A DATA MANAGEMENT INFRASTRUCTURE FOR NEUTRON SCATTERING EXPERIMENTS IN J-PARC/MLF

K.Moriyama# and T.Nakatani, J-PARC, Ibaraki, Japan

Abstract

The role of data management is one of the greatest contributions in the research workflow for scientific experiments such as neutron scattering. The facility is required to safely and efficiently manage a huge amount of data over the long duration, and provide an effective data access for facility users promoting the creation of scientific results. In order to meet these requirements, we are operating and updating a data management infrastructure in J-PAPC/MLF, which consists of the web-based integrated data management system called the MLF Experimental Database (MLF EXP-DB), the hierarchical raw data repository composed of distributed storages, and the integrated authentication system. The MLF EXP-DB creates experimental data catalogues in which raw data, measurement logs, and other contextual information on sample, experimental proposal, investigator, etc. are interrelated. This system conducts the reposition, archive and on-demand retrieve of raw data in the repository. Facility users are able to access the experimental data via a web portal. This contribution presents the overview of our data management infrastructure, and the recent updated features for high availability, scaling-out, and flexible data retrieval in the MLF EXP-DB.

INTRODUCTION

The Materials and Life Science Experimental Facility (MLF) at the Japan Proton Accelerator Research Complex (J-PARC) is the experimental facility for neutron scattering, providing domestic and international users in a wide variety of research fields with one of the highest intensity pulsed neutron beam in the world. Twenty neutron experimental instruments equipped with large-area neutron detectors and various sample environmental apparatuses are currently in operation. MLF annually supplies beamtime of two hundreds days for about a thousand users and about several hundreds of experimental proposals are performed using these neutron instruments.

Neutron instruments create a huge amount of experimental data. A typical volume of data produced in one experiment is from several tens MB to several hundreds GB. Since a lot of experiments under various experimental conditions are carried out in a short period of time using high intensity beam, the total amount of data generated annually in a whole facility at full performance is on the order of PB.

In those situations, it is required to safely and efficiently manage a huge amount of data over the long duration. In particular, an appropriate protection and preservation of the experimental data as intellectual property produced at a large experimental facility such as MLF is required recently. Furthermore, it is required to provide facility users with a data access service enabling effective utilization of a lot of experimental data. To meet these requirements, we are operating an infrastructure for a central data management and access in the whole facility. In addition, we are updating the MLF EXP-DB, which is the core system of our infrastructure, responding to the expansion and growth of experimental environment based on an improvement plan in the facility. Since the neutron beam currently provided with bombarding of 500kW proton beam is finally increasing up to the intensity equivalent to the power of 1 MW proton beam, therefore the infrastructure should respond the enhancement of data production rate due to the intensity enhancement of neutron beam.

DATA MANAGEMENT INFRASTRUCTURE

A data management infrastructure in J-PARC/MLF is comprised of several database systems and the data repository. The schematic overview of the infrastructure is shown in Fig. 1. The MLF EXP-DB is the core system of the infrastructure, and responsible for managing data and providing data access. This system catalogues experimental data and manages measurement raw data centrally in the whole facility. Measurement raw data is preserved in the data repository. The MLF Business Database (MLF BIZ-DB) collects application information such as experimental proposal, primary investigator, and sample from the front end system of facility users. Also, there are an integrated authentication system (User DB), which manages user credentials of systems comprising infrastructure, and a sample database (Sample-DB) for a safety management of handling samples. The MLF EXP-DB collects automatically every variety of information related to experiment by interacting with these database systems.

In local system of neutron instrument at MLF, the MLF control software framework "IROHA" [1], which is adopted as standard software for measurement, coordinates measurement with controlling data acquisition and sample environmental devices. In response to the message from IROHA, the data acquisition system (DAQ) produces raw data files into the data storage. Also, measurement log file including measurement conditions such as sample device configuration and results is created as "experimental meta-data" in XML-format by IROHA. This experimental

#kentaro.moriyama@j-parc.jp

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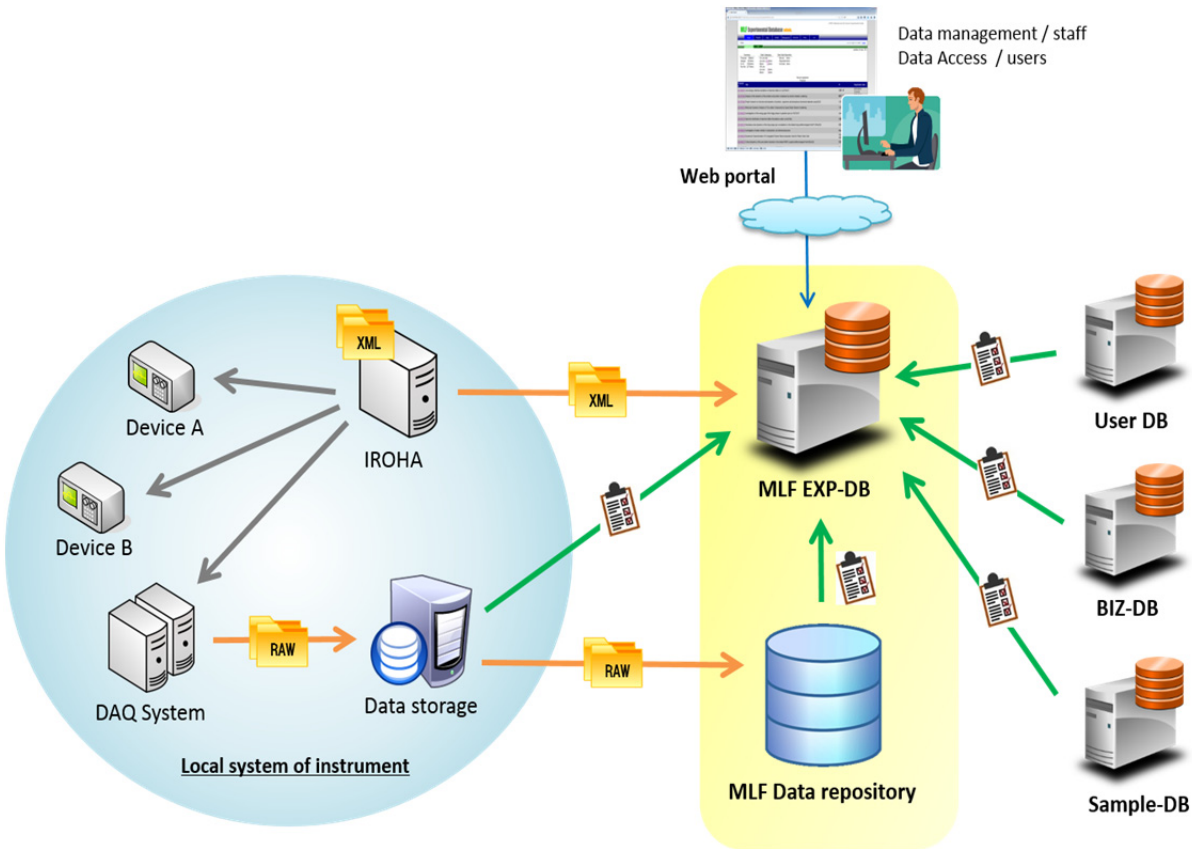

Figure 1: The schematic overview of the data management infrastructure in J-PARC/MLF.

meta-data is crucial information for the management and utilization of the experimental data.

The MLF EXP-DB collects the experimental meta-data and meta-information for raw data such as file name, location path on the storage, and size from local systems of the neutron instruments, and registers them on the experimental data catalogue with associated information collected from other database systems. Raw data registered on the catalogue is transferred from local data storage at instruments to the data repository by the MLF EXP-DB. The MLF EXP-DB provides web portals with the facility staff and users. These web portals are a front-end of the infrastructure. All of data management and access is performed via web portals.

MLF EXPERIMENTAL DATABASE

System Architecture

The system employs a Java-based commercial database software package, named "R&D Chain Management System Software (RCM) [2], based on the XML-DB architecture suitable for the handling data with flexible structure such as our experimental meta-data described in XML-format. The flexibility of the XML-DB is quite suitable for the handling of the experimental meta-data.

The RCM serves an integrated web database system designed on a three-layer model consisting of three components; RCM-Web, RCM-Controller and RCM-DB. These components run on the single physical server. The RCM-Controller has a XML-based workflow engine, and executes any control of database and remote servers according to workflow templates in which settings of job sequence are described in XML-format. Therefore, all of procedures for data cataloguing, raw data management, search for data access, etc. is implemented in the workflow templates. Result of each procedure is converted from XML to HTML using XSLT [3] that is a language for transforming XML documents into other XML documents and then web page is offered to system users via the RCM-Web. The experimental data collected from remote server in local systems of the neutron instruments are registered to the XML tree held on RCM-DB.

Access control is quite important for the data management and access. A disclosure level of data such as public, private, and share should be closely managed. In RCM, information on owner and authority is imparted as attribute to the every XML element. Therefore, access to the XML tree on RCM-DB is controlled in unit of XML element by referring this attribute. Allocating group such as the instrument group or user group to the owner of the XML subset corresponding to the experimental data, the access privileges and disclosure level of data are controlled. A login authentication to the system is performed using LDAP running on User DB.

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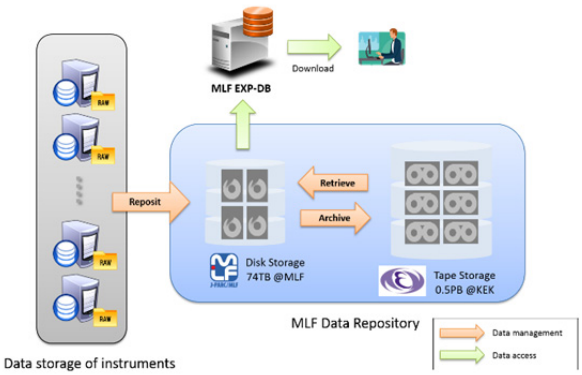

Figure 2: The schematic of the raw data management.

Experimental Data Catalogue

The experimental data catalogue can facilitate the creation of scientific results by supporting data utilization of facility users. It is useful to search experimental data necessary for analysis among a lot of data created under various experimental conditions and samples. Furthermore, it is also possible to refer information on experimental condition instead of conventional log notebook. The data catalogue is a list of measurement indicating various information related to experiment. It contains information as follows:

- **Experimental proposal:** Proposal ID, Beam line (Instrument), Title, Primary investigator (PI) and Period.
- **Measurement:** Run No., Time and date, Measuring time, Number of counts, Comment, etc.
- **Sample:** Sample ID, Name, Chemical formula, Composition, quantity, etc.
- **Device condition:** Device type, Setting parameter, Physical value, etc.
- **Data File:** Name, Size, Location path, Hash value, etc.

These kinds of the information are valuable especially for searching and analysing the experimental data taken in the time-sharing measurement varying experimental condition dynamically for transient phenomenon. A file location path enables the downloading of data stored in the data repository.

Raw Data Management

It is required to effectively and safely store a huge amount of raw data in the data repository with limited space. The data repository is composed of two data storages separately located by a distance of over 50 km. One is the 74TB disk storage at MLF campus and the other is the 0.5PB tape storage at KEK Tsukuba campus. Raw data is handled by the MLF EXP-DB within this reposit in a hierarchical way. The schematic of the raw data management is shown in Fig. 2. Raw data, produced initially in the local storage at each neutron instrument, is transferred to the primary disk storage (this process is called a "reposit") and archived into the secondary tape storage after certain period of time. The archived data is retrieved to the primary disk storage on demand. Meta-information of raw data such as the file location on the repository is updated in every data handling. Facility users are able to request and download their raw data through the MLF EXP-DB.

Web Portals

All of data management and access is performed via web portals. There are two kinds of web portals. One is a data management portal for the facility staff, and the other is a data access portal for users. The experimental data catalogue is available in both portals. Fig.3 shows screenshots of portals. The data management portal enables a various management of experimental data: a curation of data automatically registered, off-line registration after the measurement, management of raw data, quality determination of the measurement, and annotation providing. The data access portal allows the users to browse the experimental data catalogue, search with various conditions and download datasets necessary for analysis, and add annotations. It is also to execute standard data reduction and visualization, and share them among the research group.

Currently, the data management web portal is practically used at several instruments in MLF. On the other hand, the data access portal is still under trial use and development for opening service available to facility users.

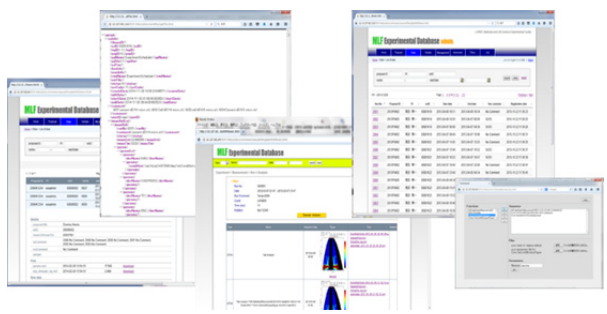

Figure 3: The screenshot of the web portal.

RECENT UPDATED FEATURES

Recently, we have redesigned the MLF EXP-DB to enhance availability and scalability, and improved a function of the experimental data retrieval in the web portal.

For the core system of the data management infrastructure, high availability is required. A service outage owing to the system failure and maintenance applying patches should be avoided as much as possible. A redundancy of system allows avoidance of such service outage, so that availability is improved. We have made the system to a redundant distributed system.

It is also necessary to consider scalability of the system especially in the data cataloguing. The data production rate in the facility is continuously rising. It depends on the beam intensity and the performance of neutron

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instruments. In MLF, the beam intensity has been increasing in phases according to the development plan for the accelerators and neutron sources. The scale of the experimental data catalogue will be the orders of tens million tags at full power operation in MLF. Also, additional installation of detector and improvement of various devices has been keeping in the instrument. Considering these situations, we have improved the MLF EXP-DB into the system capable of scaling-out responding to the scale of data quantity produced in the facility.

Furthermore, an improvement of experimental data retrieval can promote the data utilization. We have improved the experimental data retrieval with a flexible search condition according to the experimental conditions.

High Availability

The improved redundant system is composed of two servers in a switch over relationship. Figure 4 shows the overview of the system operation in this configuration. When one server is operated as active servers, which is responsible for the collect of the experimental data from instrument local systems and data access, the other is operated as hot-standby server. The database replication is regularly performed from active server to hot-standby server. In the occurrence of system failure or maintenance, the operation is switched. The data access is provided via a front-end web server, so that the user need not to take into account the access destinations.

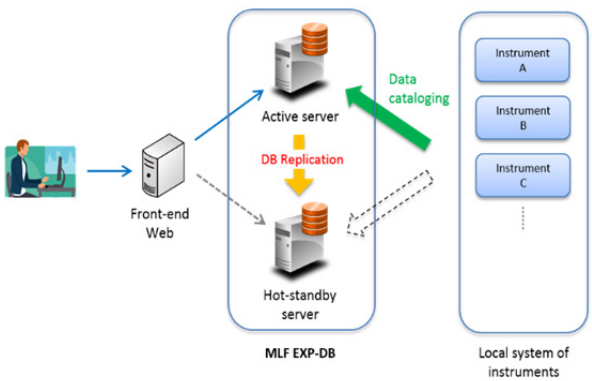

Figure 4: The schematic of the system operation in the redundant distributed configuration.

Scaling-out

The system has been scaled out to improve scalability for the data cataloguing. It is composed of two redundant system mentioned in the previous subsection. There are two experimental halls in MLF, each hall has about 10 instruments in operation. Currently, one system is allocated to the instruments in the 1st experimental hall and other system is allocated to the instruments in the 2nd experimental hall. It is capable to perform further scaling out of a load distribution by adding the redundant systems responding of the data production rate.

Flexible Data Retrieval

Since various sample environmental apparatuses in neutron instruments are used depending on the purpose of experiment, the structure of the experimental meta-data can be changed every experiment or instrument. Although every variety of information associated to experimental conditions as experimental meta-data in XML-format is registered in the experimental data catalogue, the retrieval condition is limited to some basic information on the experiment such as run No., date and time, experimental title, primary investigator in the conventional retrieval function.

In the improved retrieval, it is possible to execute a flexible data search more by specifying the search conditions for each tag of experimental metadata corresponding to the device condition. Figure 5 shows the screenshot of this retrieval.

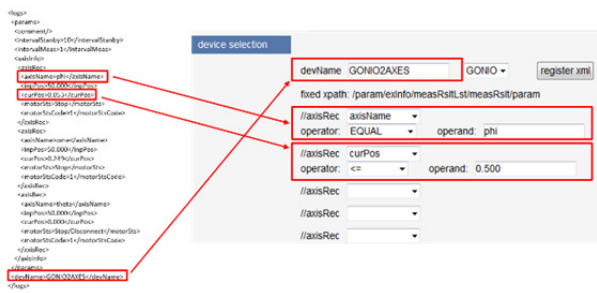

Figure 5: The screenshot of the flexible data retrieval.

CONCLUSION AND FUTURE PLAN

We are operating and updating the data management infrastructure in J-PARC/MLF. The infrastructure is mainly composed of the MLF EXP-DB, which is responsible for data management and access, and the data repository for the central preservation of experimental raw data. Currently, it manages the experimental data at four neutron instruments in MLF and plan on starting management at other instrument soon. The MLF EXP-DB provides the web portal as the interface for the data management and access. The web portal offering data access for the facility user is under trial use. We will start the data access service with this web portal including the flexible data retrieval next year.

We have also improved the MLF EXP-DB by redesigned to the redundant and scaling-out system. We have a plan for a performance evaluation in the near future.

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