DATA MANAGEMENT AT THE SYNCHROTRON RADIATION FACILITY ANKA*

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Abstract

The complete chain from submitting a proposal, collecting meta data, performing an experiment, towards analysis of these data and finally long term archive will be described. During this process a few obstacles have to be tackled. The workflow should be transparent to the user as well as to the beamline scientists. The final data will be stored in NeXus [1] compatible HDF5 [2] container format. Because the transfer of one large file is more efficient than transferring many small files, container formats enable a faster transfer of experiment data. At the same time HDF5 supports to store meta data together with the experiment data. For large data sets another implication is the performance to download the files. Furthermore the analysis software might not be available at each home institution; as a result it should be an option to access the experiment data on site. The meta data allows to find, analyse, preserve and curate the data in a long term archive, which will become a requirement fairly soon.

INTRODUCTION

The synchrotron radiation facility ANKA [3] is located at the Karlsruhe Institute of Technology, providing light from hard X-rays to the far-infrared for research and technology. It serves as a user facility for the national and international scientific community. The traditional data management for users of ANKA was based on transportable media. A user took its data home once the beam time was over. This approach is not feasible any more, for several reasons:

- Modern detectors produce more and more data
- No analysis resources at the home location
- Only manual or no bit preservation
- Poor search ability
- Difficult to share results with the global research community

In addition new regularities of the European Union research grants, request long term archiving for research data. Under discussion are periods of ten years. Therefore to preconfigure the analysis tools in a site local cloud environment would ease the usability. As a result we create a new workflow within the ASTOR project. This project is based on an Analysis-as-a-Service (AaaS) approach, based on the on-demand allocation of VMs with dedicated GPU cores and corresponding analysis environment to provide a cloud-like analysis service for scientific users [4]. In order to allow remote access to analyse and download the data, we had to implement an Authentication and Authorization Infrastructure (AAI). In this paper we discuss the workflow from a submission of a proposal to authentication and authorization towards the beamline data management, the analysis and archival of the large raw datasets.

Submission of a Proposal

For all beam time proposals a peer review process is carried out. A user has to submit an experiment proposal in the ANKA proposal submission system ANNA. This is a web interface where details about the experiment are submitted and evaluated. For accepted proposals the users have the option to supply further meta data about each sample. The beam time will be scheduled and the user can prepare the travel to ANKA.

AUTHENTICATION AND AUTHORIZATION INFRASTRUCTURE

Usually a group of people is participating in one proposal and not all of these co-proposers are traveling to ANKA, however usually all members need access to the created data and the meta data. For the workflow at ANKA several web portals and services are required. To ease the usability a Single Sign On (SSO) approach will be provided. As a result each portal becomes a Service Provider (SP) and we introduce our own Identity Provider (IDP) for ANKA. This way we will also be able to include other IDPs, like Umbrella [5] or the DFN [6] (German National Research and Education Network), to authorize people. This has the big advantage, that user do not have to remember several accounts including their passwords.

During the experiment time at ANKA, the user can log on to the beam line data management (BLDM) frontend with the same credentials already used for the submission system.

THE BEAMLINE DATA MANAGEMENT

The beam line data management (see Figure 1) system collects all relevant data from the proposal system to make them available for the experiment. As such no duplicated data is inserted into the system, and proposal meta data can directly be connected to the measurements. This includes all logging information available via Tango [7], e.g. experimental data or vacuum level, sample conditions from the SCADA system WinCC Open Architecture [8]. Each sample gets an ANKA wide distinct identifier. Depending on the sample it can be identified via QR Code or Barcode. Once the user decides that this experiment is finished, one can close this newly created dataset, which triggers the beamline data management workflow.

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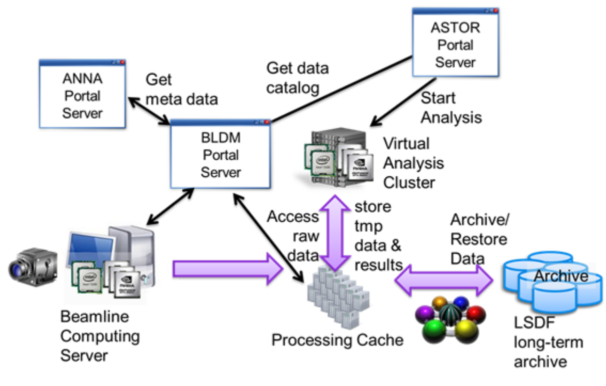

Figure 1: The Beamline Data Management.

Beside meta data acquisition and ingest into the data repository, the BLDM is responsible to hide distributed storage instances. An on site analysis is only feasible on the processing cache because the data archives are usually not designed for high-speed data access.

The BLDM is integrated into the TANGO control system and connects the storage resources to meet the requirements for data analysis and data ingest. The workflows and the current state of execution are persisted in a relational database. Monitoring and control of the data sets can be provided by the database. All TANGO devices of the BLDM are actively polling the database for work instructions like closing a dataset, computing the checksum, checking the checksum, migrating datasets or ingesting data. A message driven approach is planned to enable event driven task execution.

Storage

The idea is that each detector creates its own HDF5 file schema. When a dataset will be archived at the end of a scan, all HDF5 files produced with this scan are combined to one or more bigger file containing all data and meta data. An archived dataset can be moved around to different storage location, the analysis storage as well as the archival storage. To guarantee that each of these copies stays the same, the data cannot be changed anymore and only read access to this data is permitted. Optionally during this process a persistent identifier (PID) [9] can be created. When data will be archived for up to ten years, one has to make sure that the data can be recognised again. As time goes by, it will be difficult to remember what was measured. Keywords are needed to find this data again. As such all meta data created during a scan are stored inside of the dataset as well as inside of a database. The database can then be searched for all possible use cases.

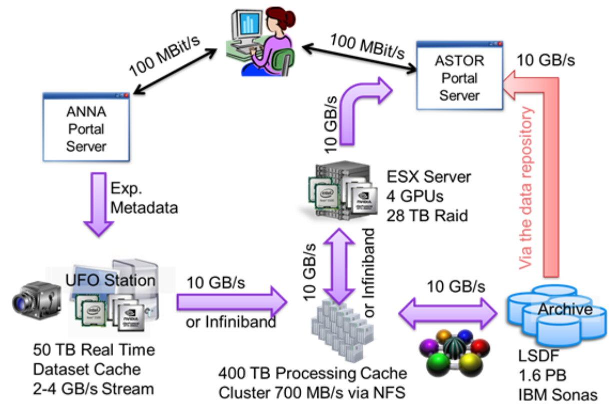

Figure 2: File based Storage.

Figure 2 shows the file based data storage approach. Another option would be to store the data not file based, within a no SQL database system (NoSQL DB) [10] as shown in Figure 3. This approach is currently being investigated to have faster parallel access of these data, if a cluster of NoSQL Nodes is used. This approach uses a key/value store, has a flexible scheme and is massive scalable. Just add more nodes to add further throughput. A NoSQL approach also supplies automatic redundancy, which results in higher performance and availability.

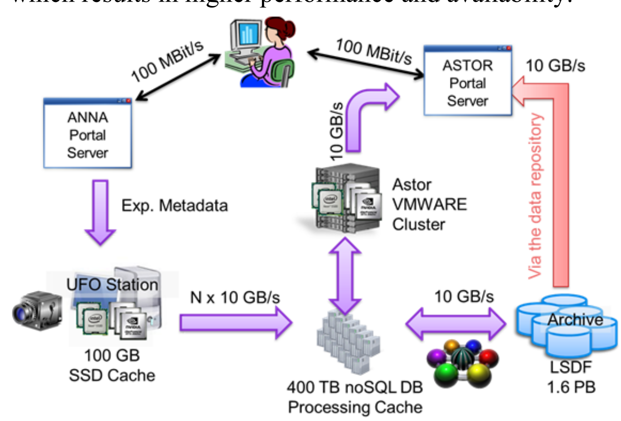

Figure 3: Storage in a NoSQLDB.

DATA ANALYSIS

Within the ASTOR project we develop an environment to analyse the data generated at ANKA with the help of virtual machines providing 3D data analysis tools like AMIRA [11] and volume graphics studio max [12] (see Figure 4). Each virtual desktop has access to its corresponding datasets through a dedicated mount point. This causes one complication. We need to map the authentication down to the file system layer in order to guarantee the access for authorized users and deny the access for others. We will have a file system group for each proposal. The members of this group will be all users participating in this proposal.

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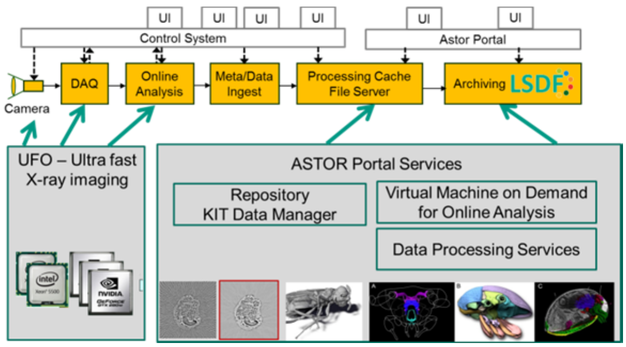

Figure 4: Astor Portal.

However users will always be able to take their data home, or download them using a web portal, to do offline analysis of their data. Data analysis results in new data. This newly created data will not be stored in the original dataset, but new datasets will be created and related to the original dataset. These new datasets will be connected inside of the database, as such duplicated storage will be avoided and the work can be easily reproduced.

DATA ARCHIVE

When a dataset will be ingested into the data repository, it can be marked as a long term dataset, even though the analysis has not been completed. This is feasible since the data will not change any more. However the user responsible for this data has to decide, for how long it will be archived if at all. Especially users coming from an industrial background might not want their data stored at a location outside of their own control. People with an academic background might want to make their data available for the public after a certain amount of time, when the initial publications are completed. At the end of the agreed archive time the data will be automatically deleted, if no new contract is negotiated. We currently create an online portal, where the user can log on with their credential and then have access to their data, either for download or direct online analysis. Inside of this portal, it will also be possible to open the access for everybody after a specified time.

CONCLUSION

Parts of the presented approach are still in the evaluation phase. We still need to discuss appropriate business models. Furthermore some political questions have to be evaluated and resolved. User tend to keep all kind of data, however storage comes not for free. We would need a way to reduce the amount of archive storage needed. Maybe there will be some costs implied for certain storage and analysis hours. Some questions need to be answered, for example, what happened to the data if a proposer of the data changes the affiliation? Will this user's access be revoked? Or if new users enter the collaboration what are the legal steps to add new users into an existing group.

ACKNOWLEDGMENT

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