

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

J. R. Corderoy, 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, integrated 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 a user 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 readably 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 work allows data coming off an instrument to be automatically reduced using a

dedicated software package such as Mantid[?], while lending transparency to the process and letting users control it through a straightforward web interface.

TO DO: some reference that automation of data reduction also pursued at other large scale facilities: Anders writing from NOBUGS conference: such as possibly mention Diamand has a batch script based system for macromolecular beamlines (talk by Dr Markus Gerstel, Diamond). Dr Martin Rehr mentioned in his talk on “Image data Management System” that auto processing was used. Dr Sergey Stepanov talk “Integration of fast detectors into.... macromolecular crystallography beamlines at the Advanced Photon Source” used auto processing - seemed to be a theme for MX beamlines.

2 Background

The autoreduction system at ISIS is based on the autoreduction setup at the the Spallation Neutron Source (SNS) at Oak Ridge National Laboratory [?].

The autoreduction implementation at ISIS uses the same underlying technologies (web framework and messaging queue software, for example) as those used for the implementation of the SNS autoreduction service but differs in that its front end client is designed to serve autoreduction users only rather than including information about the status of the neutron beamlines, which is already handled elsewhere in ISIS.

2.1 Data reduction

The autoreduction service exists to reduce beamline instrument data. An instrument produces discrete sets 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, 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 it with reduction scripts - in a specified location on a shared file archive - and sets of variables to use to reduce runs. The system watches for the completion of runs, and runs the appropriate script, with the correct variables, on them, supplying the reduced data to a data store for users to retrieve.

2.2 Requirements

The system is intended to serve both 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 implemented 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 experiments
4. Allow users and instrument scientists to see what script and parameters, was used to reduce a particular run
5. Allow users and instrument scientists to modify the parameters used for a run, and re-run reduction using new parameters or scripts

Additionally, 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 sends a request to do so to *Data Ready*. The state database consumes the request and creates a corresponding job in the database, before sending a request to process it to *Reduction Pending*. The reduction worker takes this message and executes the appropriate reduction script, sending the result to either *Reduction Complete* or *Reduction Error*, where it is consumed by the state database to update the status of the job.

3.1 Message queue

Apache ActiveMQ[?] is used as the message queueing system, with message contents as JSON-formatted objects. The intent of the message is conveyed by which queue it is 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 has 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

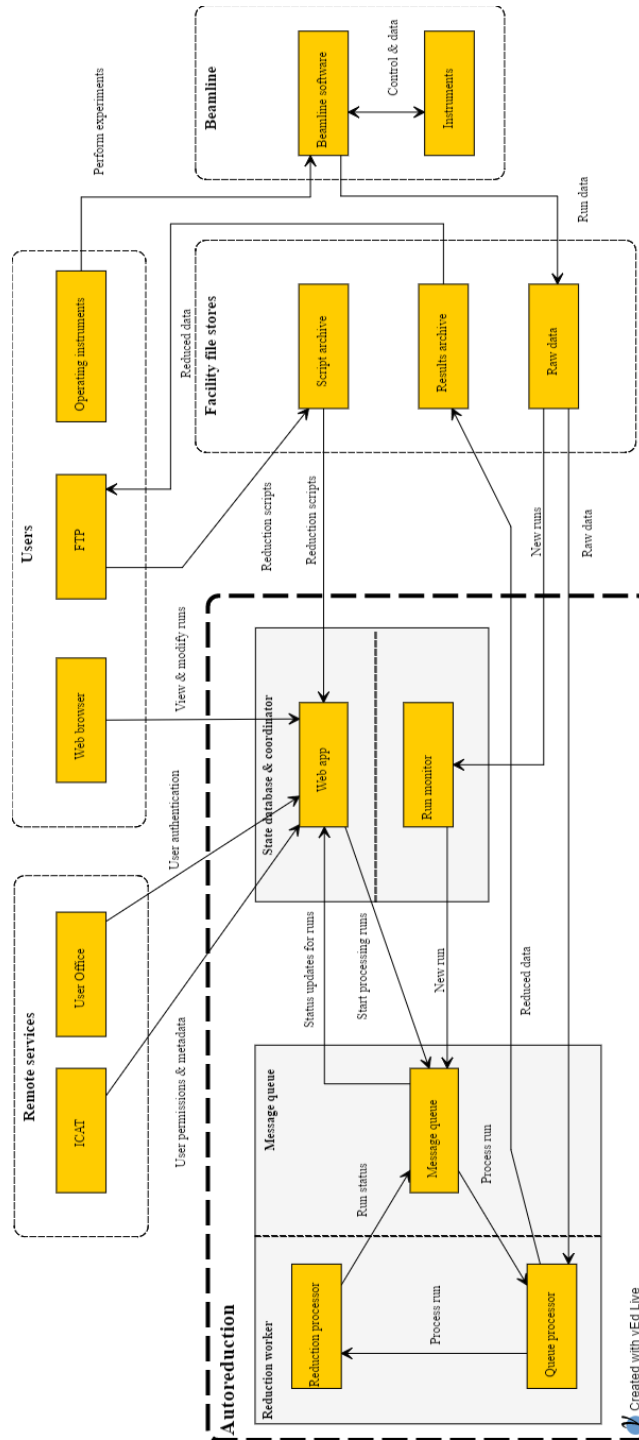


Figure 1: How the current autoreduction system fits into the ISIS workflow.

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.

As data files at ISIS typically run in the hundreds of MB they would be impractical to send directly in a message so they are 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 directly to send it removes 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, sends a message to *Data Ready* with details of the run. In the current production system at ISIS, the run monitor is on same node as the state database itself.

3.3 State database & coordinator

A node keeps track of the status of jobs in a local SQL database. This server hosts a Python service responsible for listening on *Data Ready*, to create new jobs in the database and then dispatch them to *Reduction Pending*. It manages variables for reduction, and selects the correct set for the job. The same server is also responsible for serving the Python/Django web app, and the database is accessible through Django's object interface.

The daemon receives status updates from reduction workers on *Reduction Started*, *Reduction Complete* and *Reduction Error*, making the appropriate changes to the database. On some messages in the error queue, the daemon will create and schedule the appropriate retry runs. A system for emailing notifications of run failures to administrators is also implemented here.

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 send logs of the process, and 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 data reducing. They are stored on a shared file store in a known location, where they can be modified at will by instrument scientists and the script used in reduction is 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, and the autoreduction system keeps track of the parameter

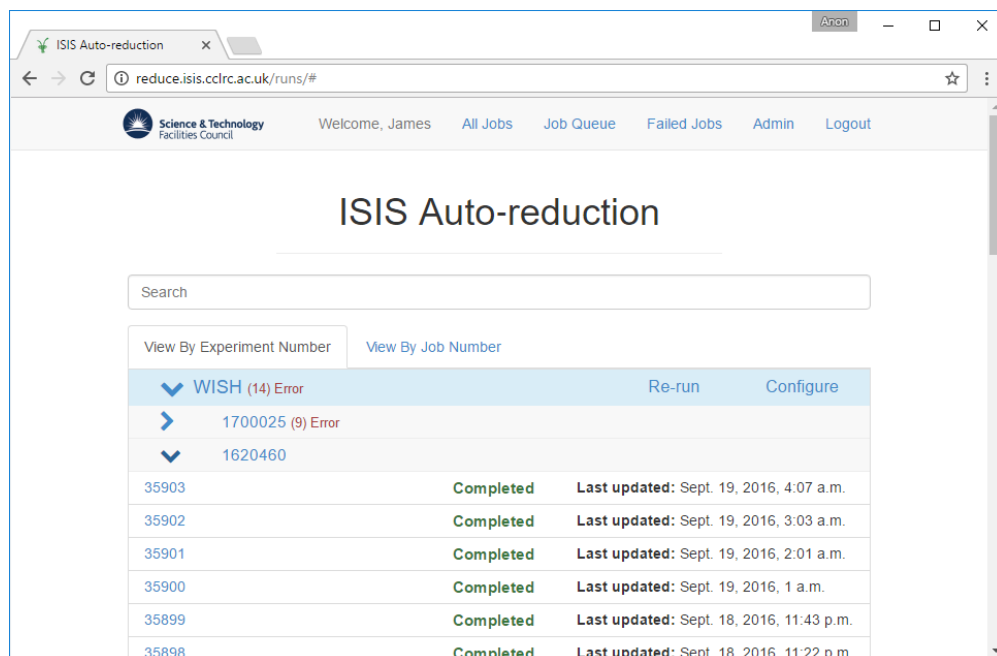


Figure 2: The web app index, showing recent runs.

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 an *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, including Mantid data reduction algorithms.

Each experiment at ISIS has a unique 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 experiments, 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 uses the state database to determine what runs to display.

Users log in via the ISIS User Office system – using credentials granted for facility-wide system – and their level of access is then governed by the ISIS data catalogue’s (ICAT) 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. Any experimenter can access this page for their runs, and it is intended that external scientists running experiments be able to control their

data reduction directly in this way.

Experiments also have summary pages, showing all 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 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 state database and web app is a Windows Server system running on a Hyper-V[?] virtualisation cluster; it serves the web app using Microsoft's Internet Information Services (IIS)[?] and FastCGI[?]. The web app is currently only accessible from inside the laboratory using the URL: <http://reduce.isis.cclrc.ac.uk>.

There is one reduction node, running Red Hat Enterprise Linux 7[?] on a dedicated server – reducing large amounts of data is memory and CPU-intensive. This node also serves the message queue; subsequent worker nodes would not have multiple message queues, and the message queue will be hosted on a separate node.

The software written as part of 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 web app accessible from outside of the STFC intranet
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

Longer term, the system may be extended to listen to live streams and starts processing such data as they come 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[?].

8 Acknowledgement

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

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