PSF Xray Newsletter 1

Quarter 4, 2013

Martin Moche

10/26/2013

The ambition of this newsletter is to create a simple summary of current actions and issues taking place at PSF Xray instead of sending out several emails.

Contents

Bruker microstar X8proteum for sale

PSF are in the process of selling its Bruker X8 protein microstar to interested research groups. Maintenance and running costs are too high for the PSF model to work in comparison to the" free" beamtime at European synchrotrons. Bruker visit on Oct 22 2013 to check instrument status since the instrument has not been running since Oct 17 2011. A brand new mirror vacuum pump in replacement of the one hit and broken by the water leak on Oct 17 2011 is available however yet to be adapted by Bruker. Vacuum and generator worked without issues while the power aggregate of the server computer had to be changed by Chad Tunell. The KryoFlex system was not tested since liquid nitrogen tank is disconnected for liquid nitrogen transport at PSF. The Montel crystal camera was not running due to AC/DC adapter failure – a known issue since the adapter was from Clas Ohlson. The Pt-135 detector background was not as uniform as it was two years ago, however Bruker expect to remotely trim and test the detector back to normal status shortly. If interested in instrument status and for questions please contact Martin.Moche@ki.se that will make you in contact with Bruker.

LCP experiments improving at PSF

Experiments conducted by Michael Raba discovered that the LCP needle of the Mosquito robot was hitting the base of the LCP plate too hard and ugly looking "eggs" of LCP. After calibration of the "Dispense height" and associated parameters the "eggs" was looking much better. Michael used the MD11-50 Laminex Glass Base (0.2 mm) and Laminex Glass Cover MD11-52 on top of a Laminex Frame MD11-56 for his LCP experiments. PSF have also the possibility to use Swiss-LCP plates with plastic base and cover to ease crystal mounting from LCP plates. Diamond and Bessy offer in-situ exposure of LCP plates however no cryo-cooling of the crystal is possible then.

After we found that LCP detection was surprisingly working in the 4C imager, Formulatrix made a software effort in improving the algorithms for LCP phase detection. After algorithm improvement still the 4C imager is better in LCP detection however the 20C imager made the best improvement going from completely failed into almost as good as the 4C imager. Plate 26029 and 26030 is visible in RockMaker – Projects/SGC Core Xray/Moche/TestExpe and several crystals have been mounted from these plates.

For Plate 26029 we recognized 68 as LCP-like experiments and the 4C imager recognized 66 of these (97%) while the 20C imager recognized 57 of these (84%). For Plate 26030 we recognized 84 as LCP-like experiments and the 4C imager recognized 61 of these (73%) while the 20C imager recognized 47 of these (56%).

Please note however that even in the 4C imager one need to check that imaging is done correctly and manually create a region for subsequent imaging event for droplets where LCP detection either fails, or simply does not look like a proper LCP experiment, for various reasons.

Recent PSF Xray repairs and replacements

The zoom mechanism of our Nikon SMZ 1500 microscope in the 20C room was recently repaired by BergmanLabora and refill of refrigerant in the 4C Hettich centrifuge performed by Thermofisher. Exchange of lamp socket in 4C imager was done at PSF. The t-shaped pipe of our Bruker liquid nitrogen tank has been repaired by Rörtjänst and a new 234 litre liquid nitrogen tank has been borrowed from MTC.

PSF firewall replacement and access to RockMakerWeb & PSF software setup

The PSF firewall power supply unit failed and firewall unit replaced by a firewall computer configured by Chad Tunell. Depending on where you try to access RockMakerWeb the procedure is slightly different.

Option 1, Access from KI-MBB:

Use a computer with good graphics card to access http://sgc.ki.se:591/RockMakerWeb/

Option 2, Access from KI-CMB, KI-MTC, LiU or from home:

First perform VPN-login to KI using the latest VPN client that can be downloaded at http://internwebben.ki.se/en/network-access-vpn-or-proxy before access to RockMakerWeb is given at the address above

Option 3, Acess from within the PSF firewall:

Please approach Martin Moche for details regarding RockMakerWeb ip-addresses

Remote access to the PSF software setup (http://psf.ki.se/Xray/PSF_Xray_Software_2013.html) demands VPN-login before running nxclient.

How to seal PSF crystal screens

All MBB research groups are now using PSF crystal screens that enable access to a broader sortiment of crystal screens. PEGs and Nucleix from Qiagen are two recent additions to the PSF crystal screens. To check availability and location of Deep Well Blocks (thawed and frozen) please visit (http://psf.ki.se/Xray/PSF_Crystal_Screens.html)

When using PSF crystal screens, please use the plate sealer for optimal sealing as pictured in figure 1

Figure 1. Demonstrate plate sealer usage for optimal sealing of Greiner deep well blocks. Use two rubber spacers on top of the Deep Well Block to be sealed with the nice rubber side facing the aluminium foil (left). Slide the Deep Well Block with rubber spacers into the plate sealer and adjust the rubber spacer position on top of the Deep Well Block and press the handle (right). Wait for 30 seconds – done!

Structural biology calculations at NSC and iRODS testing at Diamond

Data from three recent Diamond visits (130926, 131006 and 131010) have been transferred into pilot iRODS as a test of functionality using the irsync command. Some irsync error messages were initially confusing however using iquest one can check that data transfer continues in present of error messages. Subsequent data access has then been given using ichmod and three research groups are currently participating in the pilot iRODS project. All data in iRODS is visible to all research groups participating however data can only be accessed after granting. Data transfer speed is similar to standard rsync however the speed limitation are on the client side and PSF will push for faster disks and network at Diamond. Next step will be to write a joint PSF application for data storage in production mode iRODS and push for solving firewall issues at BESSY and push for i-Commands at ESRF and other light sources.

Members from the structural biology community (NMR, Xray and Cryo-EM) have together with NSC written an application to SNIC (http://www.snic.vr.se/) for support and installation of HPC structural biology environment at NSC. This application has been supported by SweStruct (http://swedstruct.mbb.ki.se/) and Gerard Bricogne providing the leading phasing and refinement softwares SHARP and BUSTER and the founder of GlobalPhasing (http://www.globalphasing.com/). The structural biology HPC computing application will be discussed by the SNIC board in November 2013.