MXCuBE-ISPyB joint discussion summary

MXCuBE-ISPyB project meeting, Trieste, September 2018

DRAFT

Autoprocessing

- There was a perceived need to upgrade the evaluation metrics normally reported in Table 1. Rmerge is still used despite being shown long ago to be frequently misleading.
- It was discussed whether users do (or should) expect to get publication quality data from synchrotron autoprocessing. Alun Ashton reported that where this can be ascertained, 95% of Diamond users use autoprocessing results.
- Diamond presents different processing results in the order they appear, which means that users tend to prefer the first result, i.e. the one that is calculated most quickly. At ESRF results are sorted by symmetry first, then by initial Rmerge (see comment above). There may be 20-30 different processing results for a single sample. ESRF has done work on user-settable filters.
- Both ESRF and Diamond report that different pipelines can give different quality results, but that no single pipeline is superior in all cases, and that sometimes only a single pipeline gets a good result. Pipelines that run XDS through different wrappers also can give different results.
- Clemens Vonrhein asked if pipelines could be set to send failed calculation runs to the program developers, and Alun Ashton promised to check for infrastructure problems.
- It was discussed if resulting data can be reprocessed away from the synchrotron infrastructure. It seems that this is not always the case, and it is not systematically tested. All pipelines in principle get their data from ISPyB, and file headers ‘should’ reflect the same data. There seems to be a particular problem with Eiger detectors, since for technical reasons the master file header is written before data collection starts, and so particularly the figure for the number of images collected is not reliable.
- Gerard Bricogne notes that autoprocessing lives suspended between MXCuBE and ISPyB, and suggests that there is room for standardisation in the way data and processing instructions are communicated between the two. Olof Svensson agrees that there is a need both for allowing user customisation of processing parameters, and for configuring reliable default values for parameters.

The various synchrotrons present their individual autoprocessing setups:

- Max IV uses the standard ISPyB results display. They would like to avoid depending on Phenix components (for licensing reasons) and note that EDNAproc does use some Phenix programs.
- For SOLEIL the entire question is very new. In SAXS autoprocessing uses Ses Passarelle, through ISPyB. In MX they use Dozor/autoPROC/XDSME (based on a workflow OS) The implementation is in Haskell, which is triggered by MXCuBE. Linking to ISPyB is still in progress, and a presentation layer is not yet ready.
- P11 (Hamburg) runs XDSAPP and MOSFILM. Results are in a HTML file with links, and the implementation is NOT particularly simple to change. When asked whether they would like MXCuBE to be updated to handle autoprocessing for them, the answer is that adding in ISPyB would delay them for a year.
- XALOC (ALBA) use EDNA for characterisation and EDNAProc; autoPROC is used but still not fully integrated. Results are given to ISPyB. There is a web interface to ISPyB for rerunning autoprocessing from the home lab.
- HZB Berlin use XDSAPP in automatic or semiautomatic mode (XDSAPP is a python GUI around XDS, doing multiple iterative runs). Most users reprocess their data at home. With respect to resolution cut-offs and other metrics, users always ask for another way of determining them, CC1/2, statistical significance cut-offs with various thresholds, ... The only attached software developer left in 2017. HZB is in favour of standardisation.
- Elettra is missing an ISPyB visualisation tool, and has found the ISPyB installation process very difficult.

Crystallography metrics

- Stephanie Monaco notes that the first goal of the display of processed structure metrics was for quick information to guide ongoing acquisition. There are now nearly thirty parallel processing results for a sample, and people are slowly opening to a new world. Users never ask for parameters. ESRF runs all the different pipelines, and it is a problem how to get the right metrics from all of them – and how to ensure they are calculated in the same way, so as to be directly comparable. Possibly MRFANA could be added to the pipeline as a tool to produce metrics from all the pipelines? According to Clemens Vonrhein MRFANA requires unmerged scaled data, and can produce any binning you want.
- It is further discussed how many people use autoprocessed data (at Diamond it is 95%), and how they select their data set. According to Stephanie Monaco many users use the autoprocessed data, and SM does not know what criteria they use. There is evidence that Diamond users tend to use the first result in the table (which is the one that finishes calculating first). This would bear further enquiry; one proposal is to randomise the presentation order and study which programs are selected. SM proposes an agreed default ranking system, with clearly explained criteria.

- It is mentioned that metrics are re-discussed every few years, and it would be nice to get beyond that. In practice only two small groups of people ever ask questions about (of?) the metrics: old-time crystallographers who once used to study every image in detail, and 1% of people who want to learn. The rest just use what they are given, seeing as they could not do better by hand. Of the various metrics in use, resolution is the major one, by tradition. Rmerge keeps surviving also because the PDB asks for it; it is proposed that maybe programs should collectively refuse to calculate it! Many users ask for I/sig(I) of 2.0, relying on BEST. CC1/2 is a very popular criterion. Is is suggested that one reason may be that it tends to give higher resolution cut-offs than I/sig(I). Clemens Vonrhein comments that the two criteria give the same cut-offs for genuinely isotropic data, so that the real problem comes back to how to treat anisotropy. There is agreement that data describing anisotropic diffraction are needed, but it is problematic that they do not conveniently reduce to a single number, whereas short summary descriptions strongly prefer a single number. Clemens Vonrhein suggests a diffraction limit that gives you 30% completeness could be calculated regardless of anisotropy, whereas Gerard Bricogne puts more emphasis on customisability of the displays.