New features, 2014-1 run

Both beamlines

Remote access

- NX Client-3 because it is no longer supported by NOMACHINE. Therefore it is being phased out from our remote operations as well. All templates have been updated to NX Player-4. Old templates are still available from legacy page for those who already have Player-3 installed. However, users are urged to upgrade to Player-4.
- OpenNX is no longer supported for the same reason.
- Automatic installation of NX Player-4 through the GMCA web site now requires extra steps of adding GMCA to Java and sometimes web browser security exceptions lists. Please read the GMCA remote FAQ web page for additional details.
- Portable versions of NX Player-4 for MacOS, Linux and Windows, which users can download, unpack and run without administrative privileges, are posted on our web site.

Data processing

- XDS now has a GUI for more convenient data processing. It can be started from a command line by typing xdsGUI.
- As before, HKL2000/3000 site files for both, the MAR and Pilatus detectors, can be found here: http://www.gmca.anl.gov/sitefiles/

IDD

Pilatus3 6M has been installed on the 23ID-D beamline

- It is a Pixel Area Detector with a large, 423.6 x 434.6 mm^2 sensitive area.
- When compared to CCD detectors used in macromolecular crystallography it has much higher dynamic range (20-bit vs 16-bit).
- Pilatus3 6M can handle 10 times higher count rates than previous generation Pilatus 6M detectors.
- Detector integrated in 23 ID-D beamline has 1mm thick sensor whereas most other Pilatus detectors currently in the field have 0.320 mm. This allows measuring data at higher energies more efficiently.
- Thicker sensor also produces slight parallax (spot elongation) at higher resolutions (higher angles), especially at closer sample-to-detector distances. However, data processing software seems to take it into account during integration.

Image display:

- Images are written in a Crystallographic Binary Format (cbf).
- Although the image files are binary, typical text editors can read their headers.
- ALBULA is image display and analysis software which is provided together with the detector. It has many useful tools for image analysis. Free copy can be downloaded from here: https://www.dectris.com/Albula_Overview.html#main_head_navigation
- ADXV is still an option for users.
- MARccd GUI can also be used to display images. It can be started on the MAR computer by clicking on the detector icon, or on any computer by command line command *marview*. Beware that if you are using MARccd GUI, the beam center is

reported correctly in pixels but not in millimeters. As a consequence, the resolution is not reported correctly.
- Both ALBULA and ADXV report the origin in pixels and therefore resolution shown in these programs is correct.

Data collection:

Much work still remains to establish optimal protocols for data collection with Pilatus. However, some preliminary recommendations can be offered already:

- Due to higher dynamic range (20-bit vs 16-bit), Pilatus3 6M will "allow" users to kill the sample quicker. I.e., if the spot saturation is used as criterion for exposure levels (as was often done with the CCD detectors), the sample will be overexposed.
- Dose per diffracting volume of the sample can be spread over many frames collected with much shorter exposure times (θ-slicing). For example, 0.1° frames with 0.1 sec exposure. Using 0.2° and 0.2 sec is a good alternative reducing the number of frames twice and increasing the counts on the detector.
- If number of frames is not a concern, so called "dose slicing" is also recommended in literature. For example, instead of collecting 90 degrees of data with 0.1° slices (900 frames), 0.1 sec exposure time and beam intensity I, one collects same 90 degrees of data four times with intensity of I/4 (4-fold attenuation) for total of 3600 images. This approach can be used to collect multiple full sets (multiple 90° swaths in the example used here) with lower dose.
- If the dose slicing is used, it is recommended to move the detector slightly between each data set. This will minimize the systematic errors and will also increase the completeness as the reflections lost to the gaps in some sets will be recorded in others.
- Data are being collected in shutterless mode. It significantly decreases the time needed to collect large number of frames. It also reduces the error introduced by shutter operation. Note that in the present implementation, the shutterless mode works only for "standard" data collection mode. It is not implemented for "vector" mode or for rastering.
- In rastering, if the crystal does not diffract strongly, using 0.1° frames and 0.1 sec exposures may not be advisable as it will produce very few spots. Using wider frame widths (0.3 -0.5 degrees) even with the same 0.1 sec exposures will increase the counts in each recorder Bragg spot making the rastering results more reliable.
- For useful discussions on data collection, please read
  - Optimal Fine phi-slicing for Single-Photon-Counting Pixel Detectors MarcusMueller, Meitian Wang, and Clemens Schulze-Briese, Acta Cryst.(2012) D68,42-56.
  - Data-Collection Stragegies, Dauter, Z. Acta Cryst. (1999). D55, 1703-1717.

Data processing:

- GMCA staff has tried to process some test data sets with XDS, MOSFLM and HKL2000 and they all seemed to work as usual, without any additional steps.
- Just a reminder that automated data processing, using XDS, is implemented in JBluIce
- You will need the most recent version of HKL2000 (v704y) and you may have to contact the vendor for a license in order to read the PILATUS images.