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Unattended MX data collection and beamline monitoring at Diamond

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Diamond Light Source, the UK national synchtotron, currently operates 7 macromolecular crystallography beamlines [1]. The core suite, comprising 4 highly automated beamlines for conventional cryo-crystallography, is complemented by dedicated ones for in-situ room temperature, long wavelength and sub-micron focusing data collection.
Low-level control of equipment is operated by EPICS, while at the user level, each beamline is driven by our data collection software GDA[2-3]. Full integration between User Administration System, the ISPyB[4] database (via the SynchWeb[5, 6] interface), and GDA, grants consistency across various aspects of the experiment, including logistics and data analysis/processing.
In the recent past, Diamond introduced fully unattended data collection[7]. Users simply need to define for each sample a suitable data collection strategy (chosen from a set of optimized recipes), while on arrival of crystals at Diamond, they are loaded in the most suitable beamline and data collection occurs without any need of interaction from the User.
The heart of this is a combination of software tools which oversee the status of the beamline and coordinate the queuing and data collection for unattended experiments.
The first task is carried out by daemons interacting with EPICS to report the status of vital PVs through HTTP restful interfaces, database connections and on-disk file analysis. Beamline health reporting occurs through systems such as Slack, Email, Signal/WhatsApp and can be configured through a Slack bot. This avoids overload of information and optimizes troubleshooting, especially during out-of-hours assistance.
On the other hand, a virtual user daemon ensures that unattended data collection is carried out every time the beamline is in a healthy state but idle. Since different instruments offer different beam properties, recipes are harmonized to capture these features. For example, at the variable focus beamline I04 dose is calculated using a built-in Raddose3D [8] calculator to ensure optimal exposure times.
This concept maximizes the performance of beamlines, reducing idle times by interleaving interactive and automated experiments and supervising the efficiency of the instruments by constantly monitoring and reporting their performance.

References

[1] https://www.diamond.ac.uk/Instruments/mx.html (shortened URL https://dls.mx)
[2] http://www.opengda.org/
[3] https://alfred.diamond.ac.uk/documentation/
[4] S. Delagenière et all. Bioinformatics, (2011) 27. 22:3186–3192
[5] S. Fisher et al., J. Appl. Cryst. (2015). 48, 927-932
[6] https://diamondlightsource.github.io/SynchWeb/
[7] https://dls.mx/udc
[8] C.S Bury et al. Protein Sci. (2018). 27:217–228.

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