

Eiger 16M @BioMAX

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About Eiger

Data Acquisition

- Arm, prepare / config detector
- Trigger, int / ext

Eiger Data

- Monitor
- Filewriter, HDF5 / NeXus





Jie Nan @ MXCuBE Workshop ESRF



Streamer, zeroMQ





Change Energy

- Important, Energy calibration, flatfiled correction, etc
- Take time, 6 9 s
 - Don't configure both wavelength and photon energy
 - Use non-default energy_threshold, double time to config
- Arm also becomes longer, over 3 s
- Readout time is energy depaendent, 4 10 μs
 - Pilatus, Exp period = readout time + exp time
 - Eiger, Frame time >= readout_time + count_time
 - Use frame_time as exposure time?
 - Simple, Frame time = 10 μs + count_time
 - Precise, Frame time = readout_time + count_time (change energy first!!)



Arm

- Configs are "locked" after arm
- Interleave, inverse beam
 - Energy
 - Image number
- Solution!?
 - Energy, don't change the energy setting, OK within 200eV (internal commu. with DECTRIS)
 - Image number
 - Streaming, rename image number
 - Repack HDF5 data
 - Can also correct the wrong energy in the master file



ROI Mode

- 16M and 9M, have 4M mode
- ROI changes,
 - Dectector "sizes" change → resolution (UI)
 - Frame_time min changes, 4M 1.3 ms vs. 16M 7.5 ms
- Resolution dependent on energy, distance, ROI (UI)



NeXus/HDF5 - 1

Master file, meta info, extened imaged header

- NeXuS, http://www.nexusformat.org/, NXMX
- Eiger Data is not 100% NXMX
 - Missing rotation axis
 - Different unit, beam_center_x, beam_center_y, pixel position

This is a length, not a pixel position, and can be outside of the actual detector.

-from nexusformat.org

- Generate_XDS.INP from XDSwiki works directly
- We also add /entry/instrument

```
def add_header(self, filename):
    h5file = h5py.File (filename)
    beamline = h5file.require_group("/entry/instrument")
    beamline.attrs['name'] = 'BioMAX@MAXIV'
    omega = h5file.require_group("/entry/sample/transformations/omega")
    omega.attrs['vector'] = (0.0, -1.0, 0.0)
    h5file.close()
```



NeXus/HDF5 - 2

- Master file, fixed size, 350 MB for 16M
 Characterization, CBF or HDF5?
 - CBF (18 MB/img)
 - HDF5, 350 MB + data file
- Data file
 - h5 container, how many imgs per file?
 - Available until the last image in the container is collected



Data handling

- Data compression
 - Bslz4, avg. ~10 fold
 - Concern, the current 10 Gb/s interface not fulfill <4 fold compression for highest frame rate
- Data size
 - 900 imgs, 5 GB, after gzip 2.6 GB
 - Ultra fine-slicing, 1/10 of mosaicity
- Data transfer
 - EPU or in-house solution
 - Minimize data transfer
- Data processing
 - Shared HPC Cluster

Benchmark test

EIGER_16M_Nov2015.tar.bz2, 900 images in 9 containers, 0.1 osc, from Dectris website

Server	Time(s)
MAXIV HPC - 4 nodes (20 cores, CPU E5-2650 v3 @ 2.30GHz)	78.2
MAXIV HPC - 8 nodes (20 cores, CPU E5-2650 v3 @ 2.30GHz)	53.7
SLS - 4 nodes (24 cores, E5-2697v2 @2.70 GHz)	76.6
Kay (32 cpus, HT)	120
BioMAX BufferServer (24 cores, CPU E5-2643 v4 @3.4GHz)	136



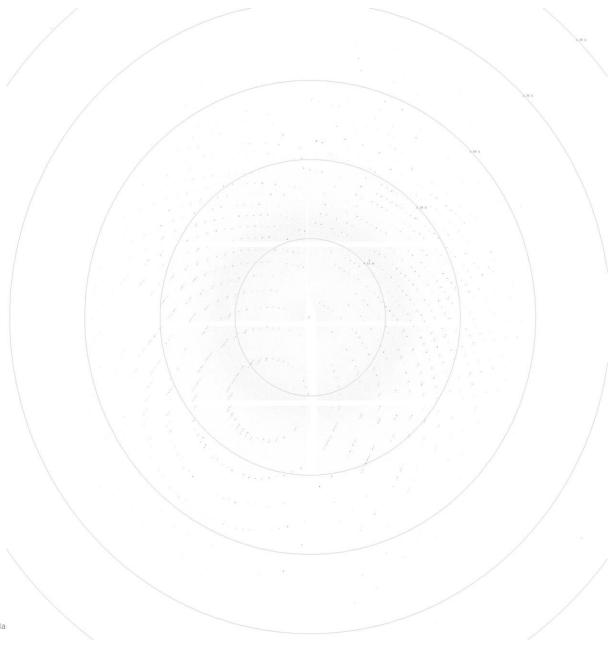
Useful tools

- A list of tools, hdrmx.medsbio.org
 - Processing
 - Filewriter interface
 - Streaming interface
 - Many more



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- Thumbnail generation (from Vicente)
 - Binning / summation
 - Eiger 1/4/9/16 M & ROI
- Detector calibration
 - pyFAI, MX-calibrate
 - CBF, converted with eiger2cbf https://github.com/biochemfan/eiger2cbf





15-17 March 2017 MAX IV Europe/Stockholm timezone

Overview

Scientific Programme

Timetable

Registration

Modify my Registration

Organizers

Sponsors

Travel

Accommodation

Contacts

The 4th High Data-Rate Macromolecular Crystallography (HDRMX) Meeting

The organizers warmly invite you to attend this meeting at the MAX IV Laboratory in Lund Sweden, 15-17 March, 2017. The meeting will be held in conjunction to the MAX IV User meeting(UM17) in Lund Sweden, 13-15 March, 2017.

This is the fourth in a series of meetings that began in spring 2016 on changes needed to existing major software packages for support of very high data rate macromolecular crystallography. The first HDRMX meeting was held at Brookhaven National Laboratory, 26 – 28 May 2016, the second meeting held at an informal dinner gathering at the meeting of the American Crystallographic Association in Denver Colorado, 22 – 26 July 2016. The third meeting was held at Biozentrum in Basel on 2 September 2016.

https://indico.maxiv.lu.se/event/233/

