XPD 2017 Cycle 3 Release

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Features

- General Refactor
- Enhanced Metadata
- Tramp/Tlist shutter protocol
- Data Reduction and Visualization Pipeline

General Refactor

Many pieces of the XPD stack needed to be refactored due to the changes in Bluesky and Databroker, including:

- Removal of "dot" access from headers
- Databroker named configurations
- Removal of dereferencing of documents

Enhanced Metadata - Motivation

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- Metadata is very important for searching data, mineing data, and using data effectivly.
- The XPD stack is designed to make the additon of metadata as easy as possible, enabling users to insert sample data via a spreadsheet and tacking metadata about the experiment (eg calibration data) automaticaly.
- Two major features were implemented:
  - Long Term Beamline Configuration
  - Server Client keys

Long Term Beamline Configuration

- There is a dedicated file `.../xpdConfig/XPD_beamline_config.yml` in yaml format to hold this kind of information.
- Please feel free to put whatever information you deam nessisary in this file.
- This information will be very helpful to make sure that when the data is queried one can make certain that the beamline configurations are comparable.

Server Client keys

- xpdAcq now has a system of "server" and "client" keys to match these data sets.
- In this system "clients" and "servers" will have a shared key. Thus, if one wanted to search for which calibration(s) go with a given data set one just searches `db(detecter_calibration_server_uid= header['detector_calibration_client_uid'])`.
- This system will allow for (in a future release) overriding calibrations and other pieces of linked data and data analysis when calibrations are taken after the sample data.

Tramp/Tlist shutter protocol

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- Keeping the detector as clean/sensitive as possible
- Some scans don't take images continously (eg while waiting for temperature equilibration)
- Temperature based scan plans now have the option to close the shutter when not taking images (see documentation for details)

Data Reduction and Visualization Pipeline - Motovation

- Users walk away with resonably analyzed data (using some of the best tools in the community)
- Users use XPD/NSLS-II/BNL's high powered computational resources
- Allows for human-in-the-loop experiment tuning (does my data look good?)

Usage and capabilities

The system is designed to do what you expect:

- Visualizes data as it comes off the detector
  - dark subtracted image
  - mask
  - $I(Q)$
  - $I(2\theta)$
  - $F(Q)$
  - $G(r)$
- Writes files to `tiff_base` as data is analyzed
  - dark subtracted image
  - calibration `.poni` file
  - mask `.msk` file
  - $I(Q)$
  - $I(2\theta)$
  - $G(r)$
  - metadata

Live Demo

Conclusion

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Much of this release is infrastructural, some of which is easy to see (live visualization), others less so (server client links). Long term these will help us to accive many of our goals:

- database of analyzed data
- adaptive scan logic
- automated experimentation