New features, 2019-1 run

New focusing optics on the IDD beamline

We have ordered new x-ray mirrors for the both ID-beamlines, and Compound Refractive Lenses (CRL) for microfocusing on ID-D. However, in the mean time we have installed some CRLs on ID-D to improve the focus with the current mirrors. As a result, the beam intensity is much higher and nearly back to the intensity we had during the 2016-3 run. At the moment, there are also some limitations on the accessible energy range (11 – 13.5 keV) and beam sizes. Table 1 and Table 2 below show the energy range, the beam sizes and the beam intensity at various settings. The two tables contain the same data, sorted differently.

Accessible beam sizes can be requested from a pull-down menu. The option to enter a beam size is not available currently.

New Robot on IDD

The prototype large capacity (18 puck) automounter on the IDD beamline has been replaced with a new improved version based on the 18 puck model operating in the IDB endstation. These automounters perform best with unipucks and ALS- or SPINE-pin bases. We have loaner kits with unipucks that are available on request.
If you are unsure about loading the pucks into the automounter dewar, please ask your host for a demo.

Screening

Additional columns are supported to provide prior information for data processing and structure determination pipelines.

- “Metal”: defines a metal in the crystal, if defined, the data will be processed as anomalous data.
- “ModelPath”: defines the PDB file used for ligand screening using DIMPLE. The files must be located in Downloads or Desktop directory if only the filename is given. Otherwise, the filename should be in the full path.
- “Spacegroup”: space group name, defines a space group to be used in data processing.
- “SequencePath”: define the sequence file to be used by MR (not yet implemented).

Strategy

- Multi-crystal strategy (MCS) subtab removed and its functionality moved to the Analysis/Screening tab. To run MCS in the Analysis tab, collect some screening snap shots as usual, rerun xds_strategy (via the "reproc" button in the corresponding Analysis/Screening tab entry), and provide the path to the partial data (XDS or SCALEPACK formats).
- Analysis/Screening allows users to select non-default strategy to export

Data collection

- Shutterless data collection in Vector and Inverse Beam modes are faster.

Table 1. Beam size and Intensity at different energies with different collimators on ID-D with the KBM and 15 CRL lenses

Energy_collimator	Horizontal size (microns)	Vertical size (microns)	Intensity (photons / s)
With Scatter Guard (sg), largest beam			
13.50keV_sg:	28.4	33.8	6.13E+12
13.00keV_sg:	24.3	26.7	7.42E+12
12.66keV_sg:	23.3	19.6	8.51E+12
12.00keV_sg:	21.5	20.0	9.85E+12
11.50keV_sg:	23.3	20.0	1.02E+13
11.00keV_sg:	30.3	30.0	9.13E+12
With 20 µm collimator			
Energy_collimator	Horizontal size (microns)	Vertical size (microns)	Intensity (photons / s)
13.50keV_20:	13.3	13.8	1.19E+12
13.00keV_20:	13.7	12.4	1.66E+12
12.66keV_20:	13.3	12.8	2.13E+12
12.00keV_20:	15.1	10.5	3.06E+12
11.50keV_20	16.0	9.5	3.49E+12
11.00keV_20:	17.8	6.2	2.25E+12
With 10 µm collimator			
Energy_collimator	Horizontal size (microns)	Vertical size (microns)	Intensity (photons / s)
13.50keV_10:	8.6	8.6	4.81E+11
13.00keV_10:	9.6	8.5	6.47E+11
12.66keV_10:	10.1	7.7	8.24E+11
12.00keV_10:	11.9	8.6	1.32E+12
11.50keV_10:	12.4	5.8	1.86E+12
11.00keV_10:	10.4	5.2	1.20E+12
With 5 µm collimator			
Energy_collimator	Horizontal size (microns)	Vertical size (microns)	Intensity (photons / s)
13.50keV_05:	7.8	5.7	1.45E+11
13.00keV_05:	7.8	5.7	1.99E+11
12.66keV_05:	8.6	6.8	2.59E+11
12.00keV_05:	10.9	6.1	4.32E+11
11.50keV_05:	8.7	5.2	6.13E+11
11.00keV_05:	8.7	5.3	4.73E+11

Table 2. Beam size and Intensity with different collimators at different energies on ID-D with the KBM and 15 CRL lenses

Energy_collimator	Horizontal size (microns)	Vertical size (microns)	Intensity (photons / s)
At 13.5 keV			
13.50keV_sg:	28.4	33.8	6.13E+12
13.50keV_20:	13.3	13.8	1.19E+12
13.50keV_10:	8.6	8.6	4.81E+11
13.50keV_05:	7.8	5.7	1.45E+11
At 13.00 keV			
13.00keV_sg:	24.3	26.7	7.42E+12
13.00keV_20:	13.7	12.4	1.66E+12
13.00keV_10:	9.6	8.5	6.47E+11
13.00keV_05:	7.8	5.7	1.99E+11
At 12.6keV			
12.66keV_sg:	23.3	19.6	8.51E+12
12.66keV_20:	13.3	12.8	2.13E+12
12.66keV_10:	10.1	7.7	8.24E+11
12.66keV_05:	8.6	6.8	2.59E+11
At 12.0 keV			
12.00keV_sg:	21.5	20	9.85E+12
12.00keV_20:	15.1	10.5	3.06E+12
12.00keV_10:	11.9	8.6	1.32E+12
12.00keV_05:	10.9	6.1	4.32E+11
At 11.5 keV			
11.50keV_sg:	23.3	20	1.02E+13
11.50keV_20:	16.0	9.5	3.49E+12
11.50keV_10:	12.4	5.8	1.86E+12
11.50keV_05:	8.7	5.2	6.13E+11
At 11 keV			
11.00keV_sg:	30.3	30	9.13E+12
11.00keV_20:	17.8	6.2	2.25E+12
11.00keV_10:	10.4	5.2	1.20E+12
11.00keV_05:	8.7	5.3	4.73E+11

Raster

- All JBluIce spot-finders are running in parallel during data collection or rastering.
- Because of the limitations on available beam sizes on IDD as discussed above, the beam size selections in raster scans have also changed. Be default, 10μm collimator will be used. This leads to different size at different energies and can be verified in the tabes 1 and 2 above. To change the beam size, numbers from the pull-down menu should be selected. There is no limitation on the cell size.
- On IDB, everything works as before.

Analysis

1. Autoprocessing can be disabled, or processing output location be changed, through User/Options or the Settings button (the latter is at the bottom of the Analysis tab).
   1) Default: put processing files next to where diffraction images are located
   2) Put all processing files in a separate tree
   3) Disable analysis

2. Automated structure determination, SAD phasing or Ligand screening are supported (only for fast_dp and gmcaproc pipelines). User may inspect the maps via the “Map” button in the analysis interface after a job completes.
   - SAD phasing: if anomalous signal is detected, SAD phasing using fast_ep (Diamond) will be run. No user input is required.
   - Ligand screening: if user provides a model via ModelPath column in the screening spreadsheet, ligand screening via DIMPLE will be run.

3. KAMO, a software for processing partial data sets from multiple crystals is integrated into jBluIce. User can start KAMO after one data collection by clicking the KAMO button at the bottom of the Analysis tab, or using the Process button and then selecting a KAMO option (kamo_xds or kamo_dials). KAMO should be kept open so that it will process any new data automatically. User can merge periodically to evaluate data quality and their overall process.

4. The updating behavior of Analysis tab is changed, it now will update frequently only when the tab is visible. Otherwise, the page contents update once per hour. The pages will be updated immediately when user switch to it (similar to the behavior of camera tab), so there is a bit of delay. User may open a peel-out analysis window if they prefer to see analysis updates constantly.

5. Documentation
   Short summary of autoprocessing in JBluIce and the pdf version of the full manual are posted on the GMCA web site
   https://www.gmca.aps.anl.gov/computing/jbluice-autoprocessing.html