Case Study

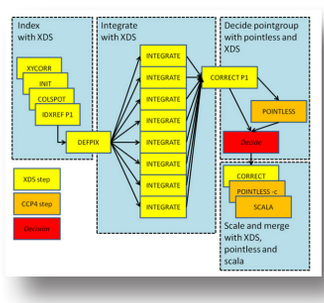
Auto-processing software pipelines at Diamond's MX beamlines

The Problem

As fast Pilatus detectors have become the gold standard at Diamond's MX beamlines, the time needed for collecting a complete dataset is now less than two minutes. This gives a user very limited time to process data and subsequently decide what would be the best strategy for collection of data from remaining crystals.

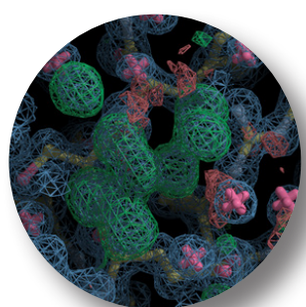
The Challenge

A user needs automated software which will provide information about data quality and completeness before the next sample has been loaded on goniometer. The main requirements for this system are to be fast and to produce reliable results. This is especially critical to maximise efficiency for our industrial clients who often come to Diamond with large numbers of protein-ligand complexes produced for fragment-based and structure-based drug discovery.



The Solution

Diamond's auto-processing pipeline includes strategy calculation using the EDNA and Mosflm programs which gives a user information about space group and resolution, and suggests the strategy for collection of complete data. The second part of the pipeline is automatic data processing performed by Fast_dp and Xia2. Fast_dp provides immediate data quality statistics in less than two minutes after data collection. Xia2 is more thorough, and processed data from this program are perfectly suitable for downstream analysis without additional re-processing by the user. The final part of the pipeline is represented by Dimple and Fast_ep. Dimple uses an apo-protein model and allows the user to rapidly check if the drug candidate is bound in their crystal. Fast_ep is SHELX based software for the automatic phasing of heavy atom substructures.



The Benefits

Auto-processing pipelines are now an essential and constantly developing part of the MX beamline package. Autoprocessing helps users decide how to collect the best data and plan the most efficient use of the available beamtime. As a result, users not only get the optimum results from their samples but can also often achieve these in shorter timescales.

"As an industrial experimentalist, high throughput/output crystallography i.e. knowing that the data set is good and also that my ligand is present during my collection time, through real time calculation and visualisation of my experimental electron density maps, ensure I get the most productivity from my synchrotron visit. The real time analysis allows me to choose which experiments to repeat/fine tune to provide customers with fast turnaround times for complexes of ligands with their target proteins."

Prof Dave Brown, Charles River Laboratories

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