

Autoreduction - an automated data reduction system for beamline instruments at the ISIS Facility

J. R. Corderoy, T. Gowland, L. Greenwood, M. Noble, D. Oram and A. J. Markvardsen
(code contributors)

ISIS Facility, Rutherford Appleton Laboratory

Email: someone with an STFC email account

23/09/2015

Abstract

A key step for users of large research facilities is the processing of instrument data before use. Autoreduction is a software system designed to automate this process, integrate with other pre-existing facility systems and software packages, and provide an interface for users to control it.

This article describes the system setup for Autoreduction at the ISIS Facility; its motivation and design, its use and interface and its current status in production at ISIS.

1 Introduction

Large scale research facilities, such as the ISIS Neutron and Muon Facility, allow users in academic and industrial research to perform experiments using instruments set up to probe the inner structure and dynamics of materials. Common to most instruments is the need to process – ‘reduce’ – raw data collected from an instrument into a form that users can interpret or do further analysis on. For example by removing instrument specific artifacts from the measured data, transforming the data into different units and/or into data formats readable by further analysis software.

The purpose of the autoreduction system is to provide a useful automation step in this process. The system described in this paper allows data coming

off an instrument to be automatically reduced using a dedicated software package such as Mantid [1], whilst also lending transparency to the process and letting users control it through a straightforward web interface.

Automated data reduction is a concept which is actively pursued at other large facilities. At the NOBUGS 2016 Conference [7], there were several talks given by delegates from other large scale facilities which mentioned the automated reduction of data at a variety of facilities.

Data Analysis Infrastructure for DLS MX/CX [5] discusses a batch script based system for macromolecular beamlines. It makes use of ActiveMQ [4] (which will be discussed later in this paper) and also has a front end status monitor to show the health of the system during run-time. Integration of Fast Detectors into Beamline Control [6] also mentioned the use of automatic data processing. To keep up with the data rates from faster detectors, they are now automatically reducing data immediately so that users can see the results as soon as the dataset is taken.

2 Background

The autoreduction system at ISIS was inspired by an autoreduction setup at the the Spallation Neutron Source (SNS) at Oak Ridge National Laboratory [2].

The autoreduction implementation at ISIS uses the

same underlying technologies (choice of programming language and queue node software for example) as those used for the implementation of the SNS autoreduction service. However, the ISIS implementation differs in that its front end client is designed to serve autoreduction users only and was not originally part of the SNS implementation.

2.1 Data reduction

The autoreduction service exists to reduce beamline instrument data. An instrument produces discrete tranches of data, referred to as ‘runs’, in service of experiments. This raw data typically needs to be processed – ‘reduced’ – before it can be used by scientists. This is done by running a script on it. Although the script itself need not change often, it may have configurable parameters – variables – which might require more frequent updating.

The autoreduction system is intended to automate this process. Instrument scientists provide the system with reduction scripts - in a specified location on a shared file archive - along with sets of variables to use to reduce runs. Firstly, the system watches for the completion of runs. Once a new completed run has been found, the system will then run the appropriate script with the correct variables on the new run. Once the script has finished execution, reduced data will be saved to a data store for users to retrieve.

2.2 Requirements

The system is intended to serve the instrument scientists (who manage beamline instruments) and users who use the instruments to run experiments. The key requirements from these users, which have been completed to date, are:

1. Automate the reduction of data from beam instruments, using scripts provided by instrument scientists
2. Show the status of reduction on runs, as well as the results and locations of reduced data, to users
3. Allow instrument scientists to set the parameters used for reduction in advance of experiments and

optionally schedule these to be different for particular experiment

4. Allow users and instrument scientists to see what script and with which parameters was used to reduce a run
5. Allow users and instrument scientists to modify the parameters used for a run and re-run reduction using new parameters or scripts

Additional constraints are:

1. Limit access to the system to ensure that only staff and scientists can access runs and instruments
2. Utilise existing authentication systems to validate identities and permissions for (1)
3. Allow scalability for processing large amounts of data in a timely manner

3 System architecture

The architecture is based on a queue node which coordinates communication between all components of the system. This maintains separate message queues which allow components to act on messages from other components and update the system. These components are:

- A monitor for new instrument runs
- The state database & coordinator
- A worker for reduction processing

When the monitor detects that a new run has completed on an instrument, it will send a message to the *Data Ready* queue. The *QueueProcessor* process will consume this message, strip out the relevant information and creates a corresponding job in the database. *QueueProcessor* will then send the message on to the *Reduction Pending* queue. The *AutoreductionProcessor* process will be watching the *Reduction Pending* queue. When *AutoreductionProcessor* receives a message, it runs the *PostProcessAdmin* script which will send a message to the *ReductionStarted* queue such that the database remains up to date. Once reduction has finished, *PostProcessAdmin* will send the result to either *Reduction Complete* or *Reduction Error*

where it will be consumed by the *QueueProcessor* and updated in the database.

3.1 Message queue

Apache ActiveMQ [4] is used as the message queuing system using JSON-formatted objects as messages. The intention of the message is conveyed by which queue it's placed in rather than a field in the message itself. Runs can be 'scheduled' simply by using ActiveMQ's scheduled delay feature which allows a message to be delivered a given time after it's been pushed to the queue.

Messages contain metadata for the run such as a (unique) run number and version, the experiment and instrument that the data is associated with, and any logs or errors resulting from reduction. They also carry the necessary information to carry out the data reduction - the Python script to run on the data, paths to the data, and variables to be used by the script.

Data files at ISIS typically run in the hundreds of MB. They are therefore impractical to be sent directly in a message and instead they're provided as file paths on a shared file archive. Meanwhile, the reduction script to be used is sent as a string; the script is served from the state database and using the message queue to directly send it obviates the need to rely on a potentially flaky shared file store within the system.

3.2 Run monitor

When a new run has been completed on the beam line, the raw data files are placed in a shared filesystem. A node runs a Python watchdog daemon that tracks changes in this filesystem and, when a new run is detected, will send a message to *Data Ready* with details of the run. The particular choice of monitor isn't crucial; anything would work as long as it pushed the same message to the queue. In the current production system at ISIS, the run monitor is on same node as the state database itself.

3.3 State database & coordinator

The *QueueProcessor* service runs as a daemon and is the service responsible for keeping track of the status of jobs in an SQL database. The service listens on the *Data Ready* queue. When messages are first received, the service will set the correct variables for the job, create new jobs in the database and, when ready, will send a message to the *Reduction Pending* queue.

The daemon service also receives updates from the reduction worker itself. When the reduction worker reaches certain stages of its execution, it will send messages to *Reduction Started*, *Reduction Complete* and *Reduction Error*. The *QueueProcessor* service also listens on these queues and will update the database accordingly when messages are received. For some messages in the error queue, the daemon will create and schedule the appropriate retry runs. There is also a system in place for emailing notifications of run failures to administrators.

Since the database is being frequently being updated throughout the process of autoreduction, the Python/Django[8] WebApp is always up to date with the latest information. This means that users can easily check on the progress of their runs and get a good idea of how long it is going to take for them to retrieve their data at the end.

3.4 Reduction worker

The data reduction itself is performed by a worker node, running a Python daemon listening on *Reduction Pending*. When the worker consumes a message, it will spawn a process starting the job and notifying *Reduction Started*. This process tests for access to the filesystems used for storing the raw and reduced data, triggering a scheduled retry later - on *Reduction Error* - if they're unavailable. Otherwise, it will proceed with the reduction, loading and then running the provided reduction script.

On a successful execution, the daemon will notify *Reduction Completed* with the location of the reduced data; otherwise, it will send the reason for failure to *Reduction Error*, most likely without triggering a retry. In both cases, it will create logs of the process and also clean up after itself. Some runs associated

with the same experiment will write output to the same directory; to prevent clashes due to this, the node contains an internal queue holding all jobs associated with a given experiment for as long as it is actively reducing runs for the same experiment.

4 Interface

4.1 Reduction scripts

The wholly automated portion of the system revolves around running scientist-provided scripts to reduce raw instrument data. These scripts are provided as Python scripts on a per-instrument basis, typically using the Mantid software package to do the heavy lifting. They're stored on a shared file store in a known location where they can be modified at will by instrument scientists. The script used in reduction is also stored in the system database.

Aside from overall logic, these scripts typically require parameters such as calibration files, information about how the instrument was run, output settings, and so on. A mechanism for providing such parameters separate from the script itself is provided. A list of parameters and default values is provided in a Python file similar to the reduction script. The autoreduction system keeps track of the parameter configurations provided to it and applies them to the relevant jobs.

The scripts need to integrate with the automation system, and as such must conform to a certain specification: a reduction script must have a *main()* method, taking an input data file and an output directory as arguments. If the script uses system-supplied parameters, it must have a certain *import* directive which serves as a point of injection for the variables when the reduction script is executed.

A reduction script is a Python script and it can call any software callable from Python installed on the reduction worker compute nodes which includes Mantid data reduction algorithms.

Each experiment at ISIS has a unique so-called RB-number and for almost all experiments at ISIS multiple separate runs are collected. A reduction script has access to all reduced data for an experiment, which

may be used in a script to automatically combine information from multiple data reductions.

4.2 Web app

The web app provides the user-facing interface for managing reduction. It was developed in Python, using the Django web framework, and is integrated with the state database. Django provides an intuitive way to interact with databases through its use of models and Object Relational Mapping (ORM). Therefore, getting information from the database to show on the front end is quick and intuitive.

Users log in via the ISIS User Office system – using credentials granted for facility-wide use – and their level of access is then governed by ICAT's [3] information on the experiments and instruments they should be able to see. A searchable index of the runs is displayed on the front page, sorted by instrument, experiment (RB-number) and/or run number, showing their reduction status.

Each run has its own summary page with detailed information; a user can see the status of the reduction, where the reduced data is, and the script and variables that were used to reduce it. From here the run can be re-run, with or without modifying the variables used and with the choice of whether or not to overwrite the previous run's data. Any experimenter can access this page for their runs, and it is intended that external scientists running experiments would be able to control their data reduction directly in this way.

Experiments also have summary pages, showing all of the runs that are associated with a given experiment along with their status and data locations. Metadata about the experiment is retrieved from ICAT and displayed here.

Instrument scientists can access a summary page for their instruments, showing the current status of runs on an instrument, as well as current and upcoming run variables. From here, instrument scientists can assign sets of variables by experiment and run number which will then be used for new runs. Batch re-running of past jobs is also possible here. This option allows instrument scientists the convenience of re-running multiple failed jobs should this

Experiment Number	Status	Last updated
35903	Completed	Sept. 19, 2016, 4:07 a.m.
35902	Completed	Sept. 19, 2016, 3:03 a.m.
35901	Completed	Sept. 19, 2016, 2:01 a.m.
35900	Completed	Sept. 19, 2016, 1 a.m.
35899	Completed	Sept. 18, 2016, 11:43 p.m.
35898	Completed	Sept. 18, 2016, 11:22 p.m.

Figure 2: The web app index, showing recent runs.

be required.

Administrators can access everything above and additionally have access to pages displaying all queued and failed jobs. These pages provide an overview of the status of the system at a glance and have controls for batch operations on failed jobs such as to re-run them.

5 Deployment

The system is deployed at ISIS. The node managing the WebApp is a Windows Server 2012 running on a Hyper-V[10] virtualisation cluster and it serves the WebApp using Apache's HTTP Server[9]. The WebApp runs on a Windows server for security reasons but since it runs on a basic Apache server, it could easily be moved across to a Linux machine if it needed to. The WebApp is currently only accessible from inside the laboratory using the URL: <http://reduce.isis.cclrc.ac.uk>.

There is then a second node which runs Red Hat

Enterprise Linux 7[14]. This node manages the parts of the system which are common between front and backend. This includes: the MySQL database, the ActiveMQ server and the EndOfRunMonitor. This node should have all the parts of the system that wouldn't need to be replicated as part of a worker node.

The third and final node manages the parts of the system that could be replicated such that we can have multiple worker nodes active in order to split the load of autoreduction and speed up the overall process. This node has the QueueProcessor and the AutoreductionProcessor installed on it. At the moment, the production system only uses one of these nodes but as the usage of the system increases, so too will the load. It might then be sensible to have multiple worker nodes.

The system is split out in this way such that if the machine with the WebApp installed were to fail, the overall process of reduction could still take place. We would still pick up new runs with the EndOfRun-

Monitor and would still be able to process them with QueueProcessor and AutoreductionProcessor.

The software written as part this project is not tied to a particular operating system since it is written entirely in Python and Django.

6 Future plans

It is planned that the autoreduction system be developed to further meet the needs of users. Future development to this will involve:

1. Expanding the system to accommodate greater volume of use – this might involve accommodating more reduction workers, for example
2. Integrating other methods of monitoring or listening for new runs – the current method of watching a file archive is specific to ISIS
3. Make the WebApp accessible from outside of the laboratory
4. Have selected reduced data automatically catalogued in ICAT
5. Improving portability and deployability of the current software; the state database/webapp is currently somewhat nontrivial to deploy
6. Having the worker node machine as a Docker [?] image for easier deployment

In the longer term, the system may be extended to listen to live streams and begin processing data as soon as it comes off beamlines rather than waiting for files to be written to disk.

7 Conclusion

The autoreduction system offers a convenient way of automating data reduction on beamline instruments. It uses a scalable architecture to allow prompt reduction of data from a large number of instruments and utilises a web app frontend to allow users to control the reduction process manually and verify that the correct reduction was executed.

The source code can be found on GitHub[15].

8 Acknowledgement

Tom Griffin, Nick Draper, Martyn Gigg, Alex Buts, other excitation group members and other testers, Shelly Ren and Mathieu Doucet.

References

- [1] O. Arnold, et al., *Mantid – Data analysis and visualization package for neutron scattering and μ SR experiments*, Nuclear Instruments and Methods in Physics Research Section A, Volume 764, 11 November 2014, Pages 156-166, [10.1016/j.nima.2014.07.029](https://doi.org/10.1016/j.nima.2014.07.029).
- [2] G. Shipman, et al., *Accelerating Data Acquisition, Reduction, and Analysis at the Spallation Neutron Source*, 2014 IEEE 10th International Conference on eScience, Volume 2, 11 November 2014, Pages 224-230, [10.1109/eScience.2014.31](https://doi.org/10.1109/eScience.2014.31).
- [3] The ICAT Collaboration, *The Icat Project.*, 2014, [10.5286/software/icat](https://doi.org/10.5286/software/icat).
- [4] Apache Software Foundation, *Apache Activemq*, <http://activemq.apache.org/>.
- [5] M. Gerstel, R. Gildea, K. Levik, A. Ashton, G. Winter. *Data Analysis Infrastructure for DLS MX/CX*, NOBUGS Conference 2016, Kbenhavns Universitet, <https://indico.esss.lu.se/event/357/session/7/contribution/51/material/slides/0.pdf>
- [6] Dr. Sergey Stepanov. *Integration of fast detectors into beamline controls at the GM/CA macromolecular crystallography beamlines at the Advanced Photon Source*, NOBUGS Conference 2016, Kbenhavns Universitet, <https://indico.esss.lu.se/event/357/session/6/contribution/17/material/slides/0.pdf>
- [7] NOBUGS Conference 2016, *NOBUGS*, <https://indico.esss.lu.se/event/357/>.
- [8] Django Software Foundation, *Django*, <https://www.djangoproject.com/>.

- [9] Apache HTTP Server Project *Apache*, <https://httpd.apache.org/>.
- [10] Microsoft Corporation, *Hyper-V*, <https://technet.microsoft.com/en-us/library/mt169373.aspx>.
- [11] Docker, *Docker*, <https://www.docker.com/>
- [12] Microsoft Corporation, *IIS*, <http://www.iis.net/>.
- [13] *FastCGI*, <https://github.com/FastCGI-Archives/FastCGI.com>.
- [14] Red Hat, Inc, *Red Hat Enterprise Linux*, <https://www.redhat.com/en/technologies/linux-platforms/enterprise-linux>.
- [15] *Autoreduction repository*, <https://github.com/mantidproject/autoreduce>.