THE AUSTRALIAN STORE.SYNCHROTRON DATA MANAGEMENT SERVICE FOR MACROMOLECULAR CRYSTALLOGRAPHY

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Abstract

Store.Synchrotron is a service for management and publication of diffraction data from the macromolecular crystallography (MX) beamlines of the Australian Synchrotron. Since the start of the development, in 2013, the service has handled over 51.8 TB of raw data (~ 4.1 million files). Raw data and autoprocessing results are made available securely via the web and SFTP so experimenters can sync it to their labs for further analysis. With the goal of becoming a large public repository of raw diffraction data, a guided publishing workflow which optionally captures discipline specific information was built. The MX-specific workflow links PDB coordinates from the PDB to raw data. An optionally embargoed DOI is created for convenient citation. This repository will be a valuable tool for crystallography software developers. To support complex projects, integration of other instruments such as microscopes is underway. We developed an application that captures any data from instrument computers, enabling centralised data management without the need for custom ingestion workflows. The next step is to integrate the hosted data with interactive processing and analysis tools on virtual desktops.

INTRODUCTION

The deposition and the wide availability of raw diffraction data have far-reaching benefits for the structural biology community [1–4]. We recently created TARDIS, a suite of tools for the deposition of X-ray diffraction images in an open access repository to facilitate their deposition using federated institutional repositories [3]. Subsequent engagement with IUCR and closer relationships with the Australian Synchrotron prompted us to develop a new framework for raw X-ray data archival and dissemination — the *Store.Synchrotron* service, which is described in this manuscript.

An earlier but more detailed description of this service is available at [5].

THE OPERATION OF STORE.SYNCHROTRON FOR THE AUSTRALIAN SYNCHROTRON

The *Store.Synchrotron* service (`https://store.synchrotron.org.au`) has been deployed to receive diffraction data from the macromolecular crystallography (MX) beamlines at the Australian Synchrotron (AS) automatically.

When a user starts collecting data at the beamline, all raw diffraction data and automated data processing results are transferred in real-time and on the next day respectively to *Store.Synchrotron* without user intervention.

This system is accessible through any web browser. Data is available immediately at time of collection to all authorised users via the internet. If desired, the data can be opened to the public.

Figure 1 shows a schematic overview of the service.

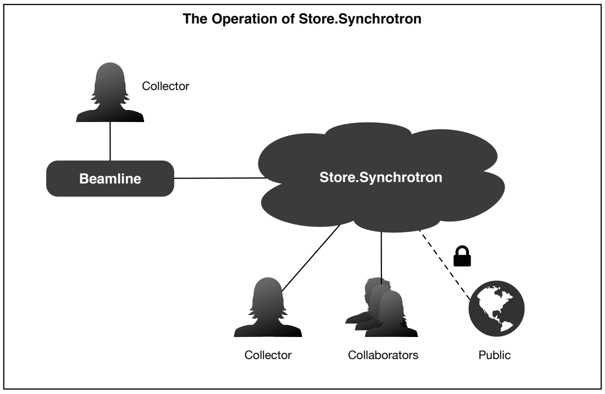

Figure 1: Schematic overview of *Store.Synchrotron*

The Need for an Automated Data Management System

At the Australian Synchrotron (AS) up until recently the most practicable solution for data management has been to take portable hard drives to the beamlines. The use of portable drives is a problem, however, because these drives may remain the lab's sole resource for raw data. After researchers have left, it may be difficult to correlate raw frames with datasets and structures, and a single disk is very prone to failure and data loss.

With *Store.Synchrotron* users now have for the first time a long-term, secure archive of their raw data, including metadata, which can be used to relate raw frames to projects and visits to the Australian Synchrotron.

In addition to the practical need for a robust data archive, new requirements by funding agencies for researchers to have a data management plan are conveniently solved by a centralised solution that takes care of the data from collection to archival and/or publishing.

The End-to-End User Experience

The default way of accessing data on the *Store.Synchrotron* service is via the web through a web browser. As a user collects a diffraction image it is available on the *Store.Synchrotron* website within minutes (Fig. 2) including instrument specific metadata.

Data is organised into three tiers. An Experiment is related to an allocation on the beamline (Fig. 2A,B). The data is then separated into Datasets (Fig. 2C). Finally, the individual diffraction images are Datafiles in their respective datasets (Fig. 2D). All or selective elements of each tier can be downloaded via the web or via SFTP.

In addition to diffraction datasets, *Store.Synchrotron* makes accessible the results of preliminary autoprocessing. Collection of the images triggers automatic indexing and full integration and scaling for complete datasets. All autoprocessing output is downloadable as well.

Design and Implementation

The *Store.Synchrotron* service is an implementation of MyTardis (`http://mytardis.org`); a web-based open-source data management platform. MyTardis began as the TARDIS [3] (`http://tardis.edu.au`) diffraction image repository but has since expanded to suit the storage and organisation of a wide range of scientific data. The interface allows browsing, data access, data sharing and publication.

The beamline registers its the raw images with *Store.Synchrotron* in real-time, triggered by the instrument control system. Different processes extract information and preview images, compute SHA-1 checksums, and copy the diffraction data to the final *Store.Synchrotron*-managed storage location. By the end of an allocation slot both raw data and auto-processing results are archived and made available on *Store.Synchrotron*. For resilience all these processes are run using a message queue. All networked communication is encrypted.

The integrity of the files stored within the *Store.Synchrotron* service is of utmost importance. As the data are the results of often non repeatable experiments, data is verified via checksums at several steps in the pipeline, starting with ingestion. If a checksum does not match, it can be re-sent if possible. All archived files are re-verified regularly to ensure the ongoing integrity of the data.

In a 12 month period since *Store.Synchrotron* began operation, only 8 out of more than 1,700,000 files had mismatching checksums. This means the vast majority of data (99.9995%) was transferred successfully in the first attempt. It also demonstrates the value of integrity checking as these 8 files could be re-transferred before the original was lost.

The *Store.Synchrotron* service receives metadata via its RESTful API. By following the REST standard we made it trivial for developers to interact with *Store.Synchrotron* programmatically, e.g. automatically or manually via different front ends.

Another important technology we use that allows space and time efficient archiving and retrieval of large datasets is SquashFS (`http://squashfs.sourceforge.net/`). SquashFS is an archive file standard that supports compression and direct random file access. *Store.Synchrotron* can transparently provide access to individual files inside SquashFS archives.

Store.Synchrotron was developed based on the web framework Django. It is running on a Ubuntu 14.04. It is hosted on the NeCTAR Project's cloud computing service (`http://www.nectar.org.au/research-cloud`). To assist the maintenance and coordination of this service, we have used an orchestration and configuration management system (SaltStack `http://www.saltstack.com/`).

Benefits from User Perspective

Protein crystallography has benefited for many years by an open-access community based approach to the constant development and improvement of data processing, structure solution and refinement tools. As these tools evolve, it is often beneficial to revisit projects where data collected has proven intractable at the time, as has been done for example in [6].

A broadly systematic approach can be taken to processing old data for new results. Data processing programs are continuously evolving. As the *Store.Synchrotron* public repository grows we can envisage a system where as new methods to analyse raw data become available they are used against old data automatically.

OPEN DATA FOR THE CRYSTALLOGRAPHIC COMMUNITY

The Australian Synchrotron is the only facility of its type in Australia, and is in constant use. As such, the organisation has actively encouraged opening up of data produced there, to encourage efficiencies and reuse. This requires services that enable effective long term storage, curation and citation.

Provision of services related to making data more easily available are timely, as Australian government research funders have been strengthening their language in this area [7, 8], bringing Australia more in-line with the global research environment and that of international funding agencies such as the US National Science Foundation (NSF) and the UK Medical Research Council (MRC).

Store.Synchrotron also represents the logical extension of a long-standing effort in the macromolecular crystallography community to ensure that satisfactory evidence is provided to support the interpretation of structural experiments. This effort has included unrivalled requirements for validation of data interpretation processes [9–12].

Other projects exist to deposit and host openly-accessible diffraction data on the web, such as DIMER (`https://dimer.uq.edu.au/`), the registration-required JCSG Repository of Crystallography Datasets (`http://www.`

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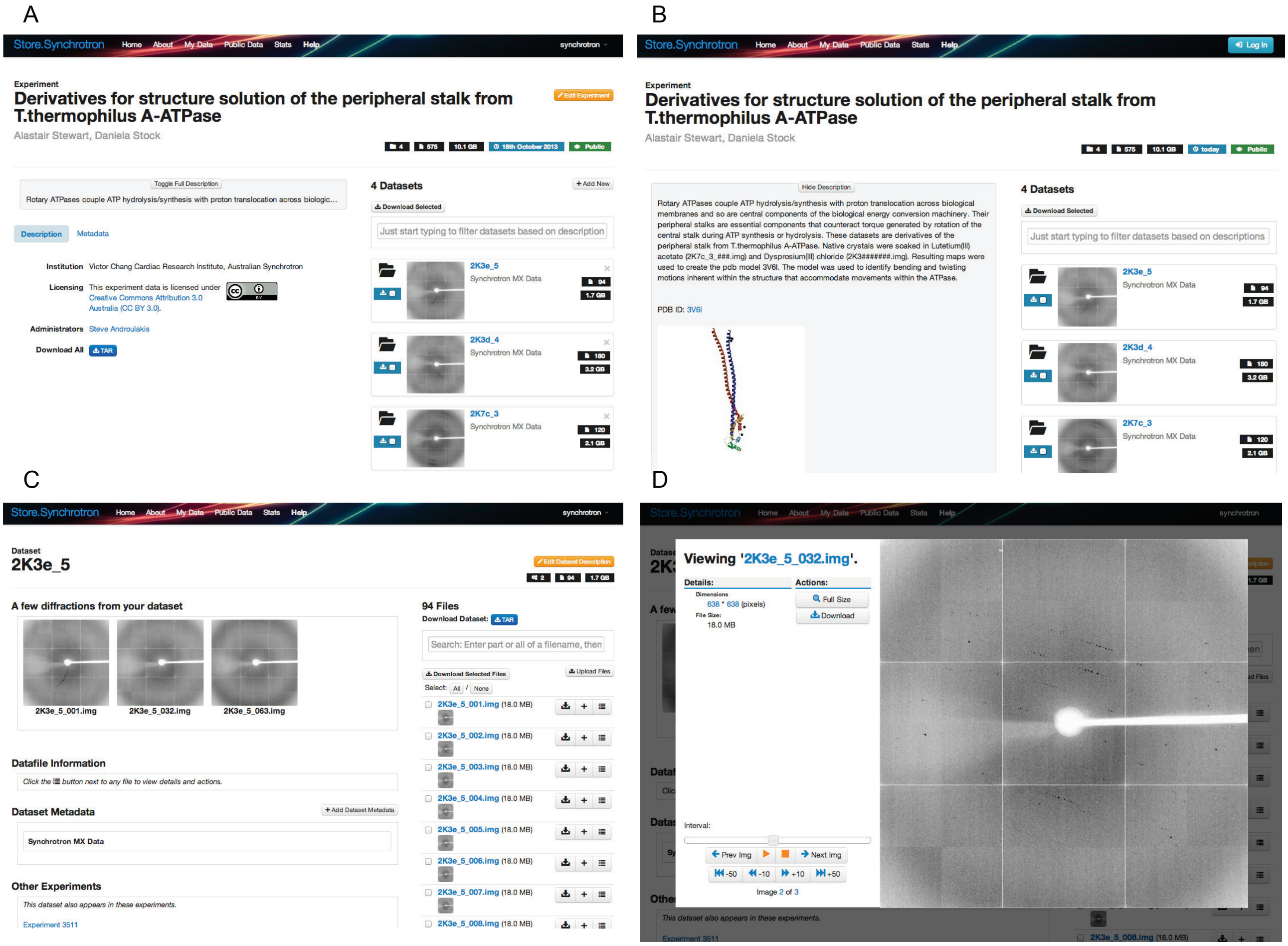

Experiment

Derivatives for structure solution of the peripheral stalk from T.thermophilus A-ATPase

Alastair Stewart, Daniela Stock

4 | 575 | 10.1 GB | 18th October 2013 | Public

Rotary ATPases couple ATP hydrolysis/synthesis with proton translocation across biologic...

Institution: Victor Chang Cardiac Research Institute, Australian Synchrotron

Licensing: This experiment data is licensed under Creative Commons Attribution 3.0 Australia (CC BY 3.0).

Administrators: Steve Androulakis

Download All: TAR

4 Datasets

Just start typing to filter datasets based on description

2K3e_5 Synchrotron MX Data 94 1.7 GB

2K3d_4 Synchrotron MX Data 180 3.2 GB

2K7c_3 Synchrotron MX Data 120 2.1 GB

Experiment

Derivatives for structure solution of the peripheral stalk from T.thermophilus A-ATPase

Alastair Stewart, Daniela Stock

4 | 575 | 10.1 GB | today | Public

Rotary ATPases couple ATP hydrolysis/synthesis with proton translocation across biological membranes and so are central components of the biological energy conversion machinery. Their peripheral stalks are essential components that counteract torque generated by rotation of the central stalk during ATP synthesis or hydrolysis. These datasets are derivatives of the peripheral stalk from T.thermophilus A-ATPase. Native crystals were soaked in Lutetium(III) acetate (2K7c_3_###.img) and Dysprosium(III) chloride (2K3#######.img). Resulting maps were used to create the pdb model 3V6I. The model was used to identify bending and twisting motions inherent within the structure that accommodate movements within the ATPase.

PDB ID: 3V6I

4 Datasets

Just start typing to filter datasets based on descriptions

2K3e_5 Synchrotron MX Data 94 1.7 GB

2K3d_4 Synchrotron MX Data 180 3.2 GB

2K7c_3 Synchrotron MX Data 120 2.1 GB

Dataset

2K3e_5

2 | 94 | 1.7 GB

A few diffractions from your dataset

2K3e_5_001.img 2K3e_5_032.img 2K3e_5_063.img

Datafile Information

Click the ☰ button next to any file to view details and actions.

Dataset Metadata

Synchrotron MX Data

Other Experiments

This dataset also appears in these experiments.

Experiment 3511

94 Files

Download Dataset: TAR

Search: Enter part or all of a filename, then

- ☐ 2K3e_5_001.img (18.0 MB)
- ☐ 2K3e_5_002.img (18.0 MB)
- ☐ 2K3e_5_003.img (18.0 MB)
- ☐ 2K3e_5_004.img (18.0 MB)
- ☐ 2K3e_5_005.img (18.0 MB)
- ☐ 2K3e_5_006.img (18.0 MB)
- ☐ 2K3e_5_007.img (18.0 MB)
- ☐ 2K3e_5_008.img (18.0 MB)

Viewing '2K3e_5_032.img'.

Details:
Dimensions: 638 * 638 (pixels)
File Size: 18.0 MB

Actions:

Interval:

Image 2 of 3

Figure 2: Screenshots of the web interface to the *Store.Synchrotron* service. **A**: A public experiment. **B**: A detailed description with images and links. **C**: One dataset highlighting a selection of images from the set. **D**: Image file preview.

jcsg.org/), and TARDIS (http://tardis.edu.au/). *Store.Synchrotron* differs from these services by automatically archiving all diffraction data produced from beamlines at time of data collection. This act eliminates the need for manual diffraction data deposition by the user as a step toward open crystallography data.

A European project, PaN-Data (http://pan-data.eu/) has also created infrastructure for the automatic archival and dissemination of raw diffraction data from facilities such as the Diamond Light Source and the ESRF. This is achieved through a combination of an information management and real-time data monitoring system ISPyB [13], metadata store ICAT (http://icatproject.org/) and its data-browsing and access web front-end TopCat (https://code.google.com/p/topcat/). To date, access to data has been private to users who collect it. *Store.Synchrotron* extends this functionality by providing both an automatic archival mechanism from the time of data collection and a publishing interface for open access to collected data.

To facilitate the publication process the *Store.Synchrotron* has developed a publication form to assist researchers in identifying and describing the raw data associated with their experiment and adding metadata such as related PDB entries. After a final check by Synchrotron staff the Experiment link is made publicly available and discoverable via the *Store.Synchrotron* site, with a Digital Object Identifier (DOI) minted for citing the data.

Considerations for Use of the Store.Synchrotron Model in Other Facilities

If this system is to serve as a model for evaluation by other synchrotrons and instrument facilities around the world, it is important to consider potential points of difficulty that may arise with the application of our approach. Certainly, the most difficult infrastructure requirement for *Store.Synchrotron* is the expense of storage and compute servers. When operating a data intensive service, a significant challenge arises: Who will pay to keep this data alive?

Monash University is a partner operator of VicNode (http://www.vicnode.org.au), the local node of the Research Data Service (RDS, http://www.rds.edu.au). VicNode provides a multi-location, tape-archived, large volume cloud data storage service that is utilised for all the data stored at the *Store.Synchrotron* service. Storage initially provided to *Store.Synchrotron* by the VicNode is over 200 terabytes in size and is a combination of disk and tape, with an off-site backup.

The minting and ongoing maintenance of Digital Object Identifiers (DOIs) represent an ongoing cost. *Store.Synchrotron* uses the federally-run Australian National Data Service (ANDS) who provide a service that allows the free minting and maintenence of DOIs resolving to Australian research data.

As discussed above, the MyTardis data management and instrument integration application is free, open-source, and able to be deployed on a compute cloud or web server in an automated fashion. We envision that our service could offer an attractive model elsewhere for raw data deposition, access, archival and dissemination.

Integration with Current and Future Instrumentation

Structural biology increasingly harnesses and integrates multiple approaches to attack challenging problems. In addition to protein crystallography, these include electron microscopy, X-ray scattering, and multiscale computational modelling. This creates a real need for integrated, end-to-end data management solutions. Similar services are also being operated that manage data from over 25 instruments at other facilities, including Monash University Micro Imaging platform (Electron Microscopy), the Monash University Medical Proteomics Facility (Mass Spectroscopy) as well as instruments at the Australian neutron source ANSTO. All this work is built upon the MyTardis data management platform and thus forms a common interface and data organisation strategy.

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