

New features in data collection and beamline controls

As of October 1, 2013

General

- Few changes have been made in preparation for integration of Pilatus detector. They are transparent to users.
- Focusing mirrors on IDB have moved closer to the sample, increasing the flux.
- Beam X/Y are correctly calculated in runadxv for binned images. Image size and pixel size are taken from the image header, instead of being hard-coded.

Remote access

- In addition to NxClient-3 used before, now users can also automatically install brand new NxPlayer-4. As with NxClient-3, the installation should not require administrative access to the computer, but needs Oracle Java operational in web browser.
- A patched version of OpenNX is available for MacOS Lion users at the GM/CA web site. This should resolve the keyboard mapping problem experienced by some MacOS users.
- bdxv is now available for viewing diffraction images. At the moment it runs from a command line and works properly via remote NX connections, resolving “blank images” problem seen some times with adxv.

MX software

- Please note that coot and xia2 within ccp4i are still those supplied with CCP4. For the latest versions, run the programs from command line

JBluIce Hutch tab:

- No changes

JBluIce Sample tab:

- Diffraction image viewer has improved. Images can be dragged (left or middle buttons), or zoomed in (right button). The toolbar has been streamlined and moved to the top. “Pan” arrow buttons have been removed.

JBluIce Screening tab/Sample automounter

- Screening can be paused with Start/Pause button. Once pause is clicked, current image collection will finish and then screening will pause. Clicking Start after that will resume screening from the position of the green arrow.
- When Raster option is selected for centering, it automatically centers on the first site found. BEWARE: in current implementation, other sites on the same mount will not be centered and scored.

JBluIce Raster tab:

- Processing checkbox has been removed. If processing must be disabled, users should contact their host.

JBluIce Collect and Analysis tabs:

- See the image viewer comments under “Sample tab” above.
- Strategy will now remember the software (MOSFLM or BEST) used for processing particular space group.
- In multi-crystal strategy, .sca files can now be used as reference data.
- New “Reprocessing” sub-tab has been added in the analysis tab. Here data can be reprocessed with user-defined space group and cell parameters.
- Each partial data set, processed on the fly, will be represented with its own curve on the plots. Double-clicking a curve will launch CCP4 loggraph.
- “Image Set” now displays both sets of inverse beam data which are being processed currently.

JBluIce Scan tab:

- No changes