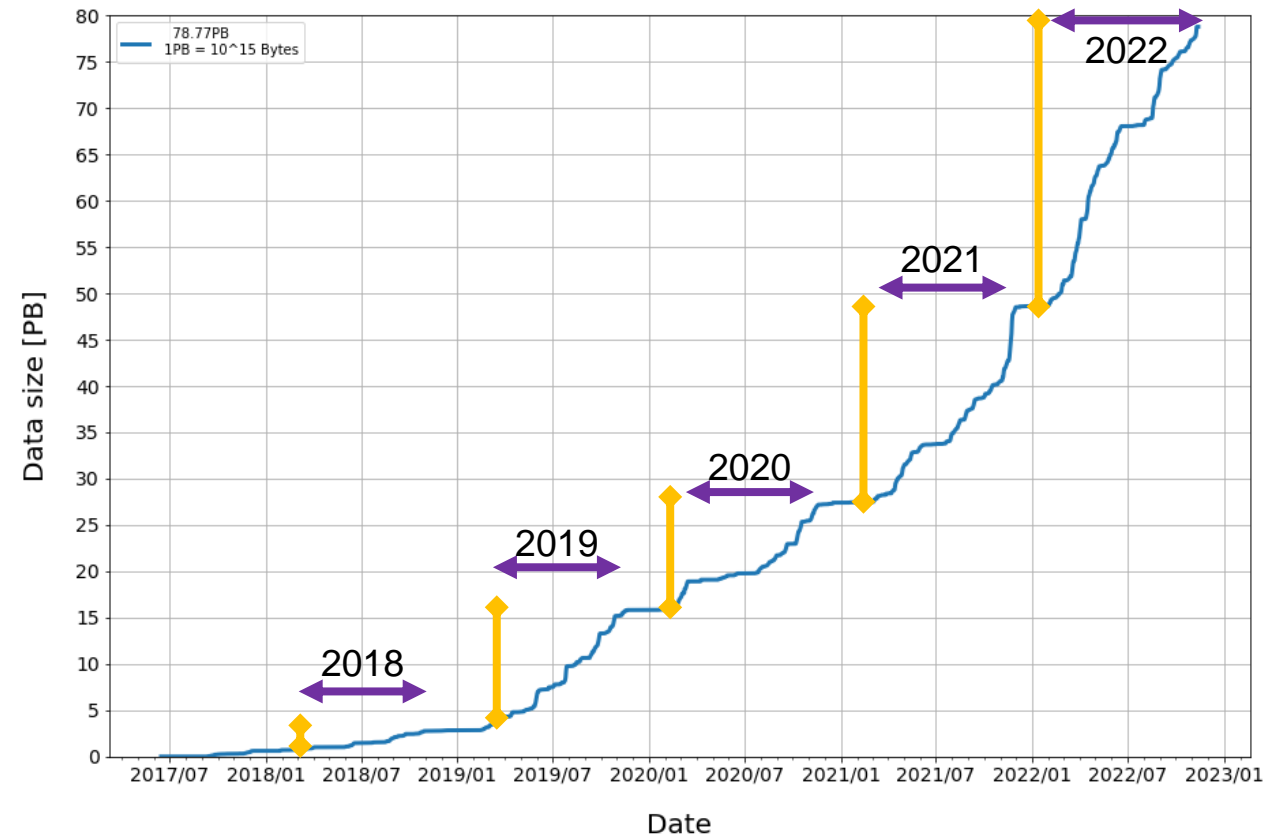
Data Storage Capacity for European XFEL
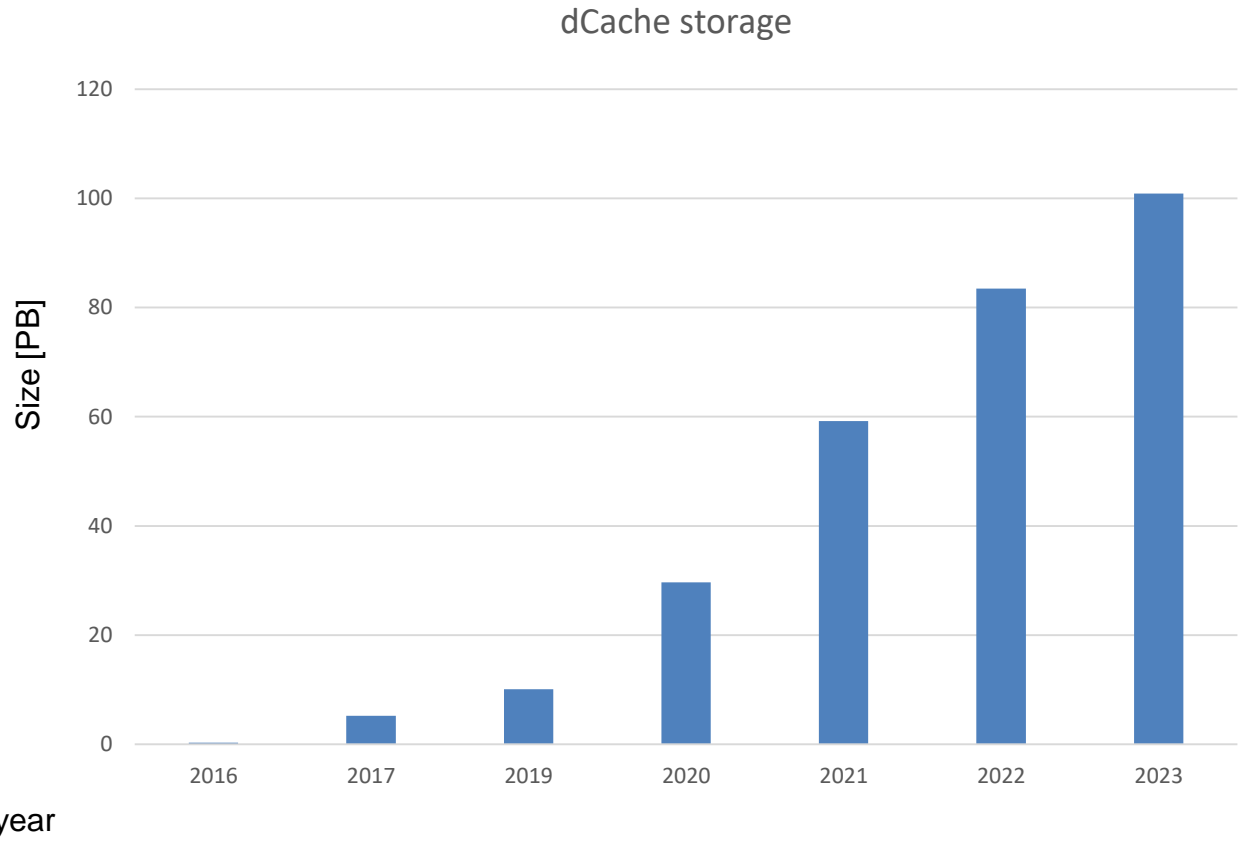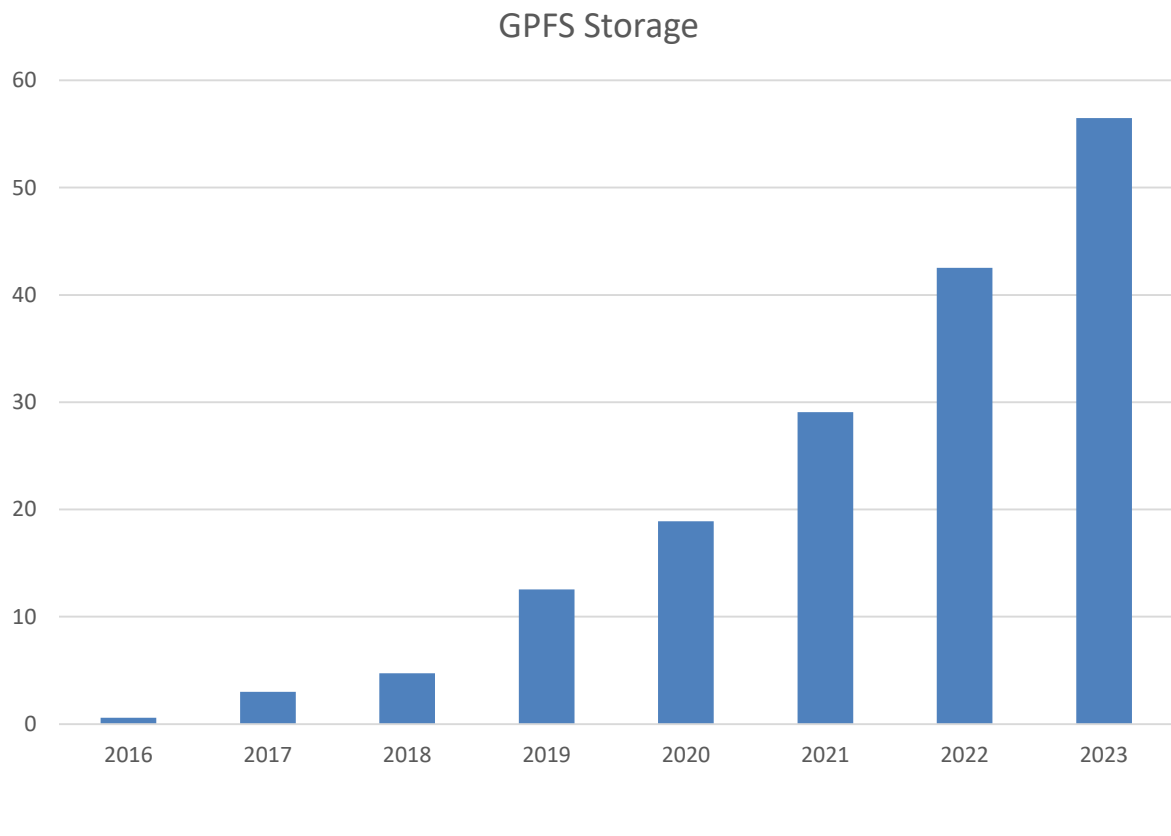
Data Reduction Becomes Unavoidable
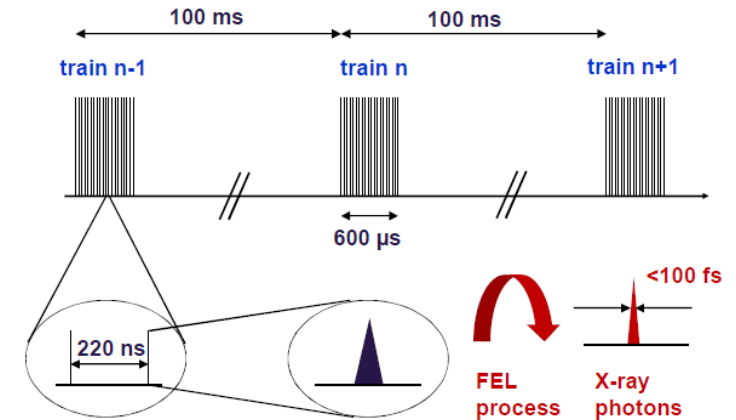
Reduce to Store

Reduce to Process
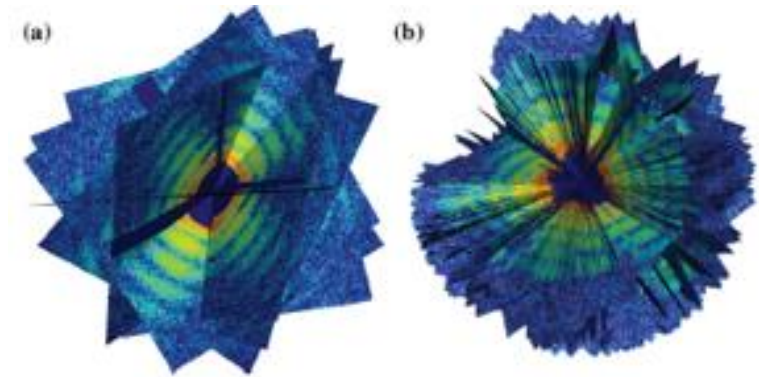
Reduce to Transport

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Can't you just use a trigger….?

Detector type	Data/sec
AGIPD 1Mpxl	~7 GB/s
AGIPD 1Mpxl Double images	~14 GB/s
AGIPD 4Mpxl	~30 GB/s *
LPD 1Mpxl	~10 GB/s
DSSC 1Mpxl	~16 GB/s

* Will not be run at full rate in current design

The data flow from all four experiments at LHC for Run 2 was anticipated to be about *25 GB/s after* data reduction
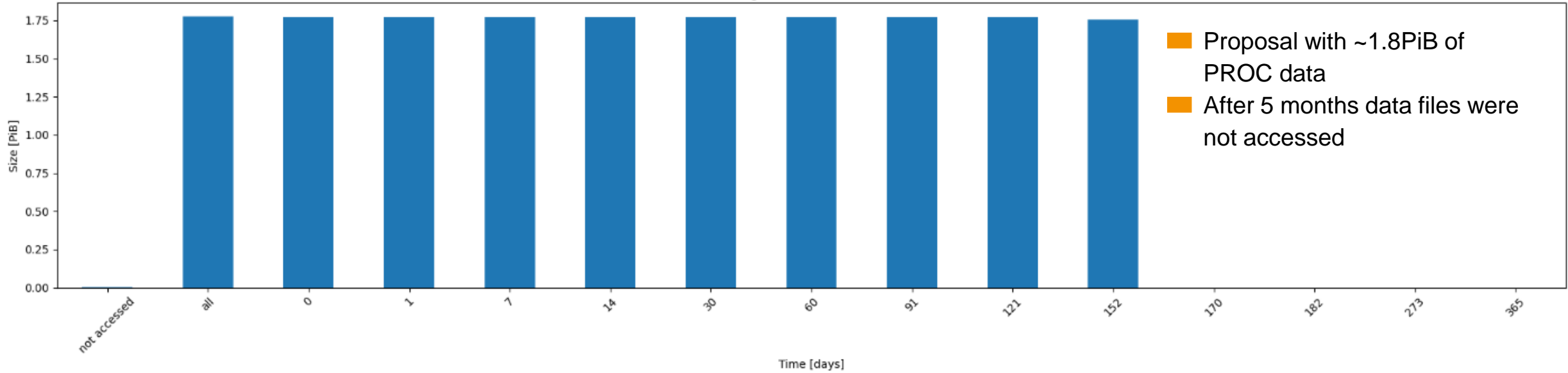
- ALICE: 4 GB/s (Pb-Pb running)
- ATLAS: 800 MB/s – 1 GB/s
- CMS: 600 MB/s
- LHCb: 750 MB/s

Data reduction in particle physics is built into it's DNA, it is intrinsic to the field's experimental viability.

The experiments are designed from the ground up on data reduction.

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Size of data accessed until a given time counted from the data creation time

- Proposal with ~1.8PiB of PROC data
- After 5 months data files were not accessed

Size of data accessed until a given time counted from the data creation time

- Proposal with 1.4PiB of PROC data
- PROC files with more than 0.5PB of data have not been accessed at all
- After 2 months less than 10% of data were accessed

Size of data accessed until a given time counted from the data creation time

- Proposal with 100TB of PROC data
- Only approx. 20TB of PROC data were accessed after two weeks

Size of data accessed until a given time counted from the data creation time

- Proposal with ~2.25PB of PROC data
- Approx. 2PB of PROC were not accessed (raw data was used)

Scientific Data Policy

Data Management Tools & Procedures

Data Management Plans per Proposal

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Collaboration

Legal aspects

TEAMWORK

Raw	Intermediate analysis step data	Metadata	Auxiliary	Simulation data
Calibrated	Analysis results	Logbook entries	Calibration constants	
Processed	Various types of data	Detector Geometry data		
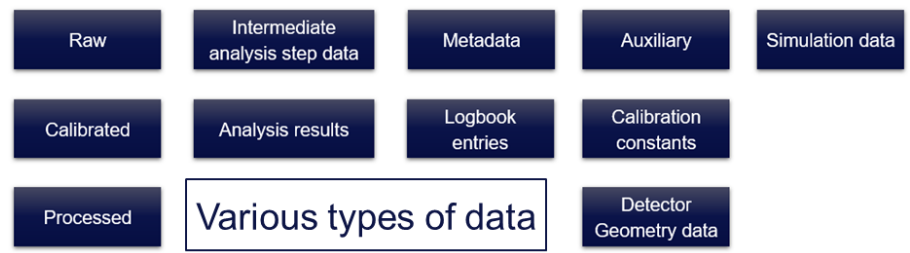
Data Retention

Why do we need a Scientific Data Policy?

Online GPFS — Cache

Offline GPFS — Performance

dCache — Capacity

Tape Archive — Safety

Data management becomes increasingly complex and expensive

Open access

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Scientific Data Policy in place

- European XFEL Scientific Data Policy was approved by the European XFEL Council shortly before European XFEL transitioned from the Construction to the Operation mode.

- The policy has is based on recommendations from the PaN-data Europe Strategic Working Group from 2011 following the majority of modifications from ILL and ESRF

- The policy defines the obligations and rights of the facility and its users with respect to the scientific data

- It allowed for a coherent approach to the data management services across different instruments and laboratories
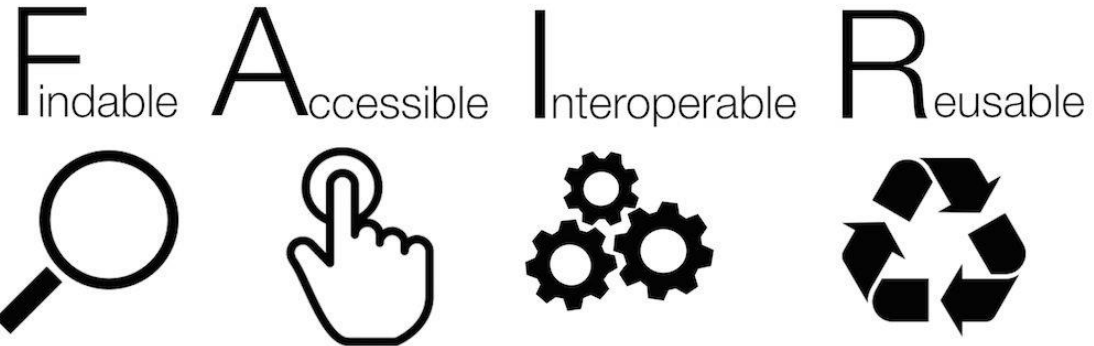
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6 June 2017

Scientific Data Policy of European X-Ray Free-Electron Laser Facility GmbH

as approved by the Council on 30 June 2017

Scientific Data Policy of European X-Ray Free-Electron Laser Facility GmbH
6 June 2017   1 of 12

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F indable   A ccessible   I nteroperable   R eusable

- In 2016, the '<u>FAIR Guiding Principles for scientific data management and stewardship</u>' were published in *Nature Scientific Data*.

- The ultimate goal of FAIR is to optimize the reuse of data

- Shifted paradigm from open to FAIR data

- "as open as possible, as closed as necessary"

- ❖ **Findable**: This is the first step for the reuse of the data, which is to find them.

- ❖ **Accessible**: Once the user has found the data, he must know how to access it

- ❖ **Interoperable**: Data needs to be integrated not only with other data, but also with applications or workflows for analysis, storage and processing.

- ❖ **Reusable**: other researchers can reuse all data.

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Highlights of Data Policy changes
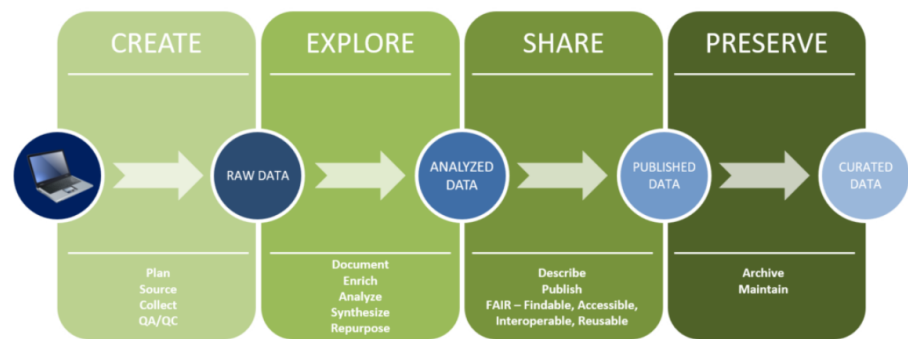
■ Introduction of the data management plan

■ Preserving user data

■ PI responsibilities and rights concerning data

■ Definition of European XFEL data format

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■ More on persistent identifiers
► DOI, ORCID

Open Access

■ Free availability
■ Anonymous access

Scientific Data Policy

······ Appendix ·····▸ Data Retention scheme

Individual DMPs are based on the Scientific Data Policy and the Data Retention scheme

Appendix

European XFEL Data Format

Data Management Plan 0001
Data Management Plan 0102
Data Management Plan 1903
Data Management Plan 2348
Data Management Plan 6001

Proposal specific adjustments

PI

DMPs are living documents defined for each proposal

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Updated definition of scientific data categories
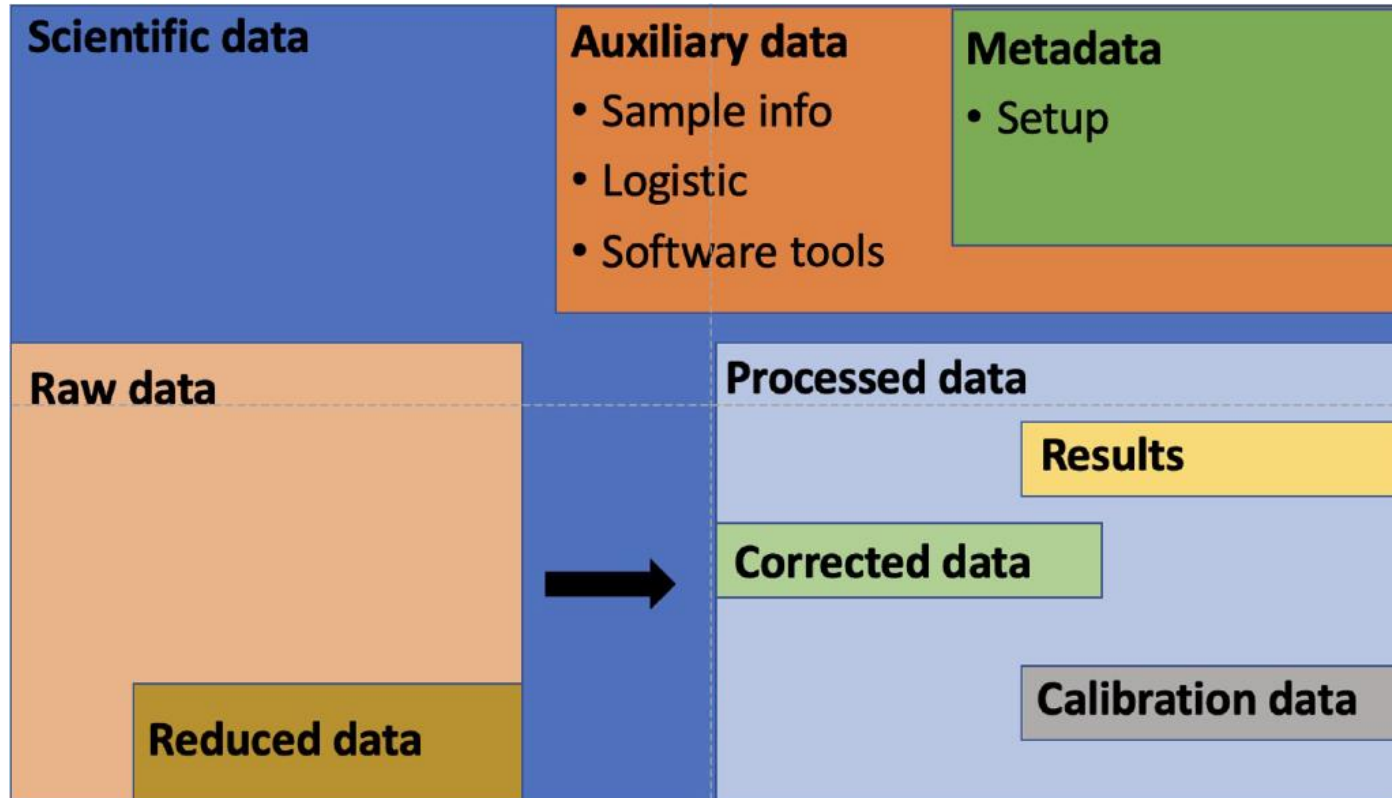
- Introduction of new data categories
    - Auxiliary data
    - Reduced data

- Changing names
    - Calibrated data becomes corrected data according to the European XFEL nomenclature

- Removal of data category
    - Alignment data – it is now included in the auxiliary data

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Data Retention in practice at European XFEL (as defined in 2017)

- **Raw data kept on dCache long term**
  - Access to tape only is not practical – up to several weeks for staging a dataset from beamtime
  - Two copies principle

- **Processed (corrected) data kept on GPFS since the beginning**
  - Could not delete calibrated data due to the lack of confidence that it can be exactly reproduced

- **Raw data are removed from GPFS immediately when the second copy is flushed to tape (but kept on dCache, see 1st point)**
  - Need more space on GPFS for new beamtimes

- **Initial implementation worked for the first stage of operation but is not sustainable for full operation**

Storage class	Quota	Safety	Lifetime	Comment
dcache.raw	None	Tape Archive	6 months	Raw data on commodity disks
raw GPFS	None	None	2 months	Very fast accessible raw data, lifetime not guaranteed
usr GPFS	5TB	Snapshots + Tape Backup	24 months	User data, results
proc GPFS	None	None	6 months	Processed data (e.g. calibrated)
scratch GPFS	None	None	6 months	Temporary data (lifetime not guaranteed)
dcache.cal	None	Tape Archive	10 years	Calibration constants on commodity disks
cal	None	Tape archive	6 months	Very fast accessible calibration data
user home	20GB	Snapshots + Tape Backup	Lifetime of the account	Home folder for user account
archive.raw	None	-	Long-term	"Long term" means 5 years and XFEL will strive for 10 years
archive.cal	None	-	10 years	

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New Data Retention Scheme

Expected to come into effect in 2025
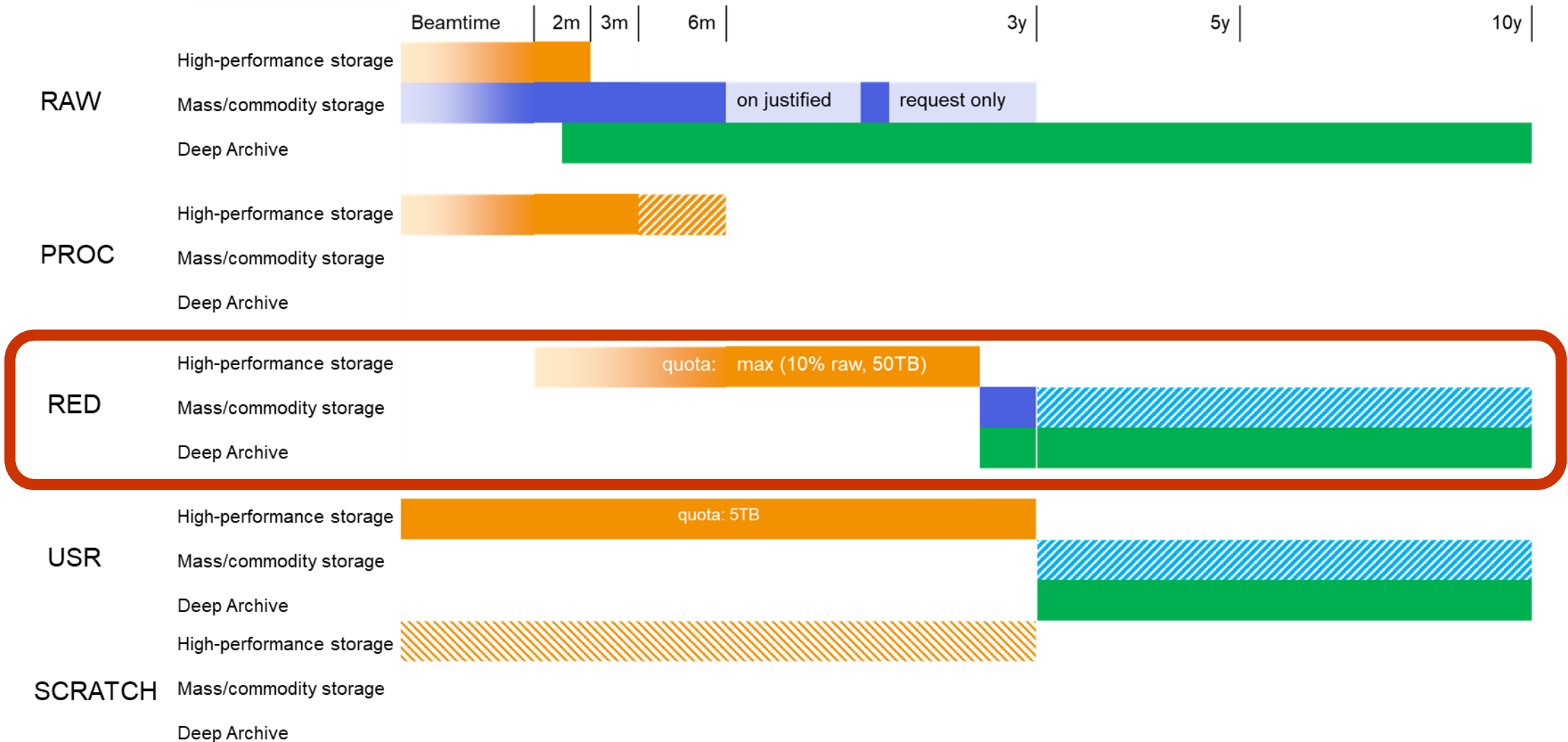
RAW data
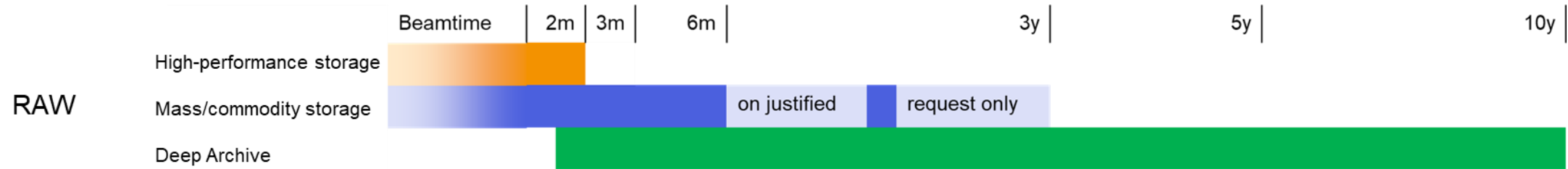
- Initially stored on high-performance disks for two months but can be removed earlier if no space is available

- Will remain on commodity storage for six months

- In exceptional cases, beyond six months, RAW data can be restored from the deep archive to the commodity storage

- Single copy of each data file is stored in the deep archive

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PROC data
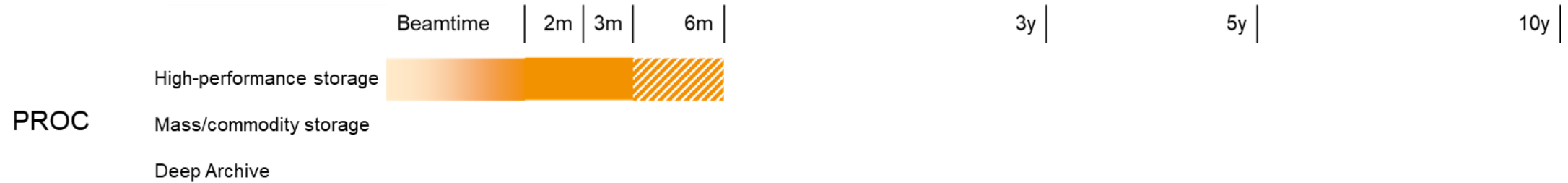
🟧 Data derived from RAW data by the facility-provided services (e.g. corrected images)

🟧 Initially stored on high-performance storage for three months

🟧 Stored period can be extended once for another three months

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RED data

RED data is a selection of RAW data, PROC data, and user-processed data adhering to the data format of European XFEL

RAW

- Selection of runs
- Selection of detector modules
- Extracted events (train/pulse)
- Removed detector gain maps

PROC

- Selection like for RAW data but contains:
  - corrected detector images
  - processed images (e.g. conversion to photons, azimuthal integration)
  - other derived data

User-processed

- Selection like for RAW data but contains:
  - User-computed properties
  - Experiment's specific data corrections
- Must adhere to the European XFEL data format
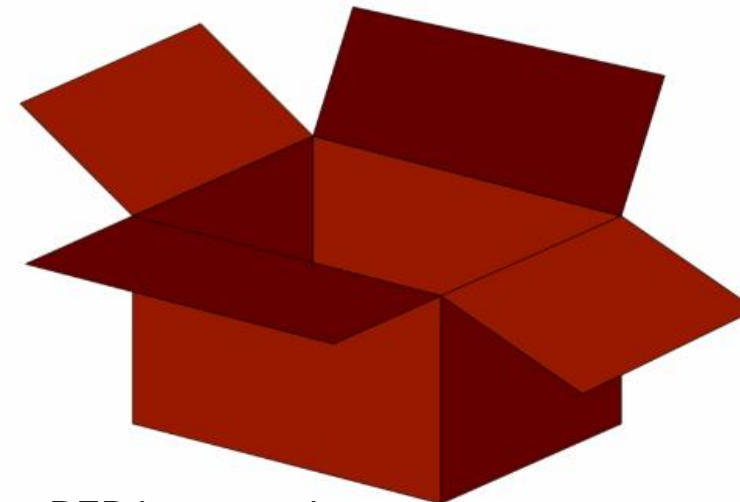
■ Examples

Raw Data size	Max. RED data size
20TB	20TB
60TB	50TB
380TB	50TB
620TB	62TB
2100TB	210TB

RED box capacity:
max(10% of RAW data size; min(50TB;RAW data size))

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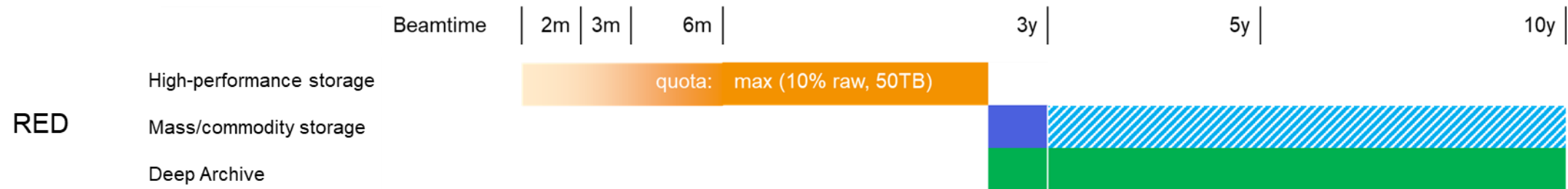
RED data

■ RED data have to be derived from RAW or PROC data within six months after the beamtime, beyond this period the content becomes read-only

■ RED data is stored on the high-performance storage system for a maximum of three years period after the beamtime

■ RED data is migrated to the commodity storage and archived during the three years period after the beamtime.

■ RED data becomes available as open access after the embargo period

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USR data

Beamtime | 2m | 3m | 6m | 3y | 5y | 10y

USR
- High-performance storage — quota: 5TB
- Mass/commodity storage
- Deep Archive
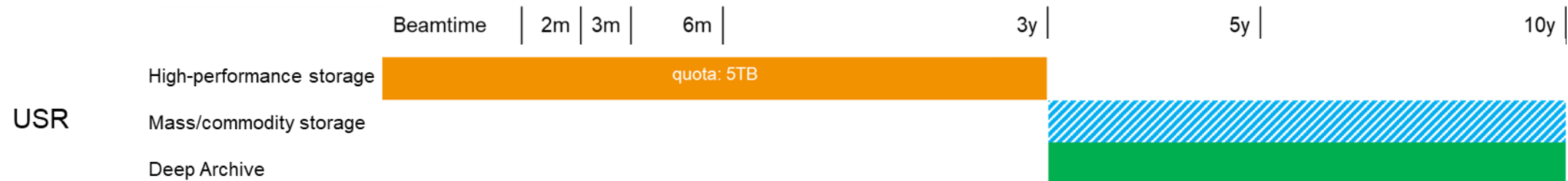
USR data are kept on the high-performance system for a maximum of three years

Maximum size of USR data is 5TB per proposal

Content of the USR folder becomes open access after the embargo period

It is the responsibility of PI that data stored in the USR folder are not violating any law (e.g. personal data protection, intellectual property rights, licensing)

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Implementation of the Data Retention Scheme

- As the first step we are going to apply the RED data concept to the internal commissioning proposals

dCache storage for RAW data from commissioning proposals
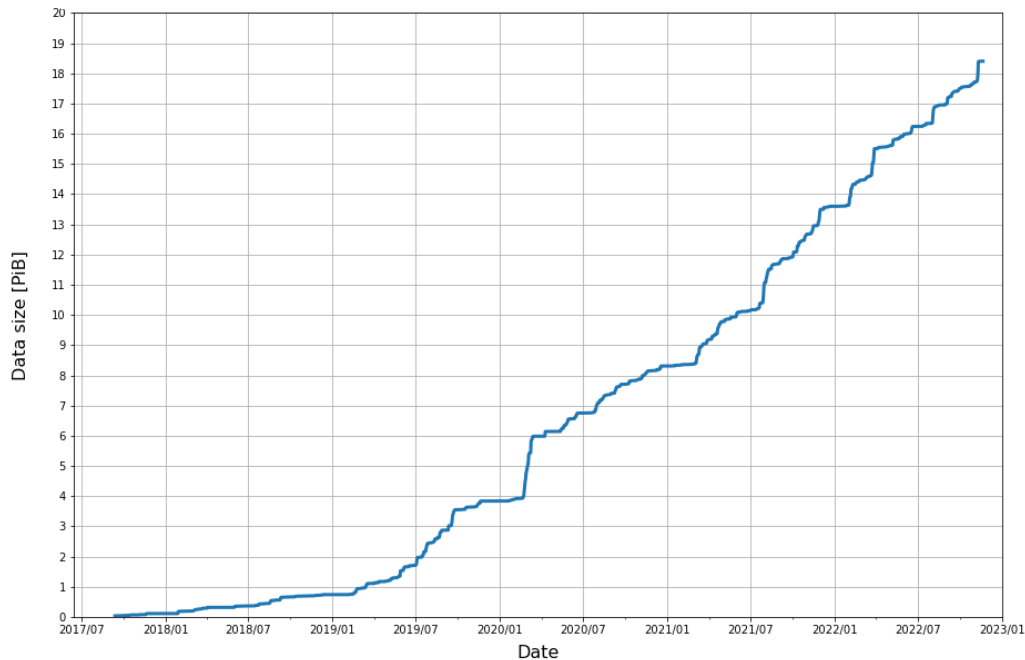
dCache storage required for commissioning proposals after applying RED data concept

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Scientific Data Policy ROADMAP

SDP – Scientific Data Policy   DRS – Data Retention Scheme   EXDF – European XFEL data format

Draft of the SDP ready
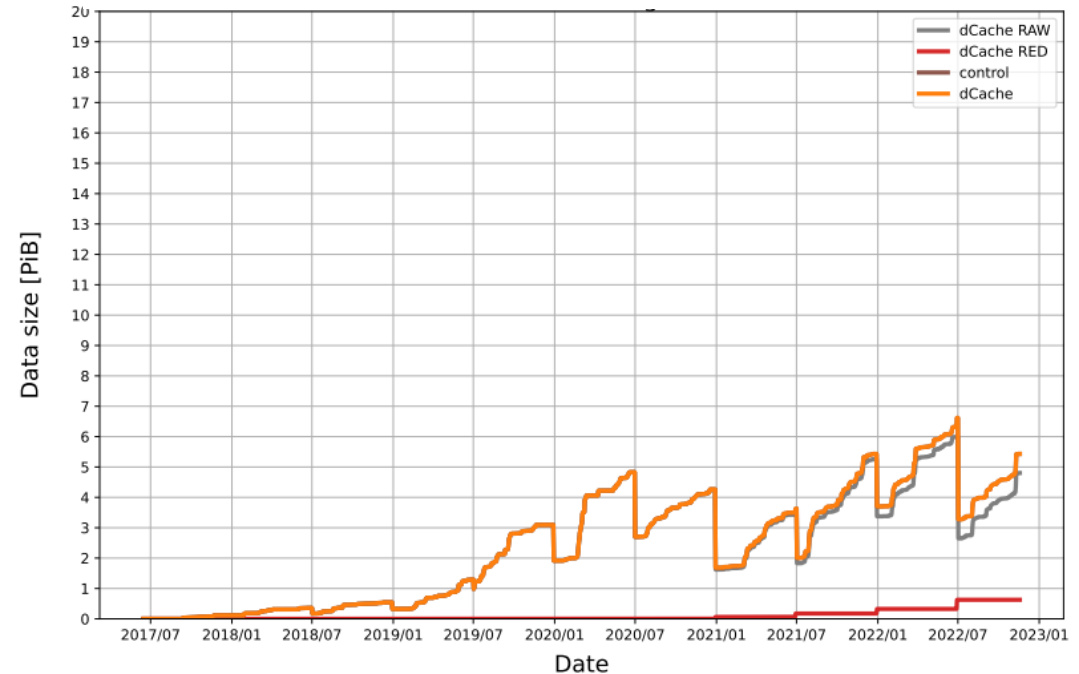
Nov 2022

SDP reviewed by Legal Office

EXDF defined and published

Users informed about the ongoing SDP work and the approved DRS

Jan 2023

Feedback from SAC on SDP

Mar 2023

Dec 2022

Presentation to the DAC committee

SDP submission for interim approval of the general concept to the EUXFEL MB

Submission for approval of the DRS to the EUXFEL MB

Feb 2023

Submission for approval of the SDP to the EUXFEL MB

Jun 2023

Adoption of SDP by EUXFEL

Implementation ROADMAP

First experiment deploying data reduction tools within the calibration pipeline

Nov 2022

Initial implementation of DMP (will be optional for the 202401 calls for proposals)

March 2023

Demonstration of real-time data reduction tools on RAW data

Aug – Dec 2023

Feb – Jun 2023

Implementation of RED data concept for commissioning proposals

Prototype of DAQ integration with data reduction tools

Development of event-finding for SFX and SPI

Jul 2023

Integration of myMdC with Globus for direct download of Open Data

Oct 2023

Revised implementation of DMP (for 202402 calls for proposals)

Summary

Stage 0: technical revision of all data sources to ensure removal of NULL data

Stage 1　　　　　　　　　　　　　　　　　　　**When: 2023   Who: European XFEL**
Finalisation of European XFEL Scientific Data Policy
Development and commisioning of data management tools and procedures needed to support implementation of New Data Retention Scheme

Stage 2　　　　　　　　　　　　　　　　　　　**When: Late 2023-2025   Who: European XFEL**
Introduction of Data Management Plans　　　　　　　　　　　　　　**Users**
User Assisted Commisioning of Data Reduction Tools and Procedures

Stage 3　　　　　　　　　　　　　　　　　　　**When: Late 2025-2026   Who: European XFEL**
Full deployment of New Data Retention Scheme for all New Proposals　　　**All Users**

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Contributors:

■ Working Group leaders: Fabio Dall'Antonia, Janusz Malka

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