DEVELOPMENT OF SPRING-8 EXPERIMENTAL DATA REPOSITORY SYSTEM FOR MANAGEMENT AND DELIVERY OF EXPERIMENTAL DATA

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Abstract

The SPring-8 experimental Data Repository (SP8DR) system is an online storage service, which is one of the infrastructure services of SPring-8. SP8DR enables experimental users to obtain their experimental data from the SPring-8 beamline on demand via the Internet. To facilitate easy searching for required data-sets, the system stores experimental data with metadata such as experimental conditions which are also useful to the post-experiment analysis process. As a framework for data management, we adopted DSpace, which is widely used in academic library information systems. We made two kinds of application software for registering experimental data simply and quickly. These applications are used to record a metadata set to the SP8DR database, which has relations to experimental data on the storage system. This data management design allows for a high-bandwidth data acquisition system. In this presentation, we report on the SPring-8 experimental Data Repository system that began operation in the SPring-8 beamline.

INTRODUCTION

Management of experimental data is important for not only the efficient operation of experiments but also for analysis of large amounts of data. SPring-8 is one of the largest synchrotron radiation facilities in the world. There are 56 beamlines currently being operated, and many kinds of experiments are carried out using high-brilliance X-rays. Each beamline has several experimental stations, and they output huge amount of experimental data. Beamline users bring this experimental data back to their own institutes for analysis. Recently, new experimental methods such as remote-controlled experiments and measurement services have become available. In those cases, beamline users may not come to SPring-8 if they can access to their data securely via the Internet. In addition, metadata that is related to the experimental conditions must be attached to the experimental data acquired under these conditions for these remote-controlled experiments. Then after the experiments, users can search and download their data at any time. However, experiments using high-performance two-dimensional detectors produce larger amounts of data, which makes data management difficult.

To maximize the data output from SPring-8, a dedicated experimental data management system was required. Therefore, we have developed the SPring-8 experimental data repository system (SP8DR) [1].

REQUIREMENTS AND CONCEPTUAL DESIGN

It is important to associate experimental data with related experimental conditions as metadata. In particular, adding correct owner information to experimental data is the most important. We can control access to the data by using this information.

An automated experiment measurement system requires writing data directly to storage in the SP8DR together with metadata. Metadata should be cataloged by database to facilitate easy data mining later, and those stored data should be preserved for some moderate amount of time. To cope with high-throughput data acquisition, a high-bandwidth storage system is required. In the case of widely the used two-dimensional imaging detector, typical write performance is several hundred Mbytes/s. Also, high-speed data transfer through the Internet should be possible, because huge amounts of experimental data will be retrieved for analysis. It is necessary to conform to contemporary rules for Internet security.

Conceptual design of the SP8DR is shown in Fig. 1. The experimental data is preserved in the storage system located in the back end of the SP8DR. The SP8DR manages the metadata as experimental conditions that include the path information of the experimental data on the storage system.

We prepared two types of data transfer methods. One is HTTP that is used in most cases, although it is slow. Therefore, we chose SkeedFileMessenger [2] for high-speed data transfer. It has a unique algorithm to improve the transfer rate.

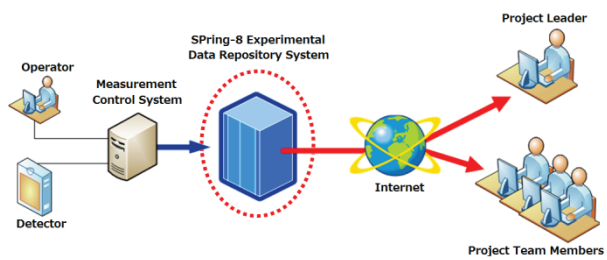

Figure 1: Outline of SPring-8 Experimental Data Repository System.

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IMPLEMENTATION

Implementation

We chose DSpace [3] as a data management framework. DSpace is a software used to build open digital repositories, and it is widely used for digital archiving by libraries around the world. DSpace uses Dublin Core [4] that is a defined extensible metadata element set as a metadata management engine. Because Dublin Core has a key-value-type database structure, its extensibility is high. As shown in Fig. 2, we originally defined the SPring-8 Dublin Core element set with a hierarchical structure for the SP8DR. The innermost part is an indispensable element set of the DSpace. The middle part is a common element set for the SP8DR. The outermost element set will be customized for specific experiments individually.

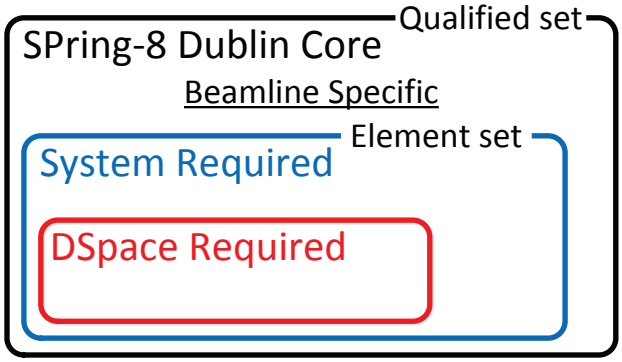

Figure 2: Schema of the SPring-8 Dublin Core.

An important component of the SP8DR is as follows.

- Path information of the data files. This describes the stored location on the storage system. It is a member of SPring-8 Dublin Core element set.
- Owner information of the data. This is used for access control and user authentication by the SP8DR. It is a member of SPring-8 Dublin Core element set.
- RegistAgent. This is a service application that stores data to the SP8DR. RegistAgent uses SWORD API of DSpace and can be controlled by a message-based interface.
- ConverterRegister. This mediates between the measurement application of the beamline experiments and RegistAgent. It was designed for general-purpose application using an extensible XML file that describes the detailed data structure. It runs as a client of RegistAgent.
- Web application. This is the user interface for data mining and downloading.
- SkeedFileMessenger. This is the data transfer boost tool. At present, it can transmit 1 GB of data in 90 seconds. Therefore, a huge amount of experimental data can be transmitted without a long wait.

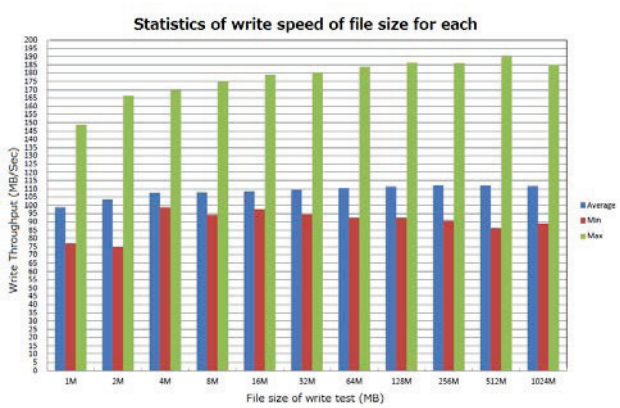

Figure 3: Performance evaluation of GlusterFS.

By following the RegistAgent protocol, it is possible to build a custom client program. By adopting the message exchange interface for data registration, it is possible to cooperate easily with other experimental measurement control systems. The experimental data are stored in the storage system. For the main storage system, we chose a scale-out-type storage architecture that enables expanding the storage area during operation. As a result of examinations of cost, performance, and availability, we adopted the GlusterFS [5]. The one side of the network port of the storage system is connected to the experimental network directly and exports disk volume information to the measurement system that runs ConverterRegister on beamlines.

Application to XAFS Measurements

We applied a subset of the SP8DR to BL14B2 as a pilot case. BL14B2 is a beamline of the Engineering Science research group. Primarily, it is used for XAFS measurements. The experimental data are spectrum observations from energy scans. It is a slow measurement, which takes considerable time for one scan. PF9809 is the data format that is most popular in Japan, and it can be as small as several megabytes. Before the installation of the SP8DR to BL14B2, we defined the SPring-8 Dublin Core Qualified Sets for BL14B2. Existing experimental data were stored in directories created by beamline users. The SP8DR records the directory structure information as metadata. Using the web interface of the SP8DR, we can access the recorded data via that directory structure as is. Also, a tree view with the metadata such as a user ID, proposal number, or experiment data as a key is implemented.

Noteworthy points of this system are as follows.

- Faster and lightweight. The SP8DR has an index that only points to real data on the storage system.
- Easy data mining. The function of the tree view of metadata enables easier data mining.
- High affinity for other systems. The message-based interface results in a high affinity for communication with other system such as an automated experiment system.
- Faster download. Skeed File Messenger enables high-speed downloading that is almost wire rate.

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EVALUATION

Performance Evaluation

We evaluated performance of GlusterFS. Figure 3 shows the results of that evaluation. Sequential writing speed performances of 25,500 trials were measured. Minimum speed, maximum speed, and average speed are described.

Data storing speed was also evaluated. Average turnover time is less than 227 ms. This is sufficient speed for XAFS experiments.

In evaluating the download speed using SkeedFileMessenger, a noteworthy result was observed (summarized in table 1). In the optimized environment, speedup of approximately seven times is achieved in comparison with HTTP.

Test at BL14B2

We started evaluation of the SP8DR with beamline scientists in 2012. After a critical bug fix, test service began in May 2013. The remote experiments using the SP8DR are scheduled soon.

CONCLUSION AND FUTURE PLANS

SPring-8 experimental data repository was developed with the goal of managing all experimental data in SPring-8 with one application. In the realization of the system, there were two large problems. One was how to manage the different metadata from each field by a single application. The other was how to register large volumes of data outputted from the detector at high speed. Both were very difficult problems.

However, the former could be solved by the database that was designed using the Key-Value-Store type under the concept of Dublin Core. The latter was solved by having the system collect file path information instead of dealing with experimental data directly. Therefore, the total amount of data handled by the system was reduced, and the system workload was lightened. In addition, the mechanism for managing the file path information of the experimental data can make the collaboration process easier with external software. So, high-speed data transfer in SkeedFileMessenger was realized by that mechanism.

Table 1: Evaluation of SkeedFileMessenger

Place	HTTP (Mbps)	SFM (Mbps)	Carrier
Author's home	8.9	61	100M FTTH (NTT-West)
Hokkaido UNIV.	34	94	SINET4
KEK	21	50	SINET4
Nagoya UNIV.	34	140	SINET4
Osaka Univ	54	66	SINET4
Riken	131	290	SINET4

This mechanism is very useful and is also being able to facilitate collaboration in the post-experimentation process.

Half a year has passed since the system was released at BL14B2, and it has been highly stable without significant problems during this period. That result means that the system is reliable.

In this system, the following are planned in the future.

1) Further reduce the transfer time with parameter tuning of SkeedFileMessenger.
2) Reduce the waiting time for data registration by up to 10 data per seconds.
3) Installing the SPring-8 experimental data repositories to the more than 20 public beamlines in SPring-8, in addition to BL14B2. We have increases the number of users with the aim of standardizing experimental data management at Spring-8.
4) Currently, the system was available for the data download service only. In the future, the system will be able to provide the final results of collaborative data processing.

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