The Implementation of Data Management and Data Service for HEPS

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Outline

1. HEPS Introduction
2. Demand and Challenges of data management
3. The architecture and design of the framework
4. The progress of the system implementation
5. Summary & Plan

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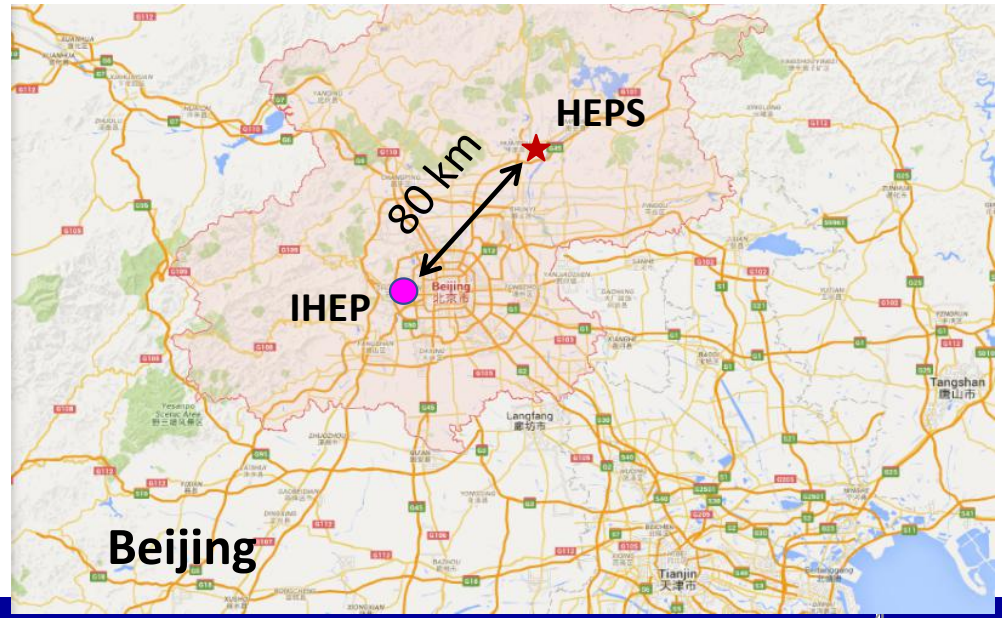
High Energy Photon Source (HEPS)

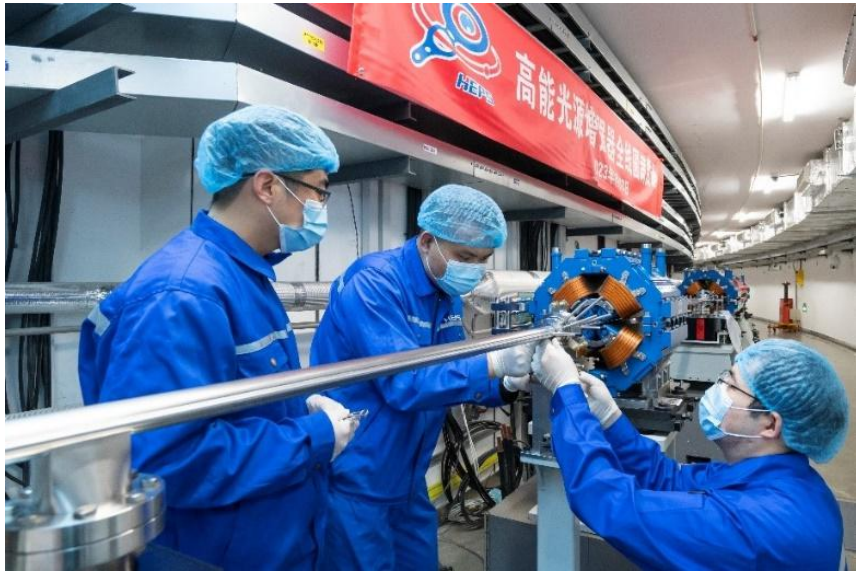
- The fourth generation light source in China — High energy, high brightness
- Located in Beijing - about 80KM from IHEP
- 15 beamlines at phase I
- The construction was started at the end of 2018
- The whole project will be finished in mid-2025

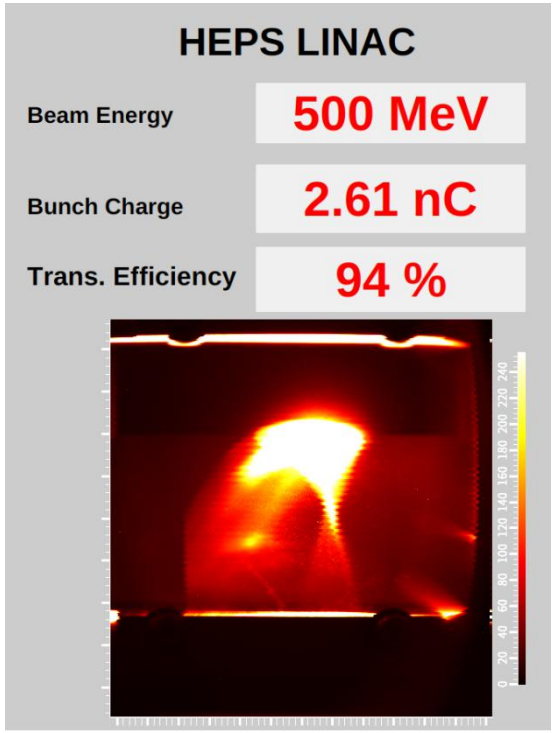
Main parameters	Unit	Value
Beam energy	GeV	6
Circumference	m	1360.4
Emittance	pm·rad	< 60
Brightness	phs/s/mm^2/mrad^2/0.1%BW	>1x10^{22}
Beam current	mA	200
Injection		Top-up



Progress of the HEPS project

- The construction of the civil structure completed. Now at the stage of equipment installation
- 2023.01, HEPS booster installation completed
- 2023.02, Start installation of storage ring
- 2023.03, HEPS achieved the first electron beam accelerated to 500 MeV.





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Data Challenges @HEPS

- Increased source brightness
  - More raw data in greater detail and less time
- X-ray detector capabilities constantly improving:
  - Increased dynamic range, faster readout rates, larger pixel arrays
  - Bigger frames, higher frame rates => more raw data
- **>24PB raw data per month** for Phase I (15 beamlines)
- More than 90 beamlines volume in total

Estimated data volume of HEPS

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

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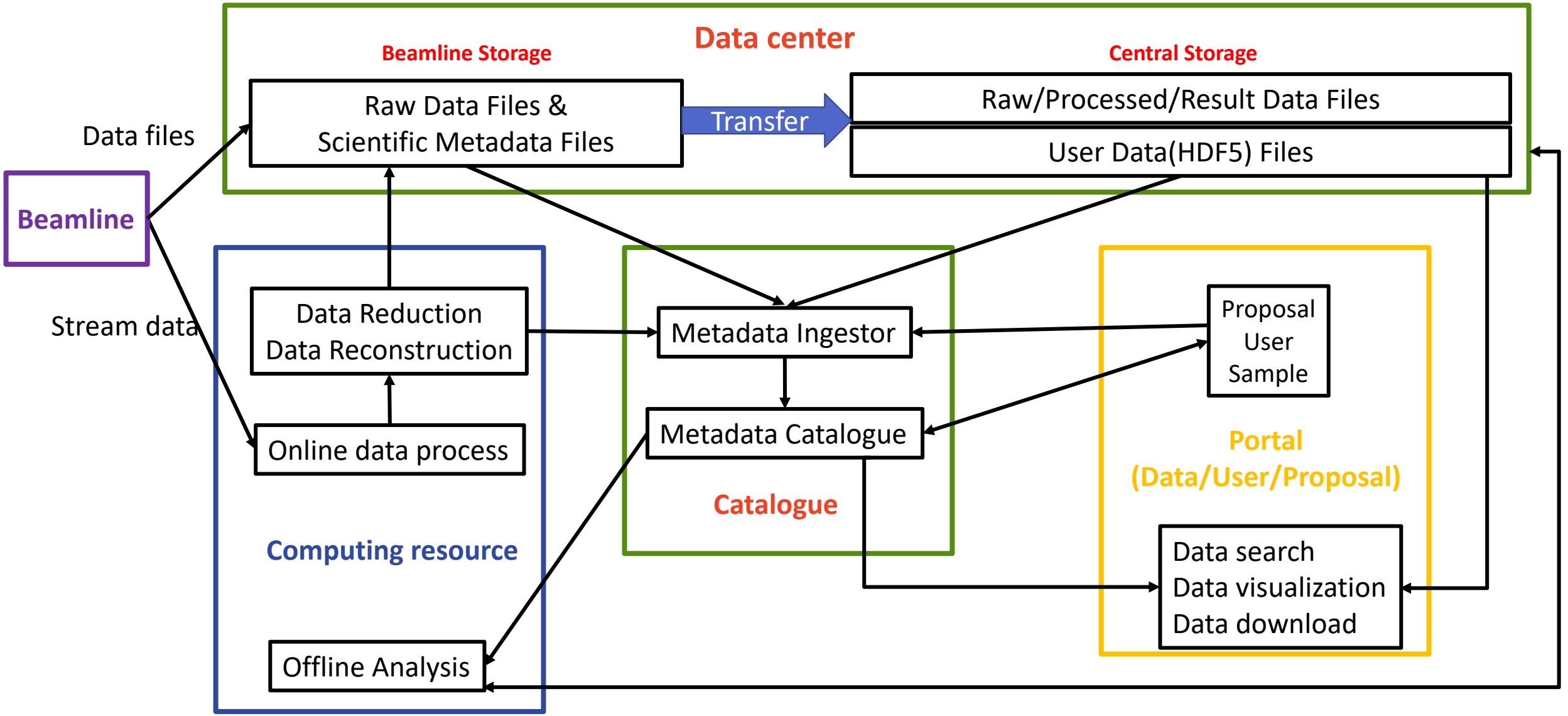
Data Flow

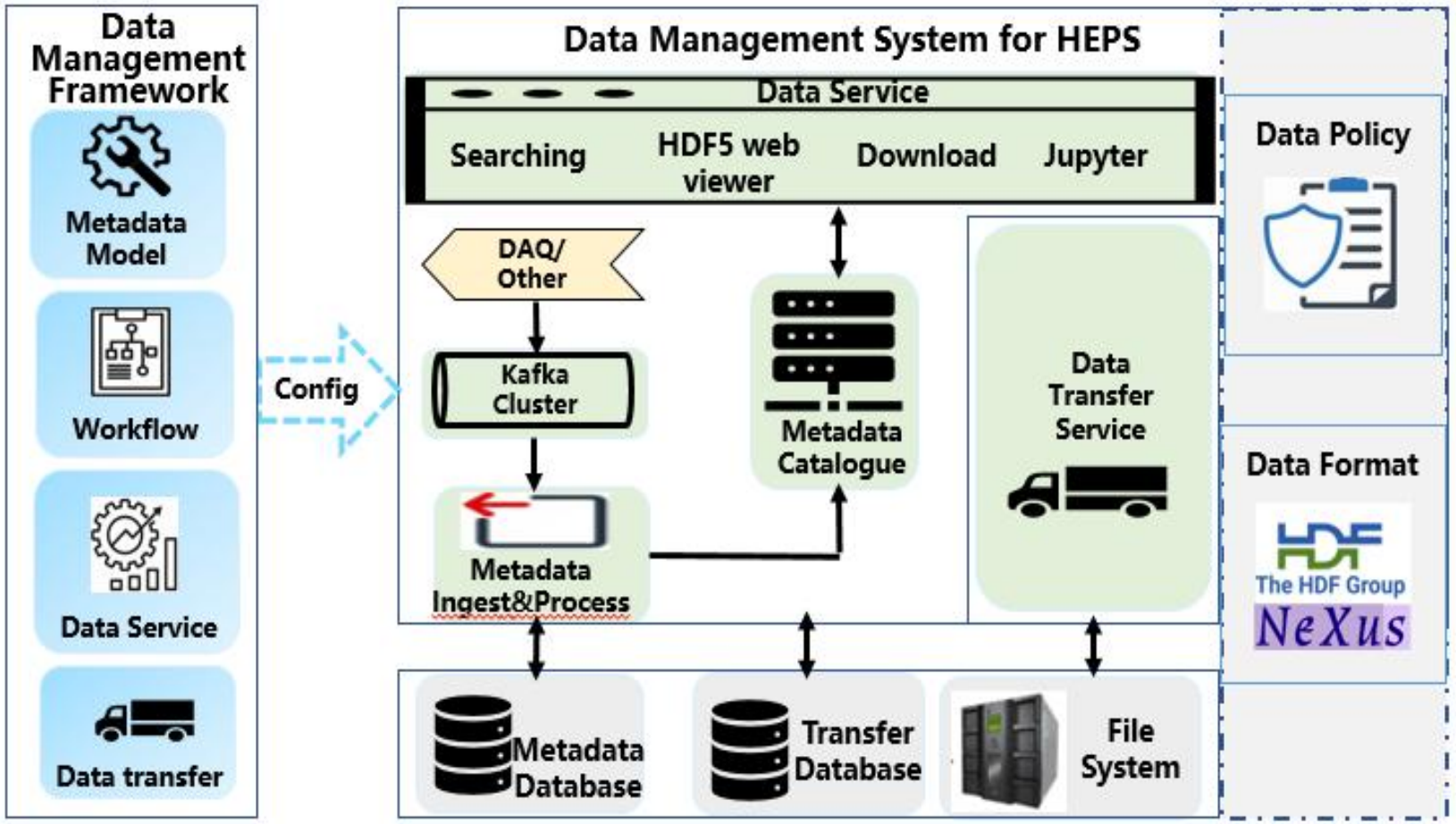

Data center
Beamline Storage
Central Storage
Raw Data Files &
Scientific Metadata Files
Transfer
Raw/Processed/Result Data Files
User Data(HDF5) Files
Data files
Beamline
Stream data
Data Reduction
Data Reconstruction
Online data process
Computing resource
Metadata Ingestor
Metadata Catalogue
Catalogue
Proposal
User
Sample
Portal
(Data/User/Proposal)
Data search
Data visualization
Data download
Offline Analysis

Tasks & Goals of Data Management

- **Data policy and Data Format**
  - The ownership, curation, archiving and access to scientific data and metadata
  - HDF5 is chosen as the standard data file format, follows NeXus conventions
- **Metadata catalogue**
  - Support the management of the whole scientific data lifecycle
  - Hierarchical storage: beamline storage → central storage → tape
  - Catalogue and provide access to scientific metadata and raw experimental data
- **Metadata acquisition**
  - Ingest metadata from other sub-systems(DAQ, transfer, storage, analysis…)
- **Data transfer**
  - Transfer all the data between beamline storage, central storage and 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

DOMAS-Data Organization Management Access Software

- Common function modules of data management
  - ✓ Metadata Model
  - ✓ Workflow
  - ✓ Data transfer
  - ✓ Data service
- Extensible and standard interface
- Be able to build data management system suitable for facilities/beamline quickly



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HEPS Data Policy

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

- Recommend providing at least 3 months disk storage and permanent tape archive (depends on final funding)
- Provide permanent storage for raw data
- Provide temporary storage for processed data, calibration data and result 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.

A draft version of ***The Data Policy for HEPS*** is finished, which will be discussed and approved by the HEPS council.

Reference:

http://pan-data.eu/sites/pan-data.eu/files/PaN-data-D2-1.pdf

https://in.xfel.eu/upex/docs/upex-scientific-data-policy.pdf

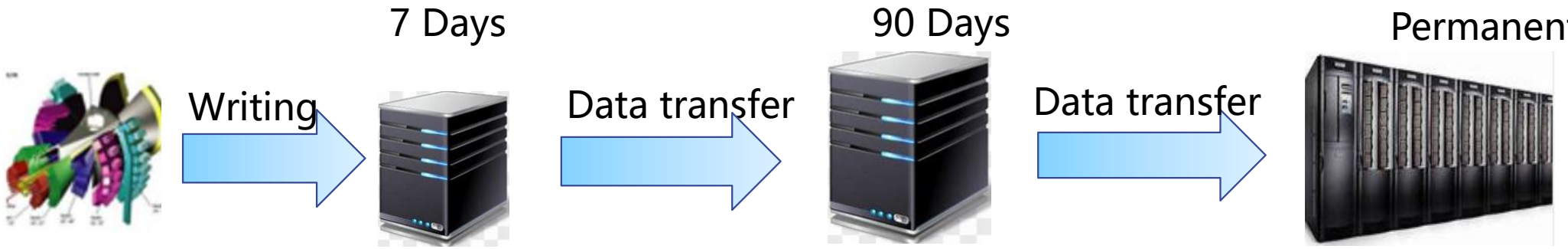
Data storage policy

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

② **Data transfer module moves data from beamline storage to central storage , data are kept up to 90 days**

③ **Data transfer module moves data from central storage to tape for permanent storage.**

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



Detector DAQ system

Beamline storage

- SSD
- High speed data IO

Central storage

- SSD+HDD
- Medium-high speed data IO

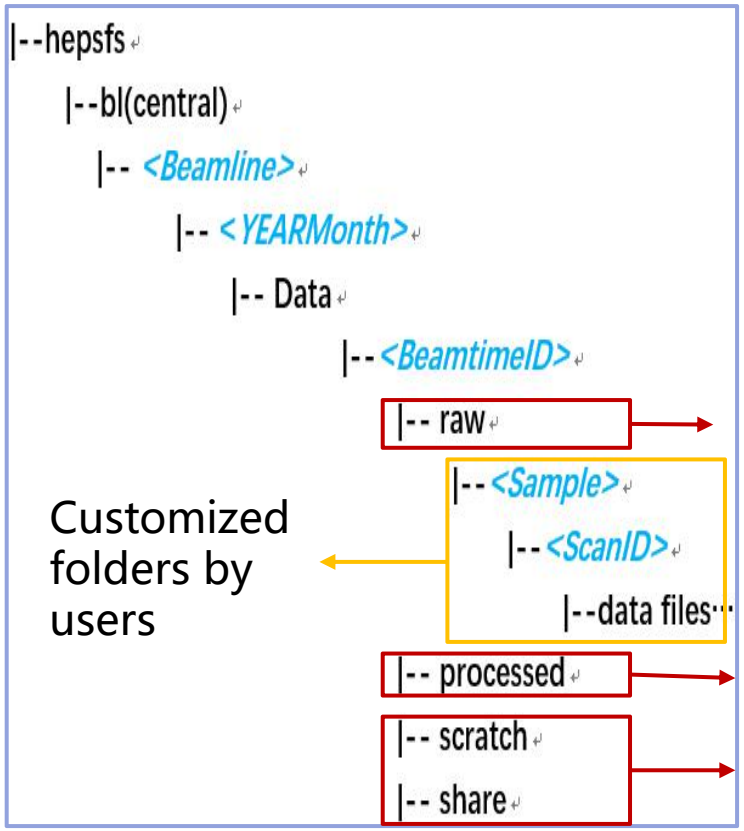
Tape

- Permanent data archive
- Prepare the data before retrieve

Data directory and ACLs

- One proposal have several experiments, each experiment is assigned beam time (BeamtimeID)
- Data path : ../<*Beamline*>/<*YearMonth*>/Data/<*BeamtimeID*>
- User access is restricted by setting ACLs of file system on folder *BeamtimeID*
- 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

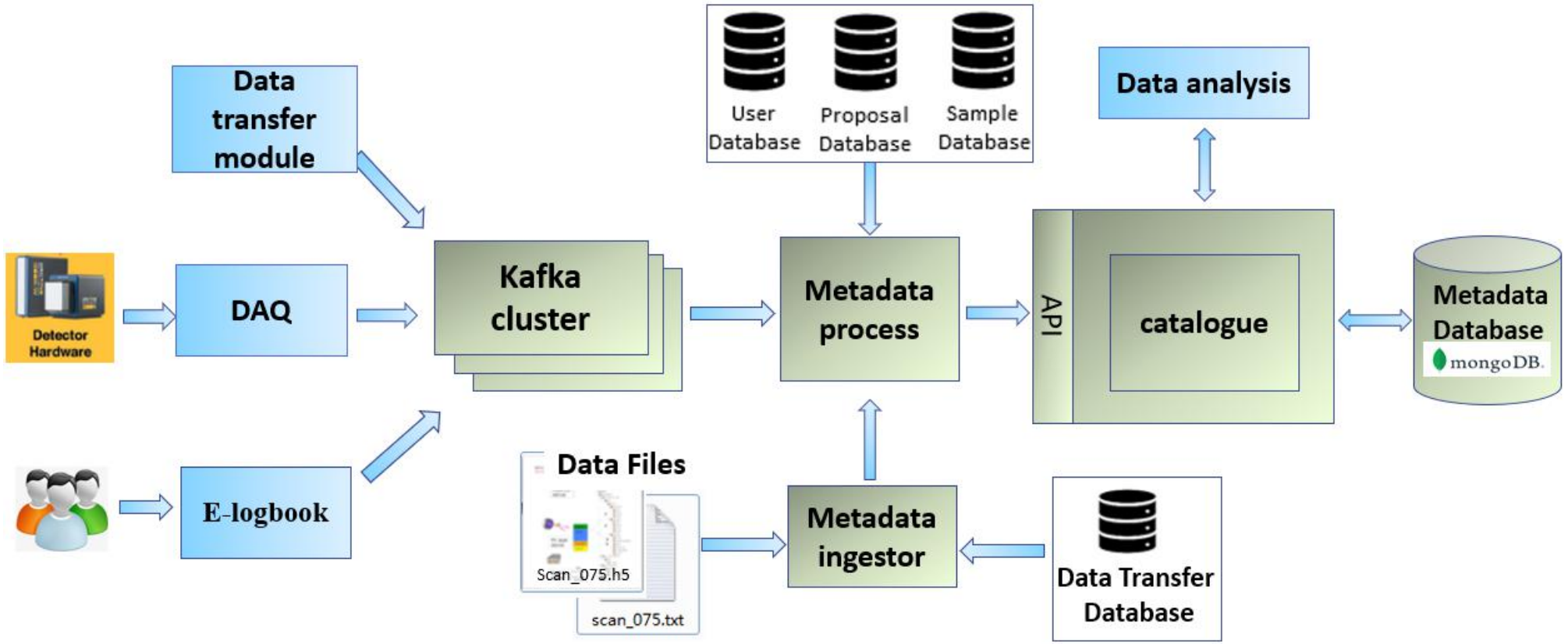


Data directory structure

Metadata items to be cataloged

Metadata	Metadata Items	From
◆ **Administrative Metadata**	• Proposal Info, User Info, Exp type, Beamline…	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,
	• Exp environment params：voltage、magnetic field、electric field… Detector Info: scan, x-ray exposure params…	DAQ system, Control system
	• E-log	E-log System

Metadata acquisition– for cataloging



Message queue

- Acquire metadata from multi-sources
- High reliability for metadata catalogue

API interfaces

- RESTful API
- Easy for other modules to call

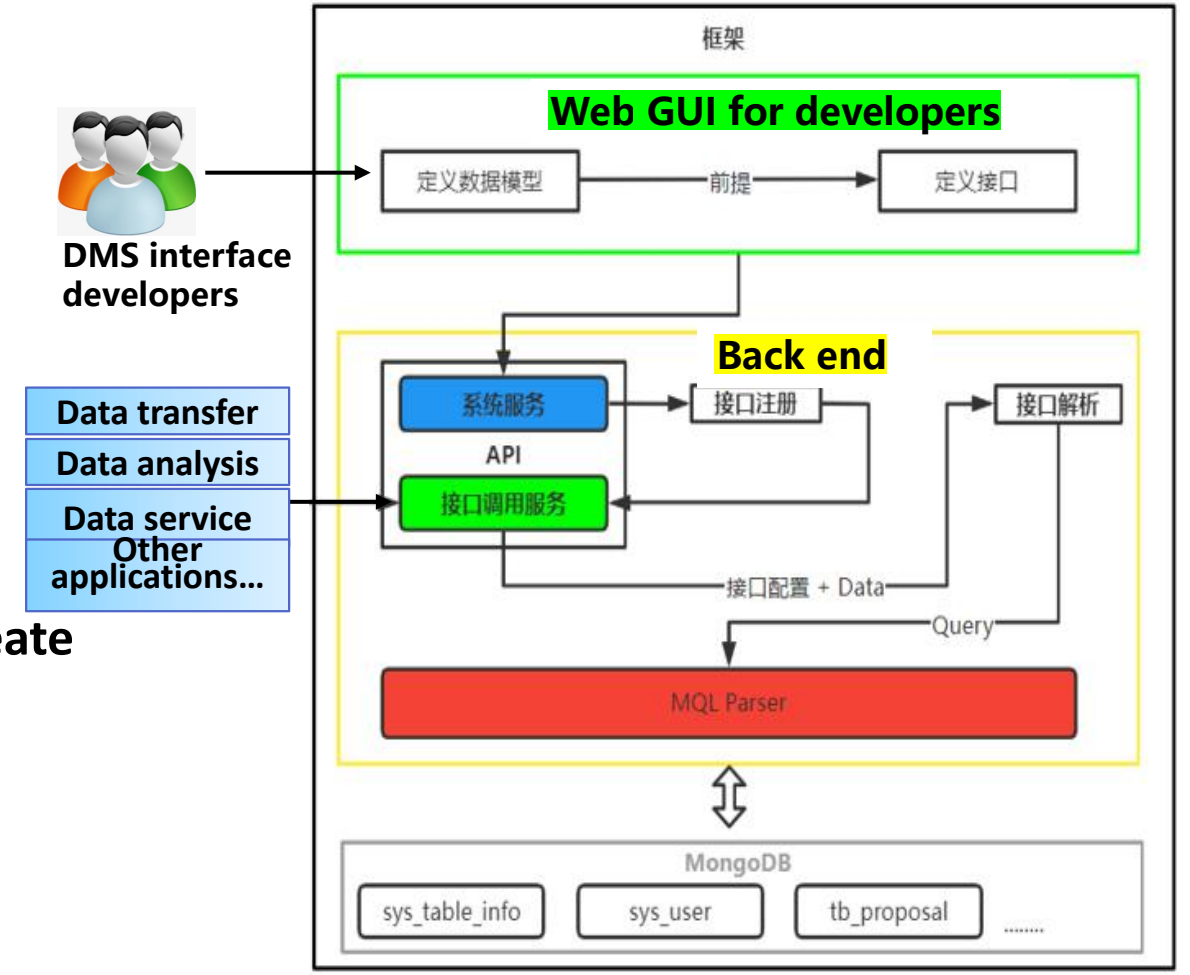
Metadata ingestor plugins

- flexible development and deployment
- Make up for lack of interfaces

Metadata catalogue

- Catalogue is the core module of data management system，which provides metadata APIs for other applications/modules
- Use MongoDB as the database because of the complicated metadata
- A tool is developed to generate interfaces automatically from metadata models

1. **Interface developer design metadata models and create interfaces from web GUI**
2. **The metadata models and interfaces are parsed and verified**
3. **The APIs can be called by other system/modules**



Data service (1)

The dedicated computer is designed for user to download data at the facility

- suitable for users to download huge volume of data
- placed at user center/user lounge
- support different storage device interfaces (NAS, disk array, mobile hard disk)

Dedicated computer for data download at HEPS

Data service (2)

Data Web Portal

- Data search/download, HDF5 file view, data analysis, logbook

数据集: | BeamtimeID: | PI: | PI Email: | ScanID: | 获取时间: 请选择日期 to 请选择日期 | 查询 | 重置

如果数据下载出现问题，请联系管理员获取数据

批量下载

数据集	BeamtimeID	样品	PI	PI Email	获取时间	ScanId	Size	操作
Fe3O4-50nm	GB06-20220718-01		刘敦一	liudy1989@swu.edu.cn	2022-07-20 09:23:31	19	157.73MB	查看数据 下载
Fe3O4-20nm	GB06-20220718-01		刘敦一	liudy1989@swu.edu.cn	2022-07-20 09:12:23	18	157.73MB	查看数据 下载
Fe3O4-20nm	GB06-20220718-01		刘敦一	liudy1989@swu.edu.cn	2022-07-20 09:05:01	17	157.73MB	查看数据 下载
Fe3O4-20nm	GB06-20220718-01		刘敦一	liudy1989@swu.edu.cn	2022-07-20 09:02:51	16	157.73MB	查看数据 下载
Cit-Fe	GB06-20220718-01		刘敦一	liudy1989@swu.edu.cn	2022-07-20 08:53:30	15	157.73MB	查看数据 下载
Cit-Fe	GB06-20220718-01		刘敦一	liudy1989@swu.edu.cn	2022-07-20 08:44:20	14	157.73MB	查看数据 下载
5D-FESO4	GB06-20220718-01		刘敦一	liudy1989@swu.edu.cn	2022-07-20 08:33:47	13	157.73MB	查看数据 下载
5D-FESO4	GB06-20220718-01		刘敦一	liudy1989@swu.edu.cn	2022-07-20 08:22:41	12	157.73MB	查看数据 下载
Fe-50nm	GB06-20220718-01		刘敦一	liudy1989@swu.edu.cn	2022-07-20 08:12:14	11	157.73MB	查看数据 下载
Fe-50nm	GB06-20220718-01		刘敦一	liudy1989@swu.edu.cn	2022-07-20 08:02:31	10	157.73MB	查看数据 下载
Fe-50nm	GB06-20220718-01		刘敦一	liudy1989@swu.edu.cn	2022-07-20 07:51:33	9	157.73MB	查看数据 下载
2-Fe3O4-50nm	GB06-20220718-01		刘敦一	liudy1989@swu.edu.cn	2022-07-20 07:38:01	8	157.73MB	查看数据 下载

Data service (2)

Data files browser in Data Web Portal

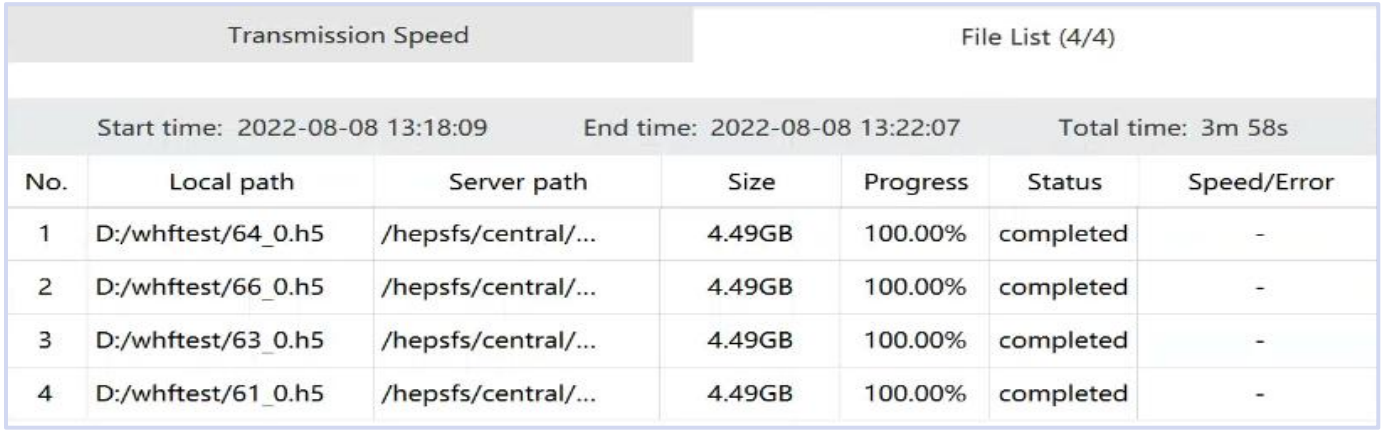
Data service (3)

Data download client in Data Web Portal

- Provide the file download client
- Maximize the utilization of network bandwidth
- Significant improvement in download speed

- Download speed test ：4*4.49GB files

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



No.	Local path	Server path	Size	Progress	Status	Speed/Error
1	D:/whftest/64_0.h5	/hepsfs/central/...	4.49GB	100.00%	completed	-
2	D:/whftest/66_0.h5	/hepsfs/central/...	4.49GB	100.00%	completed	-
3	D:/whftest/63_0.h5	/hepsfs/central/...	4.49GB	100.00%	completed	-
4	D:/whftest/61_0.h5	/hepsfs/central/...	4.49GB	100.00%	completed	-

HEPS CC system integration/Test bed/Production

Set up testbed, integrate full data lifecycle software systems to verify the system interfaces, run in the real experimental environment, move 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 DAQ system, data management system, analysis software framework, computing cluster

3

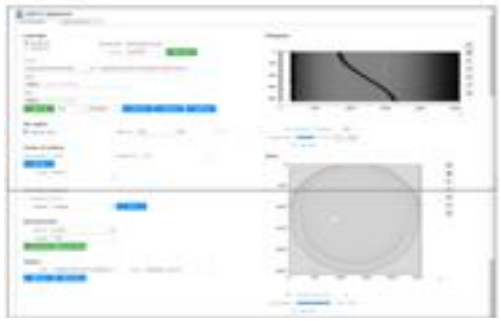
June, 2022, BSRF 4W1B

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 analysing**

Data acquisition

Analysis framework Interface



CT reconstruction

Integration test at BSRF

Summary & Plan

- The data management framework DOMAS is developed and released
- DOMAS is used to develop data management system at HEPS
- The data management and data service has been integrated with other sub-systems and verified at beamlines of BSRF
- Data management and data service are running stably at 4W1B(X-ray fluorescence microanalysis beamline) of BSRF
- Cooperation with other facilities and community is ongoing
- We also hope to have chance to cooperate with other Facilities, like PSI/MAXIV/DESY etc.

Thank you for your attention!