The Data Management and Data Service for HEPS

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Outline

1. HEPS Introduction

2. Demands and Challenges of data management

3. The system design and implementation

4. Summary & Plan

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1. **HEPS Introduction**
2. Demands and Challenges of data management
3. The system design and implementation
4. Summary & Plan
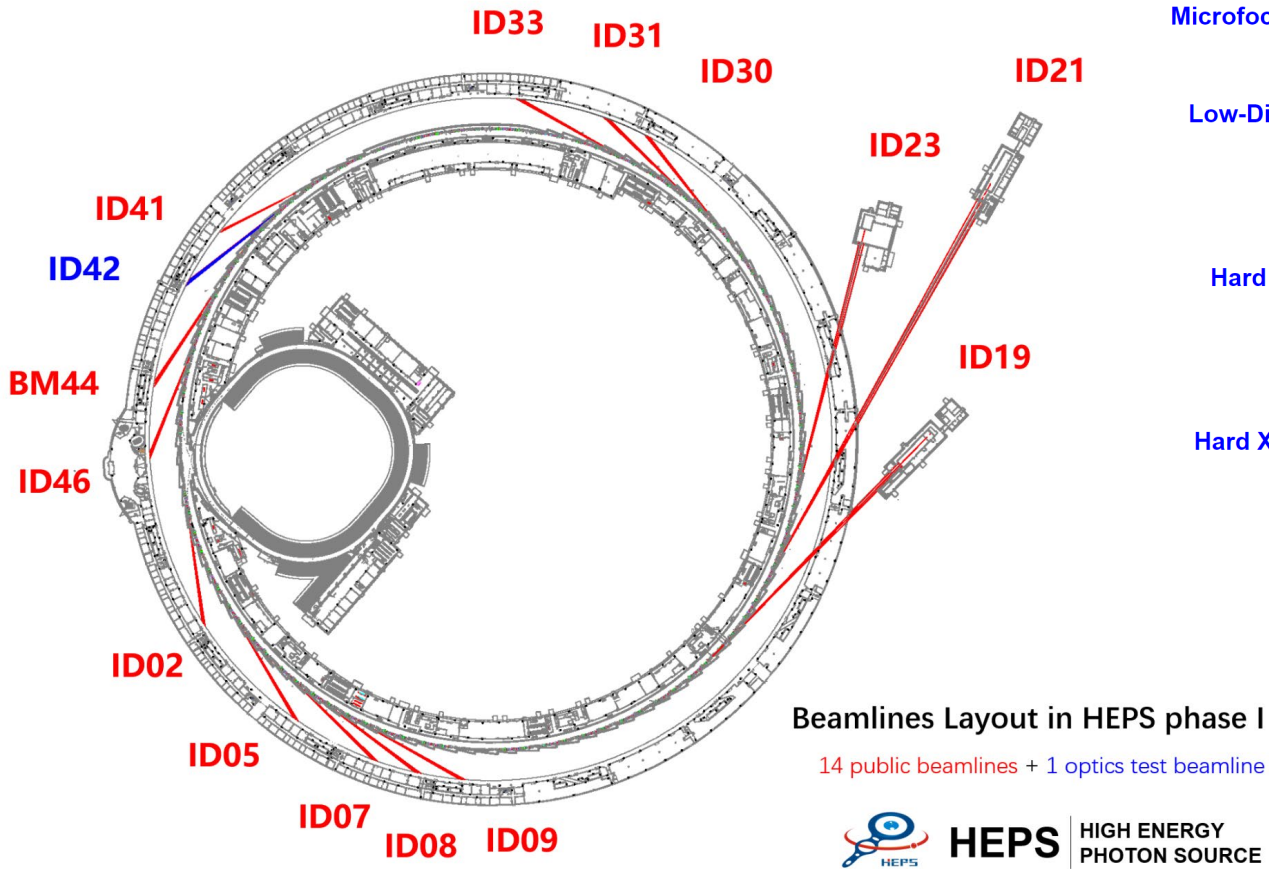
High Energy Photon Source (HEPS)

- The fourth generation light source in China — High energy, high brightness

- Located in Beijing - about 80KM from IHEP

- Officially approved in Dec. 2017, started in 2018

- The whole project will be finished in mid-2025

- The construction of the civil structure is completed

Main parameters	Unit	Value
Beam energy	GeV	6
Circumference	m	1360.4
Emittance	pm·rad	< 60
Brightness	phs/s/mm^2/mrad^2/0.1%BW	>1x10^{22}
Beam current	mA	200
Injection		Top-up

HEPS

80 km

IHEP

Beijing

Beamlines in HEPS phase I

Beamlines Layout in HEPS phase I

14 public beamlines + 1 optics test beamline

HEPS | HIGH ENERGY PHOTON SOURCE

Microfocusing X-Ray Protein Crystallography-ID02 Beamline

Low-Dimensional Structure Probe Beamline-ID05

Engineering Materials Beamline-ID07

Hard X-Ray Coherent Scattering Beamline-ID09

Pink Beam SAXS Beamline-ID08

Hard X-Ray Nanoprobe Multimodal Imaging-ID19 Beamline

Hard X-Ray Imaging Beamline-ID21

Structural Dynamics Beamline-ID23

ID30-Transmission X-Ray Microscopic Beamline

ID31-High Pressure Beamline

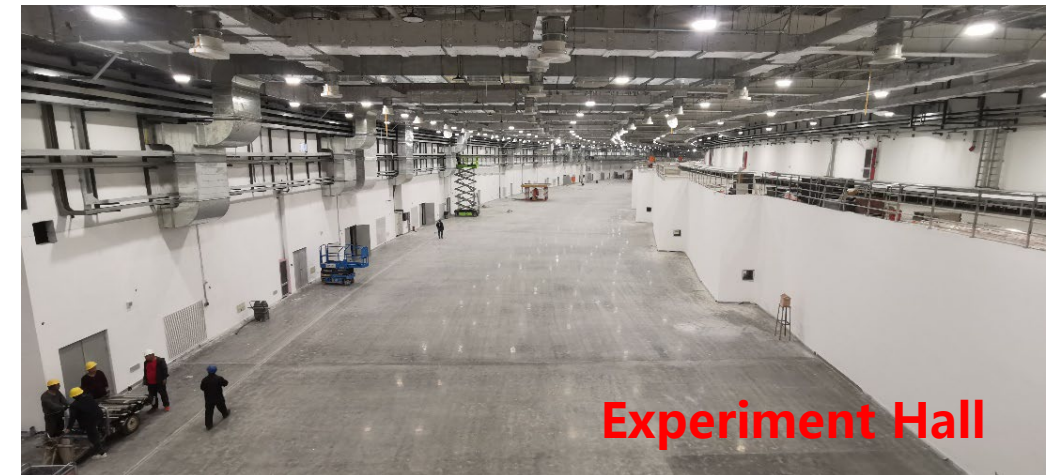ID33-Hard X-Ray High Resolution Spectroscopy Beamline

BM44-Tender X-Ray Beamline

ID41-High Resolution Nanoscale Electronic Structure Spectroscopy Beamline

ID42-Optics Test Beamline

ID46-X-Ray Absorption Spectroscopy Beamline

Experiment Hall

14 public beamlines + 1 optics test beamline in Phase I

Can accommodate over 90 beamlines in total

Progress of the HEPS project

◻ Now at the stage of beamline station equipment installation and joint commissioning.

◻ 2023.01, HEPS booster installation completed

◻ 2023.03, HEPS achieved the first electron beam accelerated to 500 MeV.

◻ 2023.11, The beam energy of the HEPS booster has reached 6GeV, with a charge exceeding 5nC.

◻ 2023.12, HEPS storage ring has been closed-looped.
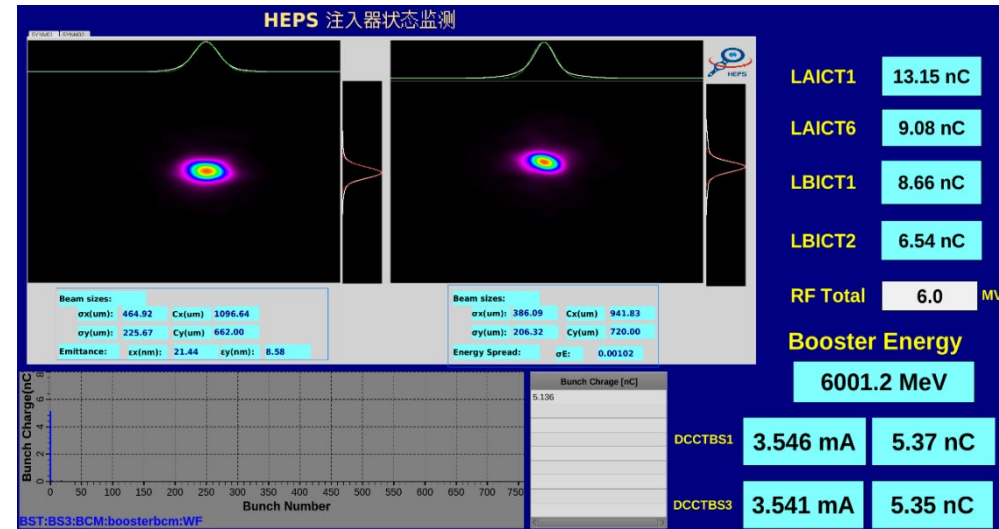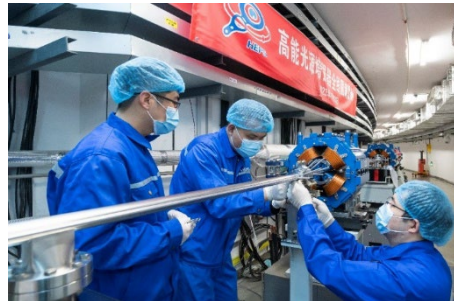
Outline

Data Challenges @HEPS

- ☐ Increased source brightness, X-ray detector capabilities have been continuously improving
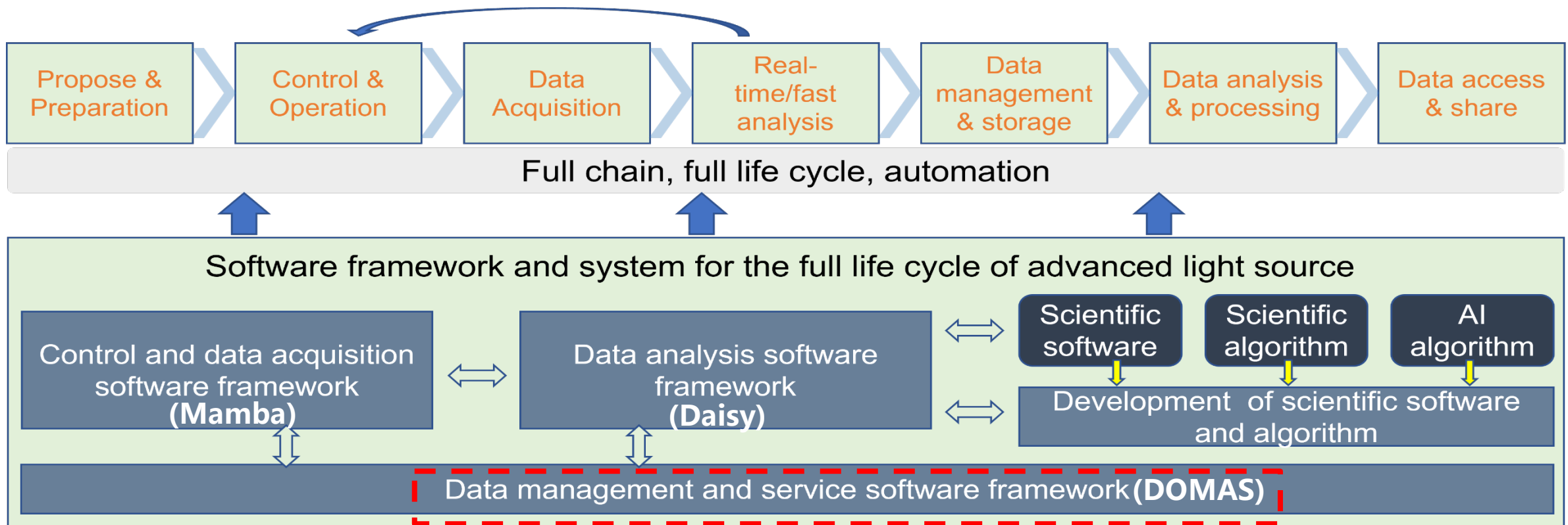- ☐ **More than 24PB raw data will produced per month**

Beamlines	Burst output(Byte/day)	Average output(Byte/day)
B1 Engineering Materials Beamline	600TB	200TB
B2 Hard X-ray Multi-analytical Nanoprobe (HXMAN) Beamline	500TB	200TB
B3 Structural Dynamics Beamline (SDB)	8TB	3TB
B4 Hard X-ray Coherent Scattering Beamline	10TB	3TB
B5 Hard X-ray High Energy Resolution Spectroscopy Beamline	10TB	1TB
B6 High Pressure Beamline	2TB	1TB
B7 Hard X-Ray Imaging Beamline	1000TB	250TB
B8 X-ray Absorption Spectroscopy Beamline	80TB	10TB
B9 Low-Dimension Structure Probe (LODISP) Beamline	20TB	5TB
BA Biological Macromolecule Microfocus Beamline	35TB	10TB
BB pink SAXS	400TB	50TB
BC High Res. Nanoscale Electronic Structure Spectroscopy Beamline	1TB	0.2TB
BD Tender X-ray beamline	10TB	1TB
BE Transmission X-ray Microscope Beamline	25TB	11.2TB
BF Test beamline	1000TB	60TB
Total average:		**805.4TB/day, 24.16PB/month**

Estimated data volume of HEPS at Phase I

Huge amount of data is a big challenge for data management and processing

Full lifecycle software system for HEPS


```
Propose & Preparation → Control & Operation → Data Acquisition → Real-time/fast analysis → Data management & storage → Data analysis & processing → Data access & share
```

Full chain, full life cycle, automation

Software framework and system for the full life cycle of advanced light source

Control and data acquisition software framework (Mamba) ⟷ Data analysis software framework (Daisy) ⟷ Scientific software / Scientific algorithm / AI algorithm

Development of scientific software and algorithm

Data management and service software framework (DOMAS)

- ☐ **Software system for the full data lifecycle of light source experiments**
- ☐ **Data management and service is the essential component and provide the interface for data access**

Tasks of HEPS Data Management

- **Data policy and Data Format**

  - Establish rules and regulations about data management

  - Design HDF5 data file format for each beamline, follows NeXus conventions

- **Metadata catalogue**

  - Design metadata model, catalogue, metadata database

  - Provide access to metadata and experimental data

- **Metadata acquisition**

  - Acquire metadata from other sub-systems(DAQ, transfer, storage, analysis…)

- **Data transfer**

  - Transfer data automatically: beamline storage → central storage → tape

  - Interact with metadata catalogue when the data storage status changed

- **Data service**

  - Provide a web-based GUI for user to search, access, download, analysis data

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HEPS Data Policy

The ownership, curation, archiving and access to scientific data and metadata

- Recommend to provide at least 3 months disk storage and permanent tape archive

- Provide permanent storage for raw data

- Provide temporary storage for processed data and calibration data

- Each dataset will have a unique persistent identifier(CSTR/DOI)

- Experimental teams have sole access to the data during the embargo period

- After the embargo, the data will be released with open access to any registered users of the HEPS data portal

Apr. 2021, The Data Policy for HEPS(draft) is finished.

Mar. 2023, The Data Policy for HEPS(draft) is revised after a lot of discussion.

Apr, 2021
The Data Policy for HEPS
--Draft Version

Mar, 2023
The Data Policy for HEPS
--Revised Draft
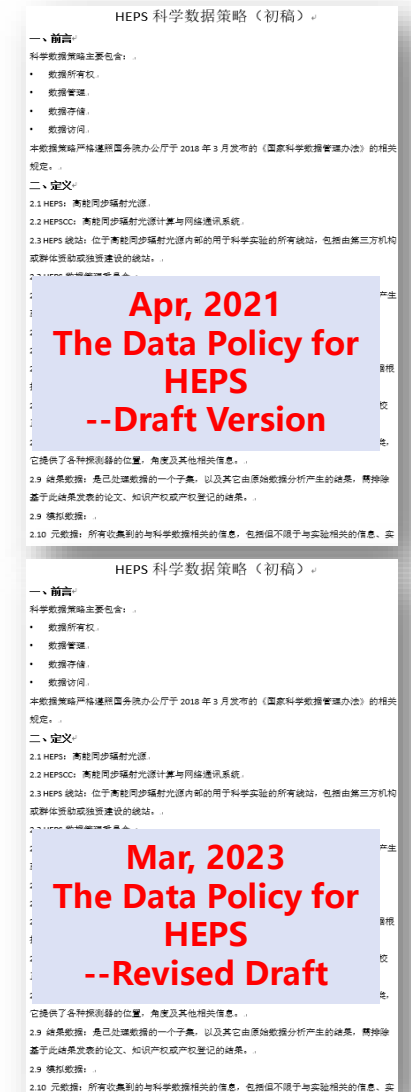
Data storage policy

① **Raw data produced from detector are saved to beamline storage directly，up to 7 days**

② **Data is moved from beamline storage to central storage，data are kept up to 90 days**

③ **Data is moved from central storage to tape for long-term storage**

Data storage policy will be adjusted according to the actual data volume and funding situation

7 Days   90 Days   Permanent

Writing →   Data transfer →   Data transfer →

Detector DAQ system

Beamline storage
- SSD
- High speed data IO

Central storage
- HDD
- Medium-high speed data IO

Tape
- Permanent data archive
- Prepare the data before retrieve
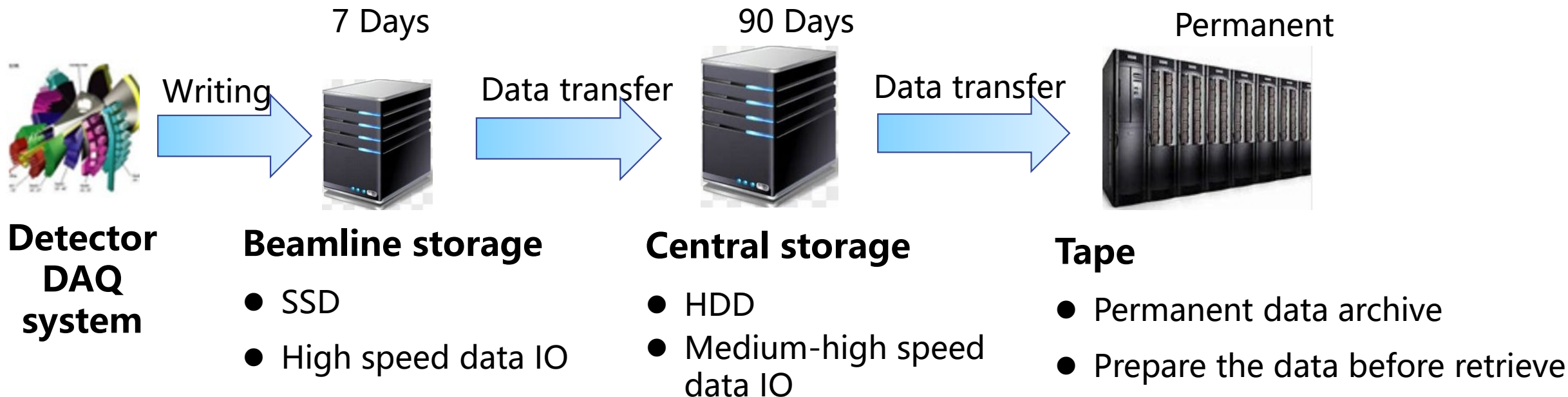
Data directory and permission

- The data is organized under the related BeamtimeID directory

- Data path : *../<Beamline>/<YearMonth>*/Data/*<BeamtimeID>*

- User access control is restricted by setting ACLs of file system on *BeamtimeID* folder

- Users will be guided to use the directories accurately

Folder	Data type	Permission	Permanent archive?
raw	Raw data/user data	Read only	Yes
processed	Processed data	Read, write	No
scratch	Temp data, snapshots, scripts,	Read, write	No
share	Snapshots, scripts, shared files...	Read, write, shared	No

```
|--hepsfs
    |--bl(central)
        |-- <Beamline>
            |-- <YEARMonth>
                |-- Data
                    |-- <BeamtimeID>
                        |-- raw                → Raw data
                        |-- <Sample>
                            |-- <ScanID>
                                |--data files...
                        |-- processed          → Processed data
                        |-- scratch
                        |-- share              → Snapshots, scripts, shared files...
```

Customized folders by users
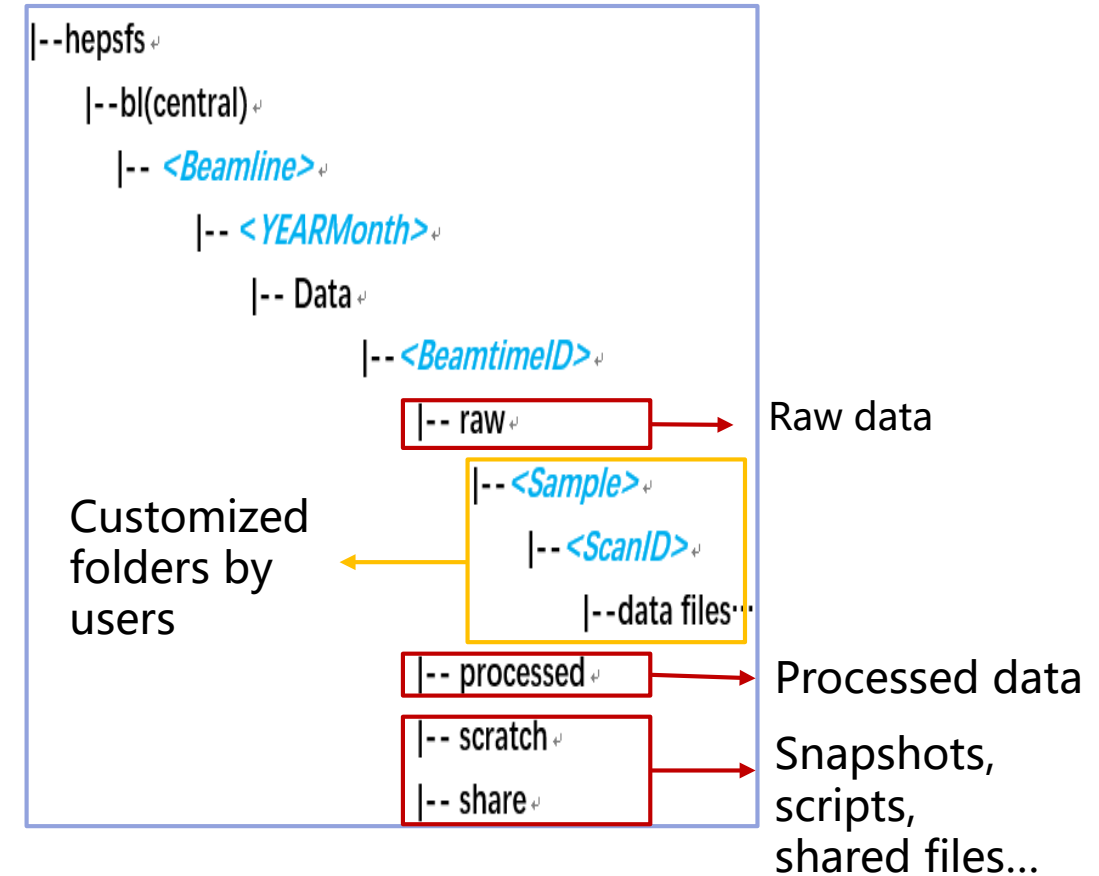
Data directory structure

Data management software framework-DOMAS

- **Functional modules**
  - ✓ Metadata catalogue
  - ✓ Metadata acquisition
  - ✓ Data transfer
  - ✓ Data service
- **Extensible and standard interface**
- **Be used to build data management system for light sources quickly**
- **Will be open-sourced progressively**
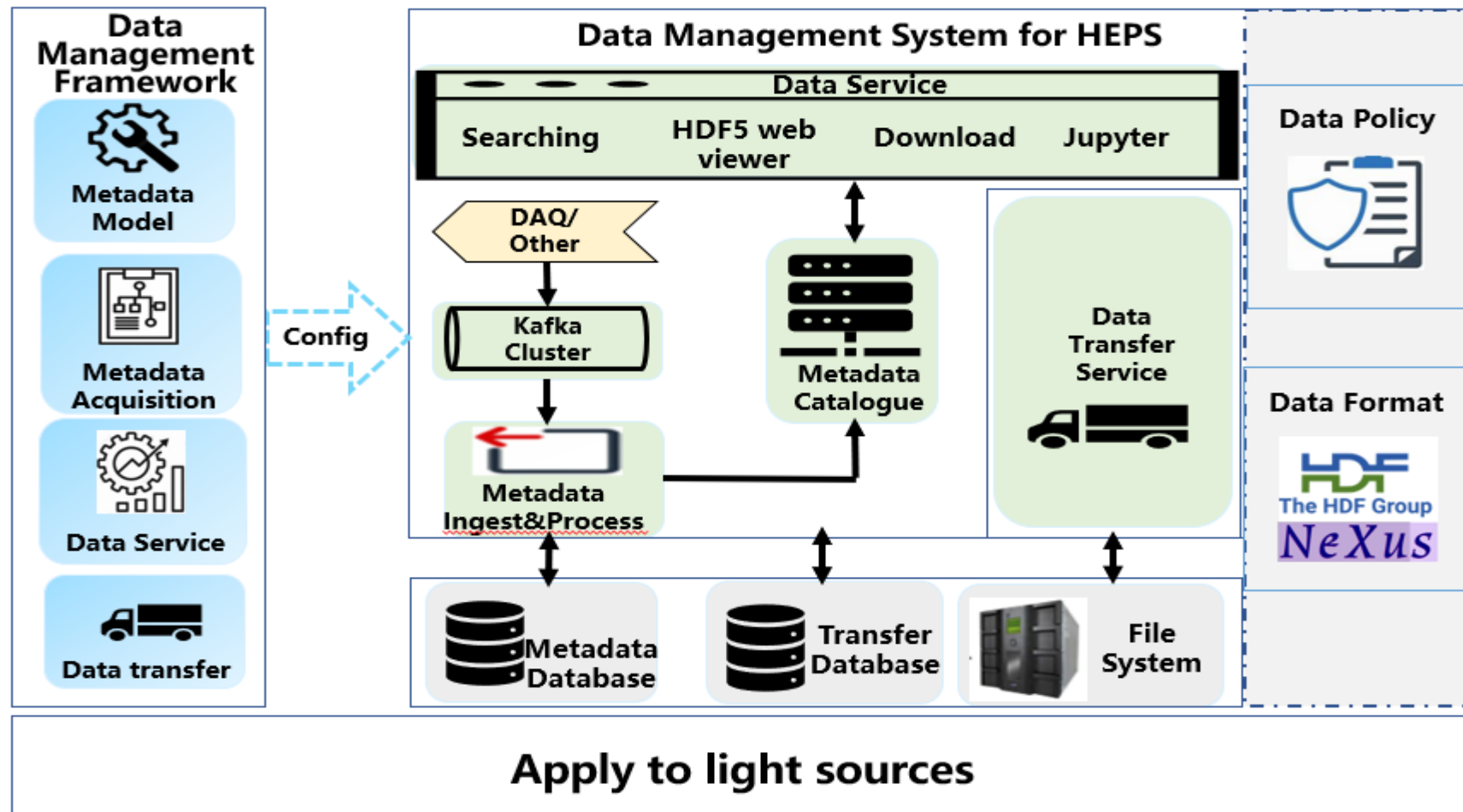
Metadata catalogue

- **Stores metadata into database and provides APIs to access metadata**
- **Use MongoDB as the database because of the complicated metadata**
- **A tool is developed to generate RESTful API automatically from metadata models**
  1. Interface developer design metadata models and create interfaces from web GUI
  2. The metadata models and interfaces can be parsed, verified and processed
  3. The APIs can be revoked by other system/modules
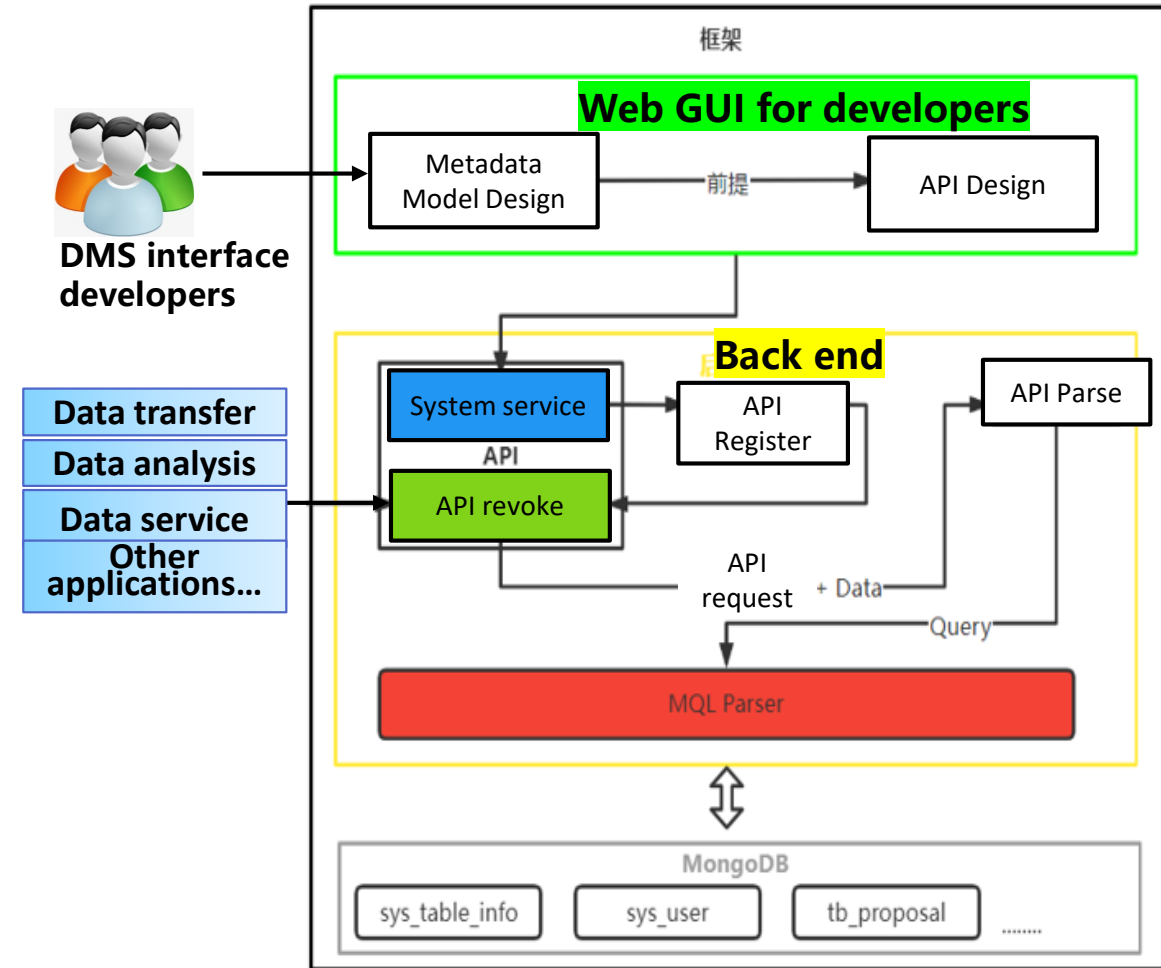
Metadata items to be cataloged

Metadata	Metadata Items	From
◆ **Administrative Metadata**	• Proposal Info, User Info, Exp types, Beamlines…	Proposal system, User service system, Transfer system, Storage, Analysis system
	• Data type: raw data, processed data, simulated data, calibration data	
	• Dataset: PID, Path, Data file list, file size, checksum…	
	• Status: disk/tape, transfer status, transfer check value	
	• Analysis software, update time…	
◆ **Scientific Metadata**	• Sample Info	Sample database, Proposal system,
	• Experimental environment：voltage、magnetic field、electric field…	DAQ system, Control system
	Detector Info: scan, x-ray exposure params…	
	• E-log	E-log System

Metadata acquisition
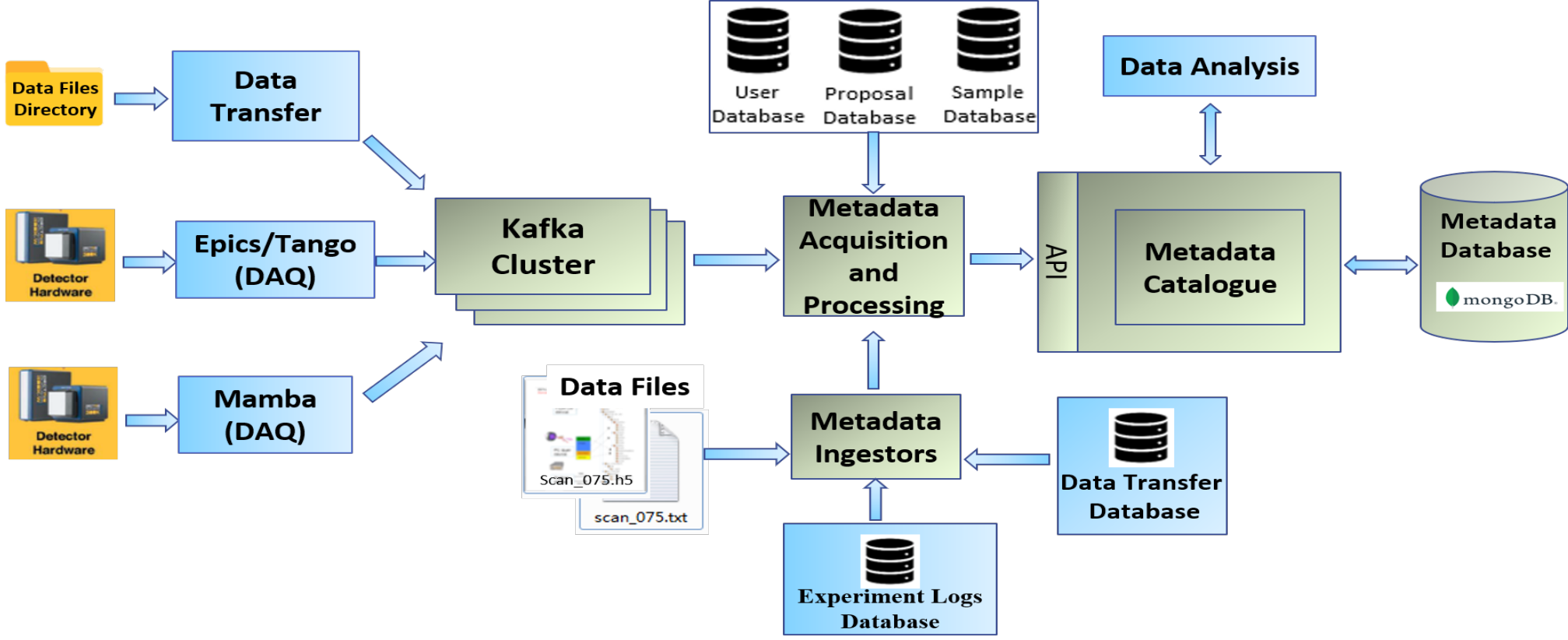
Kafka cluster

- Acquire metadata from multi-sources

- High reliability for metadata acquisition

Metadata ingestor plugins

- flexible development and deployment

- Make up for lack of interfaces

Data transfer

- Cluster deployment: control node + transfer node
- Control node: transfer task discovery, RabbitMQ, web service for configuration, Logs and cluster management
- Transfer node: transfer, logging, message interface
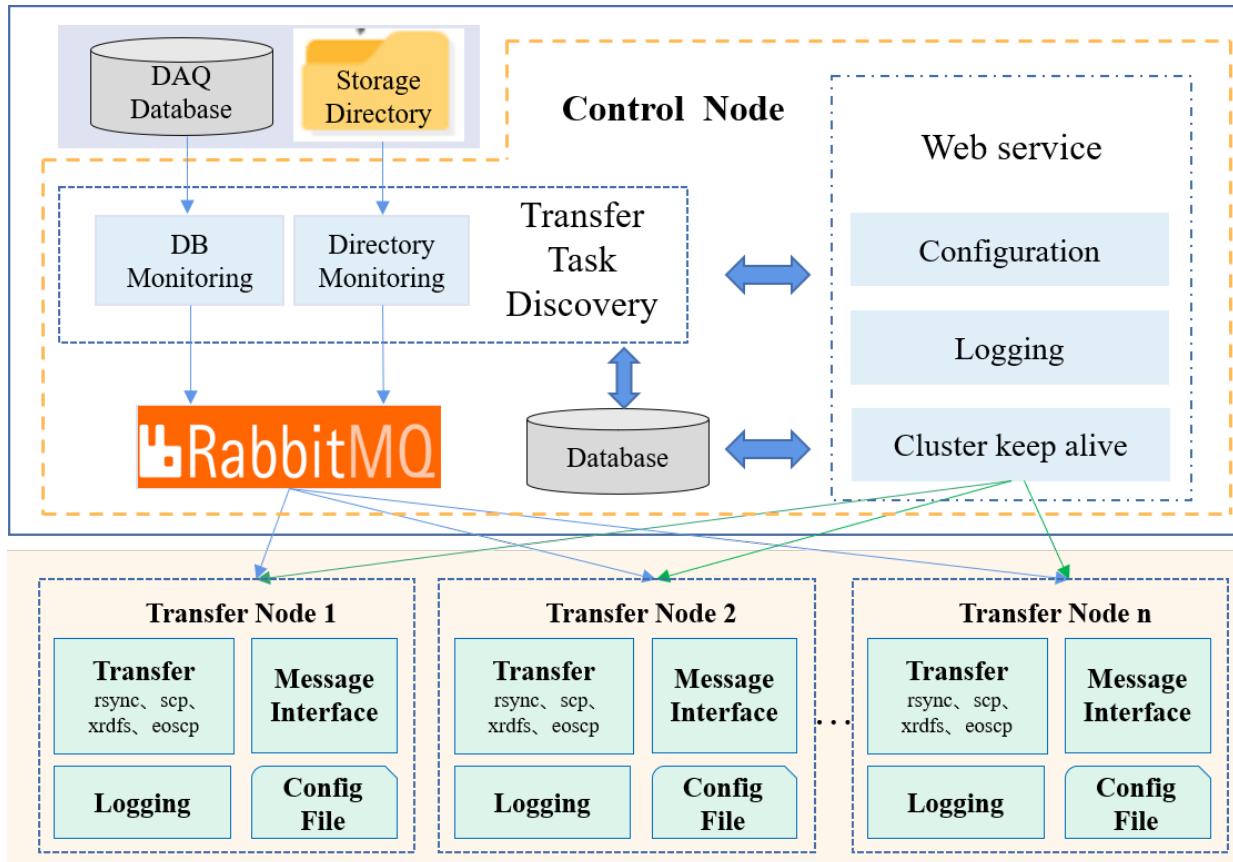
Features

1) Transfer task discovery

   Directory monitoring, Database polling

2) Transfer

   - Transfer protocols: rsync/scp/xrdfs/eoscp
   - Cluster deployment and multithreaded transfer
   - Checksum validation, retransmission

3) Configuration

   Transfer task discovery, interface, logs, cluster…

4) Logging and monitoring

   log information related to transfer failures and exceptions

An universal data transfer software, is used in other experiments (JUNO, LHAASO…)

Data service (1)-- Dedicated computer terminal

The dedicated computer terminal for data downloading

- placed at user center/user lounge

- suitable for downloading huge volume of data

- supports different storage device interfaces (NAS, disk array, mobile hard disk)

- Raw data +processed data

Dedicated computer terminal

for on-site data downloading

Data service (2)--Data Web Portal

Data search, download, access, analysis

- **Dataset search through metadata retrieval**

Beamtime ID	proposal ID	PI	PI Email	Start Time	End Time	Dataset Count	Actions
G4W1A-230723-01	2023-BEPC-PT-008641			2023-07-23 08:00:00	2023-07-25 08:00:00	1	👁 View Dataset
G4W1A-230721-01	2022-BEPC-PT-007389			2023-07-21 08:00:00	2023-07-23 08:00:00	2	👁 View Dataset
G4W1A-230720-01	2023-BEPC-PT-007867			2023-07-20 08:00:00	2023-07-21 08:00:00	5	👁 View Dataset
G4W1A-230718-01	2021-BEPC-PT-006169			2023-07-18 08:00:00	2023-07-20 08:00:00	8	👁 View Dataset
G4W1A-230717-01	2021-BEPC-PT-005200			2023-07-17 08:00:00	2023-07-18 08:00:00	2	👁 View Dataset
G4W1A-230716-01	2023-BEPC-PT-008308			2023-07-16 08:00:00	2023-07-17 08:00:00	2	👁 View Dataset
G4W1A-230714-01	2023-BEPC-PT-008530			2023-07-14 08:00:00	2023-07-16 08:00:00	1	👁 View Dataset
G4W1A-230713-01	2022-BEPC-PT-007658			2023-07-13 08:00:00	2023-07-14 08:00:00	1	👁 View Dataset
G4W1A-230711-01	2023-BEPC-PT-008278			2023-07-11 08:00:00	2023-07-13 08:00:00	1	👁 View Dataset
G4W1A-230710-01	2023-BEPC-JZ-00018			2023-07-10 08:00:00	2023-07-11 08:00:00	1	👁 View Dataset
G4W1A-230709-01				2023-07-09 08:00:00	2023-07-10 08:00:00	1	👁 View Dataset
G4W1A-230707-01	2022-BEPC-PT-006548			2023-07-07 08:00:00	2023-07-09 08:00:00	1	👁 View Dataset
G4W1A-230706-01	2023-BEPC-JZ-00006			2023-07-06 08:00:00	2023-07-07 08:00:00	1	👁 View Dataset
G4W1A-230705-01	2023-BEPC-PT-008244			2023-07-05 08:00:00	2023-07-06 08:00:00	1	👁 View Dataset
G4W1A-230704-01	2023-BEPC-PT-008244			2023-07-04 08:00:00	2023-07-05 08:00:00	0	ⓘ No Data
G4W1A-230703-01	2023-BEPC-JZ-00006			2023-07-03 08:00:00	2023-07-04 08:00:00	1	👁 View Dataset
G4W1A-230702-01	2023-BEPC-JZ-00018			2023-07-02 08:00:00	2023-07-03 08:00:00	1	👁 View Dataset

Data service (2)-- Data Web Portal

- **Browse and download data files in storage**

Data service (2)-- Data Web Portal

Integrate a client for downloading

■ Maximizes the utilization of network bandwidth

■ Greatly improves the download speed

■ Download speed test：4*4.49GB files

	Bandwidth	Duration	Speed
LAN	1000Mbps	2min52sec	839Mbps
WAN	100Mbps	28min	85Mbps

The progress of data management

1. **Finished the core functional modules**
   - ✓ Metadata catalogue, metadata ingestion, data transfer, data service
   - ✓ Interfaces with other systems, control system, transfer module, storage system, analysis system
   - ✓ Implement automatic data transfer between hierarchical storage (**beamline storage → central storage → tape**)

2. **Provide plans for data management when network interrupts**
   - ✓ when network interrupts，metadata and data are saved to local disk
   - ✓ After the network recovers, metadata will be sent to be catalogued

3. **HEPS data format design**
   - ✓ Designed and released data format for 7 beamlines

Metadata catalogue
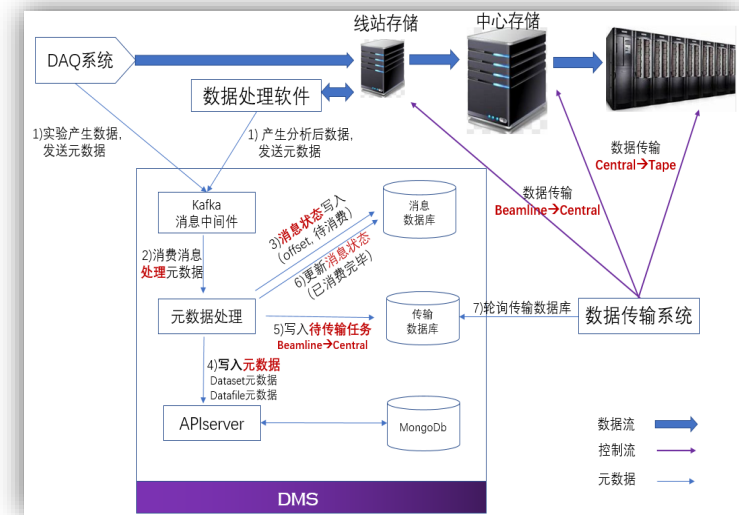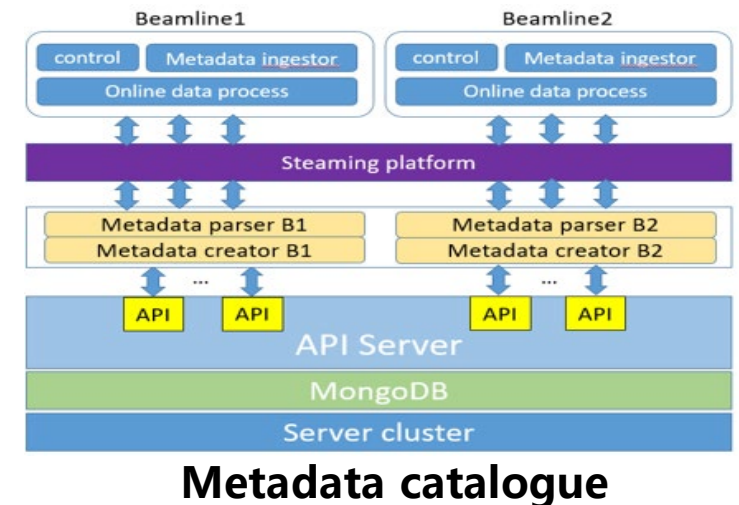
**Automatic data management flow**

HEPS CC system integration/Test bed/Production

Set up testbed at BSRF to integrate full lifecycle software systems to verify interfaces and process.

HEPS CC system has been tested in the real experimental environment, moved to production gradually.

1 **Oct, 2020, BSRF 1W1A**

Simple verification of the data management system

- Network bandwidth is 1Gb/s
- Beamline storage: **2TB** NAS, Dell EMC NX3240, NFS file system
- Central storage: **80TB** disk array, Lustre file system
- Metadata ingest, catalogue, data transfer, data service

2 **July, 2021, BSRF-3W1 test beamline**

- Network bandwidth updated to 10Gb/s
- Beamline storage & Central storage: **80TB** disk array, Lustre file system
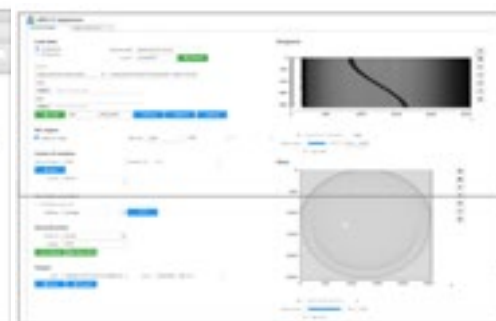- Integrate **MAMBA**,**DMS**, **Daisy**, computing system

3 **July, 2023, BSRF 4W1B/1W1A/4W1A**

Running in production environment

- Network bandwidth updated to 25Gb/s
- Beamline storage: Huawei Ocean Store 9950
- Central storage: 80TB disk array, Lustre file system
- **Follow real experiment process, provide Pymca to do analyzing**
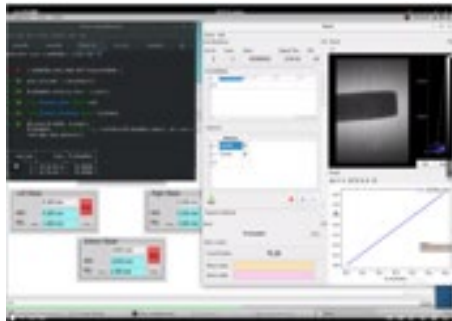
Data acquisition   **Analysis framework Interface**   **CT reconstruction**   **Integration test at BSRF**

Outline

Summary & Plan

- DOMAS is developed and will be released as open-sourced progressively

- HEPS Data Management System(DMS) has been implemented

- HEPS DMS is integrated, verified and running stably at 4W1B/1W1A/4W1A of BSRF

- The deployment of HEPSCC system on the HEPS Campus is on going, waiting for integration and testing

- Promote the application of DOMAS at SHINE and HALF

- Keep on cooperating with other light source facilities and communities

Thank you for your attention!

Comments or suggestions?