The Implementation of Data Management and Data Service for HEPS

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speaker: Hao-Kai Sun

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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
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
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

<table>
<thead>
<tr>
<th>Main parameters</th>
<th>Unit</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Beam energy</td>
<td>GeV</td>
<td>6</td>
</tr>
<tr>
<td>Circumference</td>
<td>m</td>
<td>1360.4</td>
</tr>
<tr>
<td>Emittance</td>
<td>pm·rad</td>
<td>&lt; 60</td>
</tr>
<tr>
<td>Brightness</td>
<td>phs/s/mm²/mrad²/0.1%BW</td>
<td>&gt;1x10²²</td>
</tr>
<tr>
<td>Beam current</td>
<td>mA</td>
<td>200</td>
</tr>
<tr>
<td>Injection</td>
<td></td>
<td>Top-up</td>
</tr>
</tbody>
</table>
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.

HEPS LINAC

- Beam Energy: 500 MeV
- Bunch Charge: 2.61 nC
- Trans. Efficiency: 94 %
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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

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

**Total average:**

- 805.4TB/day,
- 24.16PB/month

IHEPCC & HEPSCC
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
Data Flow

- Raw Data Files & Scientific Metadata Files
- Online data process
- Metadata Ingestor
- Metadata Catalogue
- Catalogue
- Data search
- Data visualization
- Data download
- Proposal
- User Sample
- Portal (Data/User/Proposal)
- Raw/Processed/Result Data Files
- User Data (HDF5) Files

Data files

Beamline Storage

Central Storage

Data center

Computing resource

Offline Analysis

Transfer
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
1. HEPS Introduction
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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:*

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 has 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.

<table>
<thead>
<tr>
<th>Folder</th>
<th>Data type</th>
<th>Permission</th>
<th>Permanent archive?</th>
</tr>
</thead>
<tbody>
<tr>
<td>raw</td>
<td>Raw data/user data</td>
<td>Read only</td>
<td>Yes</td>
</tr>
<tr>
<td>processed</td>
<td>Processed data</td>
<td>Read, write</td>
<td>No</td>
</tr>
<tr>
<td>scratch</td>
<td>Temp data, snapshots, scripts,</td>
<td>Read, write</td>
<td>No</td>
</tr>
<tr>
<td>share</td>
<td>Snapshots, scripts, shared files</td>
<td>Read, write, shared</td>
<td>No</td>
</tr>
</tbody>
</table>
## Metadata items to be cataloged

<table>
<thead>
<tr>
<th>Metadata</th>
<th>Metadata Items</th>
<th>From</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Administrative Metadata</strong></td>
<td>Proposal Info, User Info, Exp type, Beamline...</td>
<td>Proposal system, User service system, Transfer system, Storage, Analysis system</td>
</tr>
<tr>
<td></td>
<td>Data type: raw data, processed data, simulated data, calibration data</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Dataset : PID, Path, Data file list, file size, checksum...</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Status: disk/tape, transfer status, transfer check value</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Analysis software, update time...</td>
<td></td>
</tr>
<tr>
<td><strong>Scientific Metadata</strong></td>
<td>Sample Info</td>
<td>Sample database, Proposal system, DAQ system, Control system</td>
</tr>
<tr>
<td></td>
<td>Exp environment params : voltage, magnetic field, electric field...</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Detector Info: scan, x-ray exposure params...</td>
<td></td>
</tr>
<tr>
<td></td>
<td>E-log</td>
<td>E-log System</td>
</tr>
</tbody>
</table>
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
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

Table:

<table>
<thead>
<tr>
<th>样品</th>
<th>PI Email</th>
<th>获取时间</th>
<th>ScanId</th>
<th>Size</th>
<th>操作</th>
</tr>
</thead>
<tbody>
<tr>
<td>FeSO4-50nm</td>
<td><a href="mailto:ludy1989@swu.edu.cn">ludy1989@swu.edu.cn</a></td>
<td>2022-07-20 09:23:31</td>
<td>19</td>
<td>157.73MB</td>
<td>下载</td>
</tr>
<tr>
<td>Fe3O4-20nm</td>
<td><a href="mailto:ludy1989@swu.edu.cn">ludy1989@swu.edu.cn</a></td>
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</tr>
<tr>
<td>Fe3O4-20nm</td>
<td><a href="mailto:ludy1989@swu.edu.cn">ludy1989@swu.edu.cn</a></td>
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<td>下载</td>
</tr>
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<td>Fe3O4-20nm</td>
<td><a href="mailto:ludy1989@swu.edu.cn">ludy1989@swu.edu.cn</a></td>
<td>2022-07-20 09:02:51</td>
<td>16</td>
<td>157.73MB</td>
<td>下载</td>
</tr>
<tr>
<td>Fe-50nm</td>
<td><a href="mailto:ludy1989@swu.edu.cn">ludy1989@swu.edu.cn</a></td>
<td>2022-07-20 08:12:14</td>
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<td>157.73MB</td>
<td>下载</td>
</tr>
<tr>
<td>Fe-50nm</td>
<td><a href="mailto:ludy1989@swu.edu.cn">ludy1989@swu.edu.cn</a></td>
<td>2022-07-20 07:51:33</td>
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<td>157.73MB</td>
<td>下载</td>
</tr>
<tr>
<td>2-Fe3O4-50nm</td>
<td><a href="mailto:ludy1989@swu.edu.cn">ludy1989@swu.edu.cn</a></td>
<td>2022-07-20 07:30:01</td>
<td>8</td>
<td>157.73MB</td>
<td>下载</td>
</tr>
</tbody>
</table>
## Data service (2)

### Data files browser in Data Web Portal

![File Manager](image)

<table>
<thead>
<tr>
<th>文件名</th>
<th>类型</th>
<th>大小</th>
<th>操作</th>
</tr>
</thead>
<tbody>
<tr>
<td>Jzhang-red-1_None.h5</td>
<td>file</td>
<td>142.53 kb</td>
<td>下载</td>
</tr>
<tr>
<td>S4-1-0.1s-10mu_None_0.h5</td>
<td>file</td>
<td>142.53 kb</td>
<td>下载</td>
</tr>
<tr>
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<td>JZhang-red_None_1.h5</td>
<td>file</td>
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<tr>
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<tr>
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<td>下载</td>
</tr>
<tr>
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<td>file</td>
<td>407.81 MB</td>
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<tr>
<td>S2-1-0.2-20mu-test2_0_0.h5</td>
<td>file</td>
<td>33.53 MB</td>
<td>下载</td>
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<tr>
<td>HS2-1-0.2s-20mu_0.h5</td>
<td>file</td>
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<tr>
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<td>file</td>
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</tr>
</tbody>
</table>
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

<table>
<thead>
<tr>
<th></th>
<th>Bandwidth</th>
<th>Spend</th>
<th>Speed</th>
</tr>
</thead>
<tbody>
<tr>
<td>LAN</td>
<td>1000Mbps</td>
<td>2min52sec</td>
<td>839Mbps</td>
</tr>
<tr>
<td>WAN</td>
<td>100Mbps</td>
<td>28min</td>
<td>85Mbps</td>
</tr>
</tbody>
</table>

Transmission Speed

<table>
<thead>
<tr>
<th>No.</th>
<th>Local path</th>
<th>Server path</th>
<th>Size</th>
<th>Progress</th>
<th>Status</th>
<th>Speed/Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>D:/whitest/64_0.h5</td>
<td>/hepsfs/central/about/</td>
<td>4.49GB</td>
<td>100.00%</td>
<td>completed</td>
<td>-</td>
</tr>
<tr>
<td>2</td>
<td>D:/whitest/66_0.h5</td>
<td>/hepsfs/central/about/</td>
<td>4.49GB</td>
<td>100.00%</td>
<td>completed</td>
<td>-</td>
</tr>
<tr>
<td>3</td>
<td>D:/whitest/63_0.h5</td>
<td>/hepsfs/central/about/</td>
<td>4.49GB</td>
<td>100.00%</td>
<td>completed</td>
<td>-</td>
</tr>
<tr>
<td>4</td>
<td>D:/whitest/61_0.h5</td>
<td>/hepsfs/central/about/</td>
<td>4.49GB</td>
<td>100.00%</td>
<td>completed</td>
<td>-</td>
</tr>
</tbody>
</table>
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!