MS41 Automation in data collection and processing

MS41-03

Interactive and unattended data collection driven by target dose on the Diamond Light Source I04 beamline

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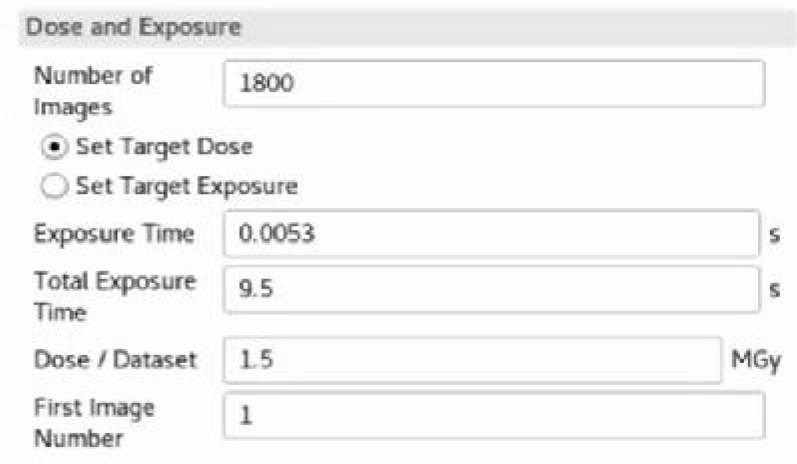
Abstract

Diamond Light Source currently operates seven beamlines for macromolecular crystallography [1]. I04 [2,3] is an energy (6-18 keV) and beam size (5-100 microns) tuneable microfocus beamline suitable for projects ranging from large scale high throughput ligand screening to difficult single or multiple anomalous dispersion experiments. These large spectrum capabilities are built on top state of the art hardware equipment and software developments. The hardware highlights are a multi-axis goniometer for crystal alignment and X-ray centring, a large and very fast frame rate pixel array detector for diffraction data collection and the use of compound refractive index lenses for focusing. The software stack includes the diamond wide data acquisition and GUI software GDA [4-5] as well as the SyncWeb interface [6] for ISPYB [7]. Collecting at its full potential I04 can load a sample, centre it automatically using X-ray diffraction at two different orientations and collect a 7.2 second rotation dataset of 360 degrees in less than 2 minutes providing on average over 32 samples throughput per hour. I04 is also part of the recent Diamond MX beamline developments on the use of Unattended Data Collection (UDC) [8] where the only interaction of the users with the beamline is done prior to the beamtime on defining how do they want to collect their data based on a series of pre-set recipes (unpublished). In addition to UDC, I04 provides onsite and remote access capabilities and has special tools like built-in Raddose3D [9] calculator to help design experiments for optimal data. Here we present a brief overview of the beamline automation in data collection including the recent enhancements on using dose to increase efficiency on both the unattended data collection as well as driving queues of experiments dialling dose instead of an exposure (Figure 1, Figure 2). The latter enhancement was critical to open the automation avenue for the available beamline energy range and beam sizes without compromising on radiation damage as well as not under exposing a well diffracting crystal.

References

[1] https://www.diamond.ac.uk/Instruments/Mx.html
[2] R. Flaig et al, Acta Cryst. (2017). A73, a71
[3] https://www.diamond.ac.uk/Instruments/Mx/I04.html
[4] http://www.opengda.org/
[5] https://alfred.diamond.ac.uk/documentation/
[6] https://diamondlightsource.github.io/SynchWeb/
[7] S. Delagenière et all. Bioinformatics, (2011) 27. 22:3186–3192
[8] https://www.diamond.ac.uk/Instruments/Mx/I03/I03-Manual/Unattended-Data-Collections.html
[9] CS Bury et all. Protein Sci. (2018). 27:217–228.

1)Using dose as the target to drive the experiment



2)Data collection queues driven by dose

Centring Mode	Number of Images	Time per Image (s)	Target Dose (MGy)	Maximum Resolution (Å)	Distance (mm)	Wavelength (Å)	Energy (eV)	Transmission (%)	Beamstop position	Horz. Beam Size (µm)	Vert. Beam Size (µm)
Auto X-ray	3600	0.0026	1.50	2.1000	313.0	0.97949	12658.0	100.000000	Standard	31.73	20.00
Auto X-ray	3600	0.0020	1.50	2.1000	167.6	1.54980	8000.0	17.166685	Standard	31.73	20.00
Auto X-ray	3600	0.0020	1.50	2.1000	313.0	0.97949	12658.0	12.506396	Standard	11.11	5.00
Auto X-ray	3600	0.0087	5.00	2.1000	313.0	0.97949	12658.0	100.000000	Standard	31.73	20.00
Auto X-ray	3600	0.0026	1.50	2.1000	313.0	0.97949	12658.0	100.000000	Standard	31.73	20.00