Streamlining the user experience of the macromolecular crystallography beamlines at Diamond Light Source

D.R. Hall

Diamond Light Source, Didcot, United Kingdom

Since the start of operations over 10 years ago, Diamond Light Source have made a concerted effort to manage and develop the macromolecular crystallography (MX) beamlines experimental workflows, data and subsequent analysis and presentation of results. This effort is built around the data acquisition gui GDA\(^1\), the database ISPyB\(^2\) and the web interface SynchWeb\(^3\) alongside multiple downstream processing and structure solution pipelines Diamond has implemented or developed. These have been key in developing a workflow for users which include organising samples from the home lab to Diamond for experiments; providing information for experiments and downstream processing pipelines and recording and presenting all experimental data and results from auto-processing pipelines. As throughput has increased greatly for example due to increases in detector frame rates, sample exchange time reduction and automation of many processes these technologies have become ever more essential and it is necessary to provide as near real time as possible experimental feedback to enable rapid decision making and make best use of beam time. Many of the tools developed for MX are increasingly available to other scientific disciplines at Diamond. The lab-beamline-lab workflow as used at Diamond for MX users will be presented, delving in more detail into aspects of the data processing pipelines and the accessibility of results that users benefit from.

\(^1\) http://www.opengda.org
\(^2\)ISPyB: an information management system for synchrotron macromolecular crystallography S. Delageniere et al., Bioinformatics (2011) 27 (22): 3186-3192.