



# Eiger 16M @BioMAX

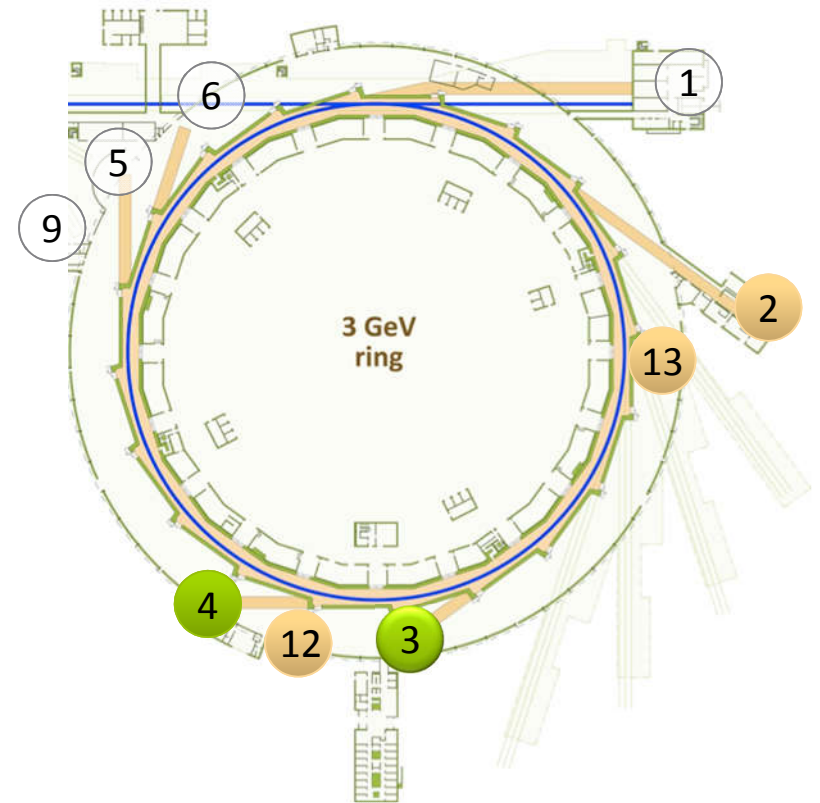
Ph.D. Jie Nan

On behalf of MX Group

Mar. 15<sup>th</sup>, 2017

# Eiger at MAX IV

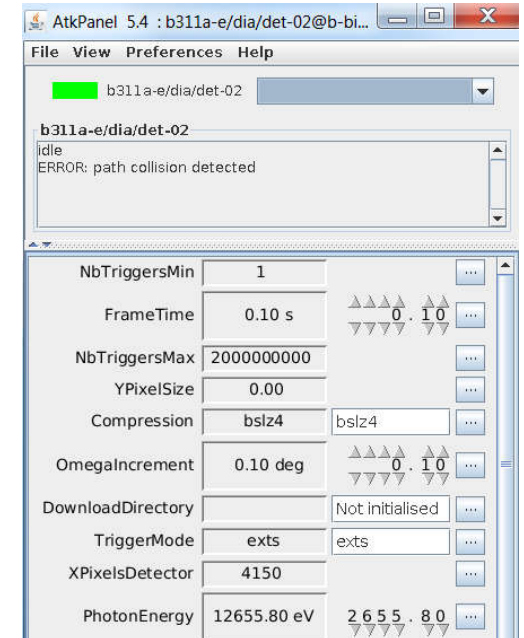
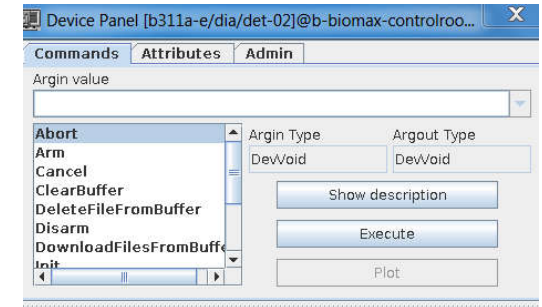
- Eiger 16M at BioMAX
  - Arrived & Comissioned in Oct. 2016
  - Data acquisition in Dec. 2016 due to shutdown
- Eiger 1M at Balder in Feb. 2017
- Growing interest
  - Eiger 4M at CoSAXS, NanoMAX, SoftiMAX?



- 2. NanoMAX**, Nano-imaging & - spectroscopy
- 3. BALDER**, Chemical spectroscopy: real-time & -conditions
- 4. BioMAX**, Protein crystallography
- 12. CoSAXS**, Geometric structure & correlation: (bio) liquids
- 13. SoftiMAX**, Microscopy & method development

# Detector control and integration into MXCuBE3

- Eiger Tango Device
  - Extended the one from Teresa Nuñez (DESY)
  - <https://github.com/MaxIV-KitsControls/dev-maxiv-eigerdectris>
  - Support control and filewriter
  - Streaming under development
- Integrated into MXCuBE3
  - Standard data collection including helical scan
  - Mesh scan not yet
  - ROI vs. resolution / distance
  - ROI vs. shortest exposure time



# Issues / surprises

- 6-9s for changing energy / energy\_threshold / wavelength
- Use non-default energy\_threshold, double time to config
- Arm becomes longer (> 3s) after changing energy
- img number, not configurable after arming
- How about interleave? Repacking the data or virtual dataset?

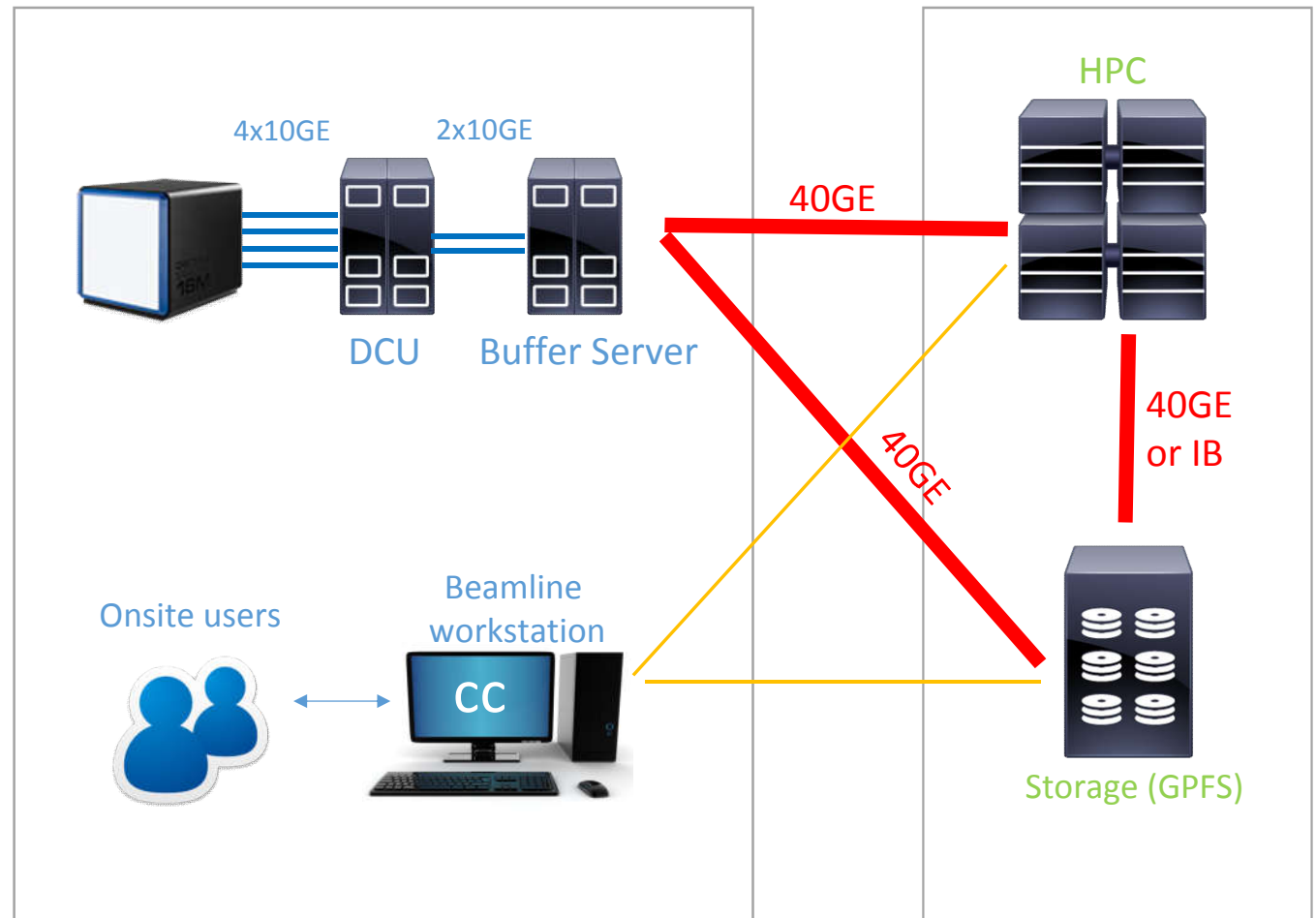
# MX IT-infrastructure (1)

BioMAX

MAX IV

## Buffer Server

- 12 TB SSD
- 500 GB RAM
- 24 cores
- GPFS



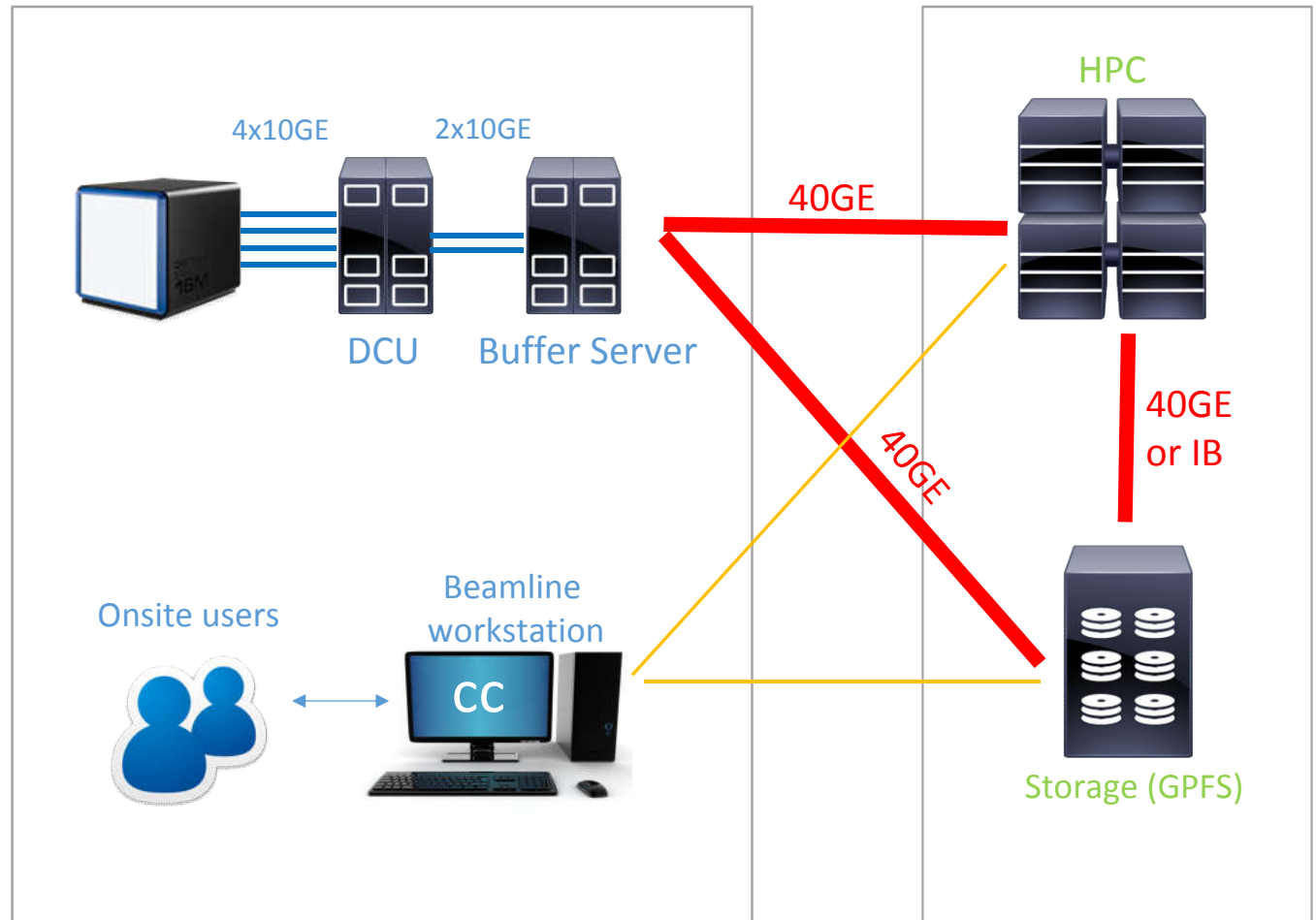
# MX IT-infrastructure (3)

BioMAX

MAX IV

## Storage

- Bulk
  - write from BS ~1.1GB/s
  - 250 TB
- IBM ESS in the future (tested)



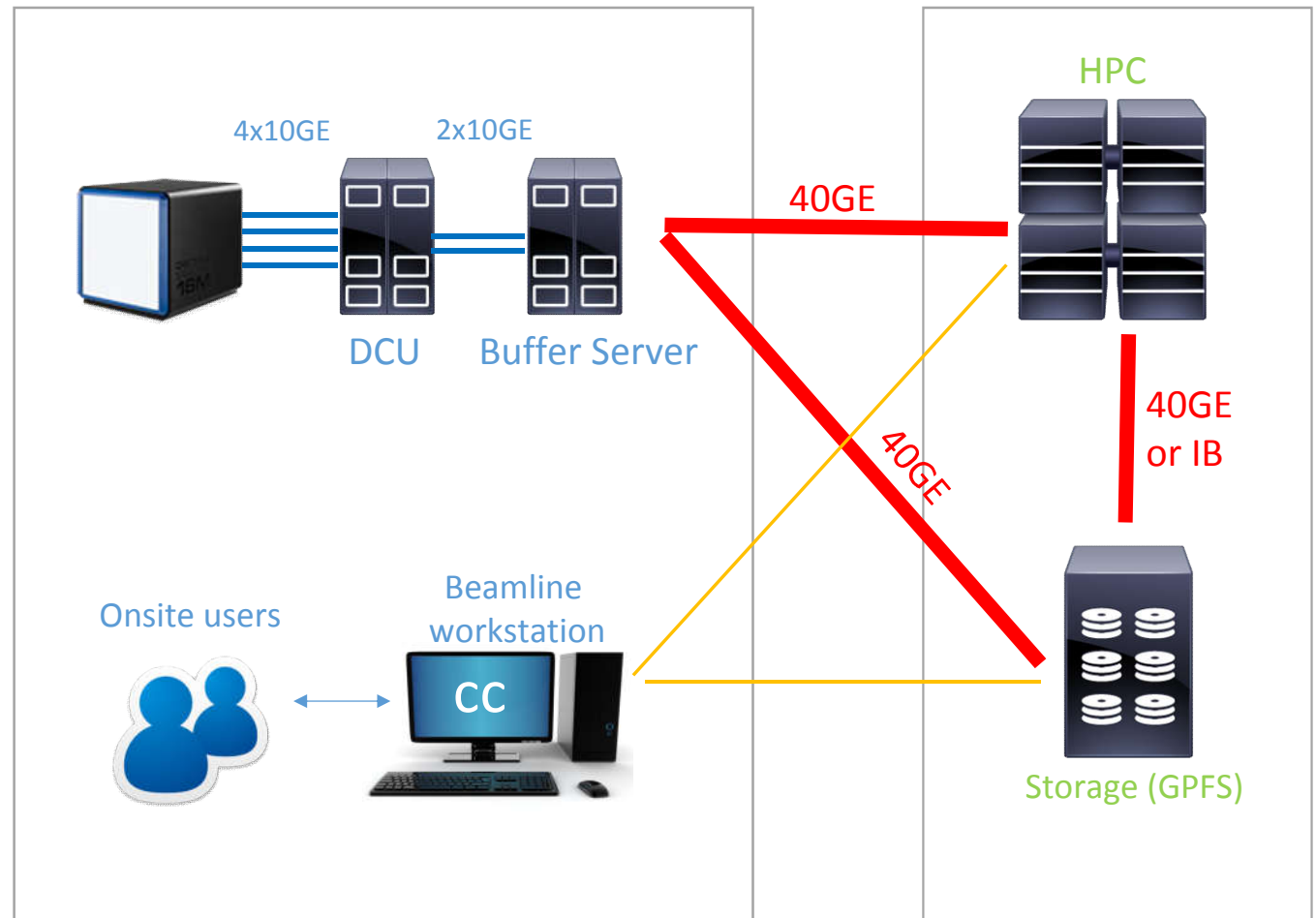
# MX IT-infrastructure (2)

BioMAX

MAX IV

## HPC

- 16 CPU node + 1 GPU node
- 8 x 20 cores + 8 x 24 cores
- Limited RAM, 64 /128 GB
- infiniband interconnects
- Growing rapidly
- SLURM



# NeXus/HDF5

- adding rotation axis, works well with generate\_XDS.INP from XDSwiki
- adding beamline name, where is the best place?
  - /entry/instrument
  - /entry/instrument/collection

```
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()
```

**Wish: to record the collection trajectory**



# Benchmark (XDS)

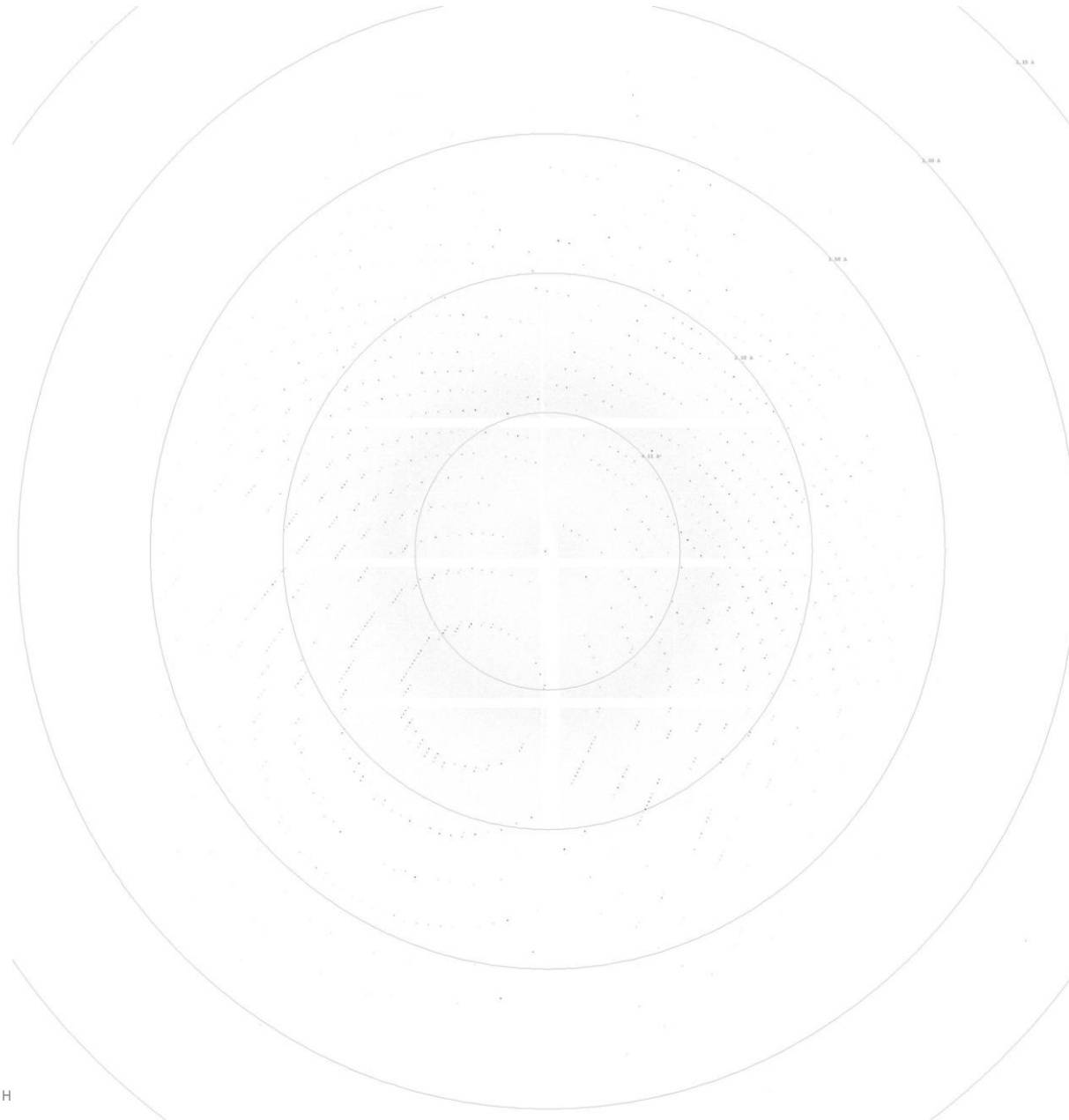
- EIGER\_16M\_Nov2015, 900 images in 9 containers, 0.1 deg, insulin from SLS  
NUMBER OF REFLECTIONS IN SELECTED SUBSET OF IMAGES **131826**
- Thau\_BIOMAX, 900 images in 9 containers, 0.1 deg, thaumatin from BioMAX (in red)  
NUMBER OF REFLECTIONS IN SELECTED SUBSET OF IMAGES **508739**

	HPC - 4 nodes(20 cores, CPU E5-2650 v3 @ 2.30GHz)	HPC - 4 nodes (24 cores, CPU E5-2650 v4 @ 2.20GHz)	HPC - 8 nodes(20 cores, CPU E5-2650 v3 @ 2.30GHz)	HPC - 8 nodes (24 cores, CPU E5-2650 v4 @ 2.20GHz)
Buffer Server (10 Gbps)	78.2		53.7	
Buffer Server (40 Gbps)	61 / <b>86.7</b>	53 / <b>74.8</b>	44.2 / <b>62.3</b>	36.3 / <b>54.8</b>
ESS (gpfs16m)	60.8 / <b>88.5</b>	53.6 / <b>75.2</b>	47.8 / <b>64.8</b>	38.8 / <b>56.7</b>

Evaluation of spot finding is on going ...

# Tools

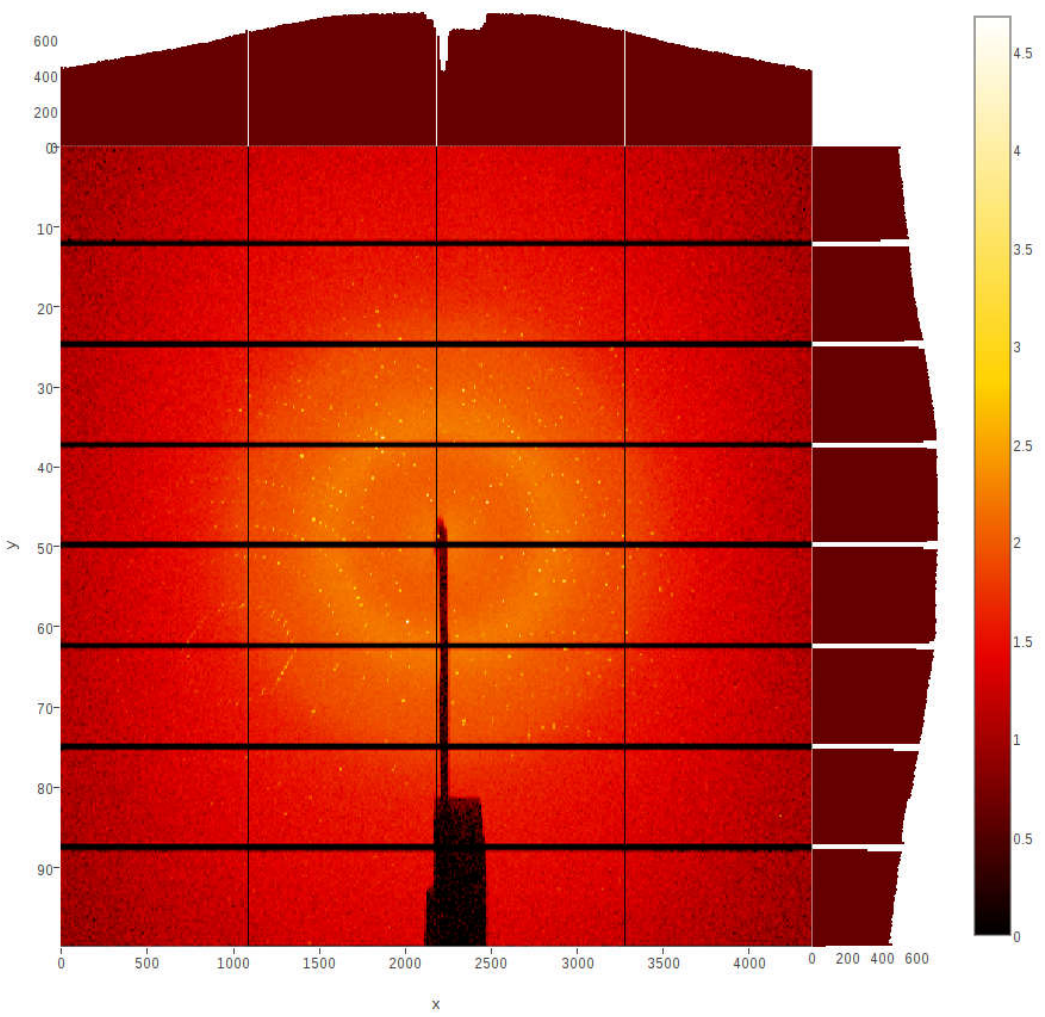
- Thumbnail generation
  - Vicente Rey Bakaikoa
  - Binning / summation
  - Eiger 1/4/9/16 M & ROI
  - <https://github.com/mxcube/EigerTools>
- Hdf5 web viewer
  - Jason Brudvik (MAX IV)
  - Under development



Data Storage

- example-subfolder
- from-vincent-m
- from-zdenek
- jie
  - tau1-tau\_2\_master
    - entry
      - data
        - data\_000003
        - data\_000007
        - data\_000001
        - data\_000008
        - data\_000009
        - data\_000006
        - data\_000005
        - data\_000004
        - data\_000002
      - instrument
      - sample
- nanomax-read-only
- public

Title goes here



# Acknowledgement

## **MX Group**

Uwe Mueller  
Thomas Ursby  
Johan Unge  
Roberto Appio  
Christopher Ward  
Ross Friel


## **HDRMX community**

## **KITS Group**

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Artur Barczyk  
Andreas Mattsson  
Vincent Hardion  
Zdenek Matej  
Jason Brudvik

many others from MAX IV

Vicente Rey Bakaikoa

A photograph of a modern building at night. The building's facade is illuminated with a large, glowing blue logo that reads "WORLDWIDE" in a stylized font. The building has a grid-like pattern of windows and a prominent horizontal light fixture near the top. In the foreground, three Swedish flags are flying on tall poles. The sky is dark, and there are some streetlights visible at the bottom of the frame.

Thank you for your attention!

Questions?