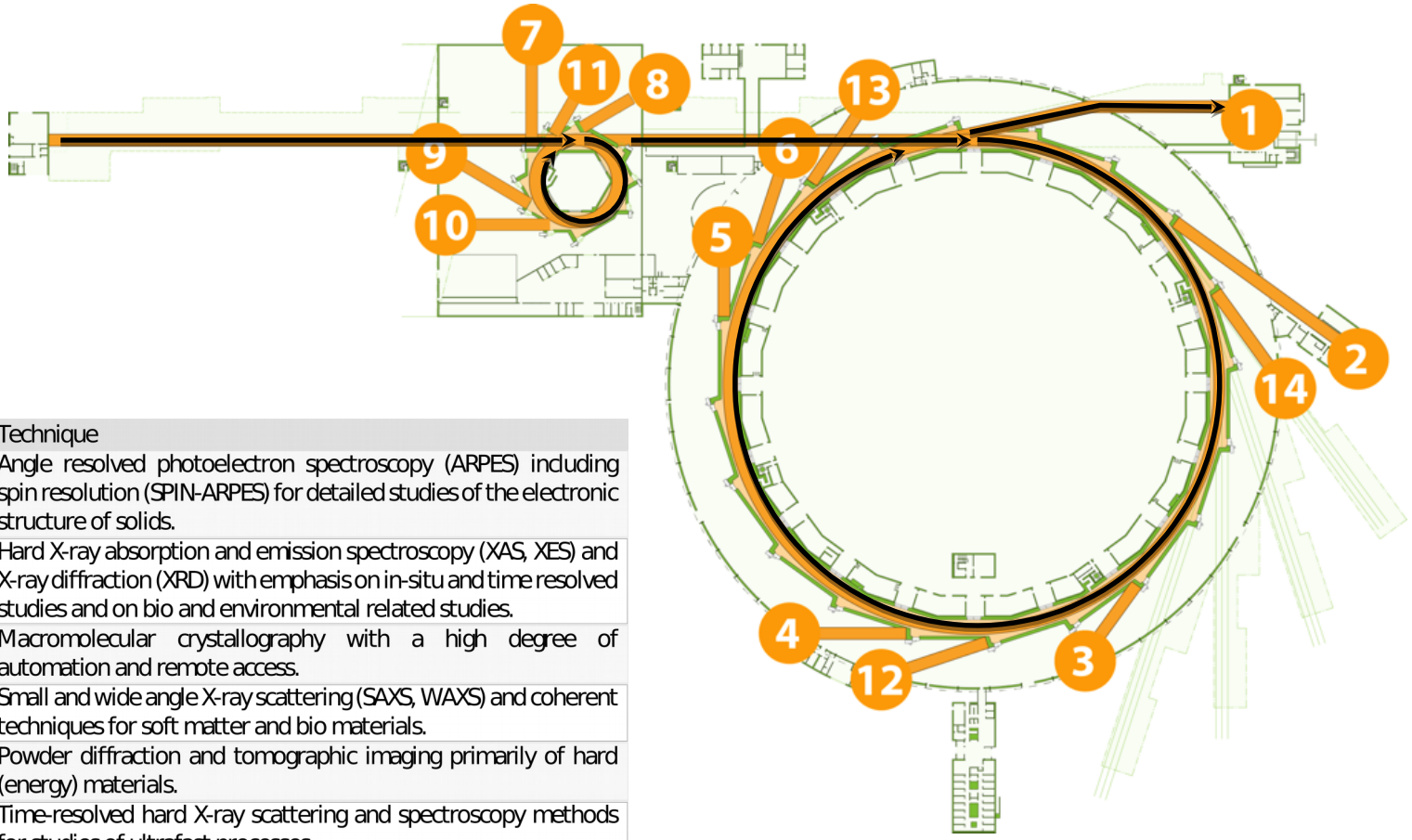
MXCuBE @ MAX IV: Status Report

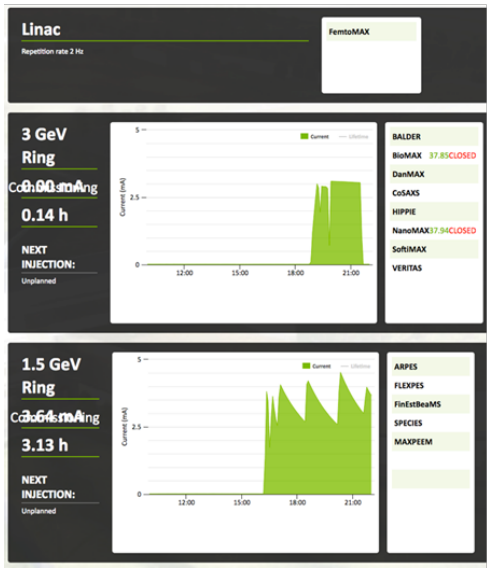
Johan Unge

January 31, 2018

1 Linac
2 Rings
15 beamlines



Beamline		Accelerator	Technique
ARPES	7	1.5 GeV	Angle resolved photoelectron spectroscopy (ARPES) including spin resolution (SPIN-ARPES) for detailed studies of the electronic structure of solids.
Balder ★	3	3.0 GeV	Hard X-ray absorption and emission spectroscopy (XAS, XES) and X-ray diffraction (XRD) with emphasis on in-situ and time resolved studies and on bio and environmental related studies.
BioMAX ★	4	3.0 GeV	Macromolecular crystallography with a high degree of automation and remote access.
CoSAXS	12	3.0 GeV	Small and wide angle X-ray scattering (SAXS, WAXS) and coherent techniques for soft matter and bio materials.
DanMAX	14	3.0 GeV	Powder diffraction and tomographic imaging primarily of hard (energy) materials.
FemtoMAX ★	1	Linac	Time-resolved hard X-ray scattering and spectroscopy methods for studies of ultrafast processes
FinEstBeaMS	8	1.5 GeV	Electron spectroscopies and luminescence methods for studies of low density matter and solids.
FlexPES	11	1.5 GeV	Soft X-ray spectroscopies for studies of low density matter and solids.
HIPPIE ★	6	3.0 GeV	Near ambient pressure photoelectron spectroscopy on solids and liquids.
MAXPEEM	10	1.5 GeV	Aberration corrected photoelectron microscopy for investigation of surfaces and interfaces.
NanoMAX ★	2	3.0 GeV	Imaging with spectroscopic and structural contrast techniques and nanometre resolution.
SoftiMAX	13	3.0 GeV	Scanning transmission X-ray microscopy and coherent imaging methods.
SPECIES	9	1.5 GeV	Resonant inelastic X-ray scattering (RIXS) with high resolving power and near ambient pressure photoemission.
VERITAS ★	5	3.0 GeV	Resonant inelastic X-ray scattering (RIXS) with unique resolving power and high spatial resolution.

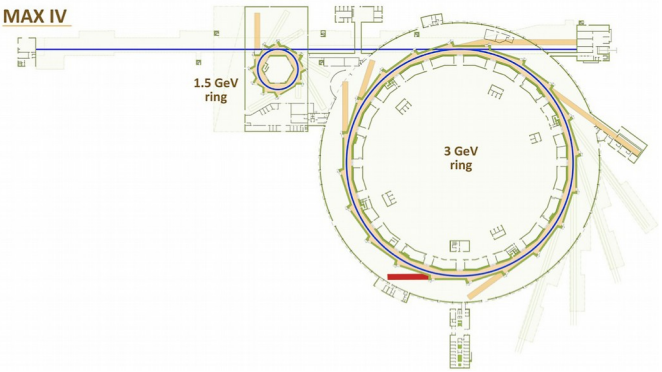


Linac:
Injector 1.5 & 3 GeV & SPF
Injects both rings & delivers light to FemtoMAX

3 GeV:
200 mA, >5 Ah
≈ (340?30) pm·rad
≈ 8.5 mA single bunch
Delivers light to users

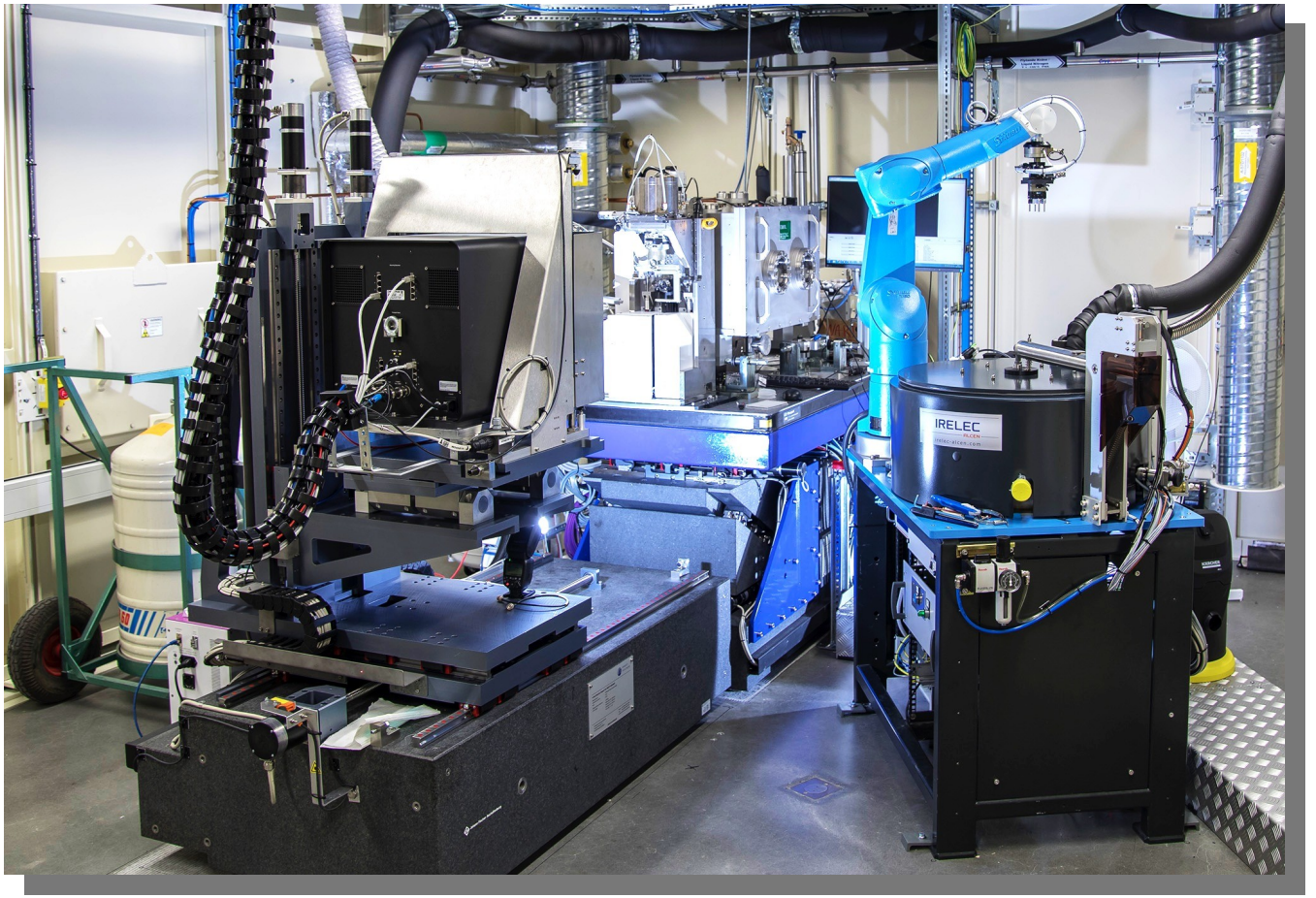
1.5 GeV:
< 200 mA
Commissioning

BioMAX experimental station



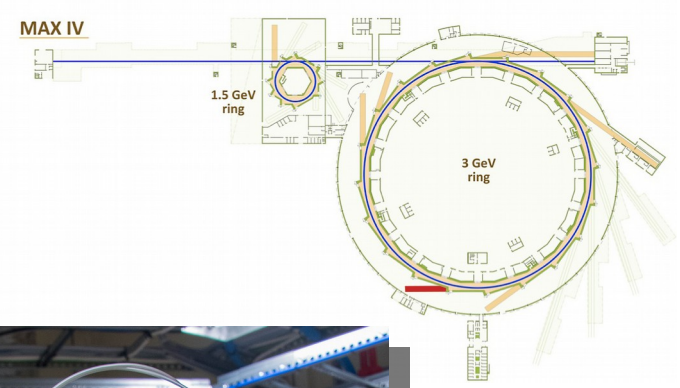
Experimental environment

- MD3 micro-diffractometer
- Eiger 16M hybrid pixel detector
- ISARA sample changer
- HCLab humidifier
- Beam Condition Unit incl. XBPM
- Amptek fluorescence detector



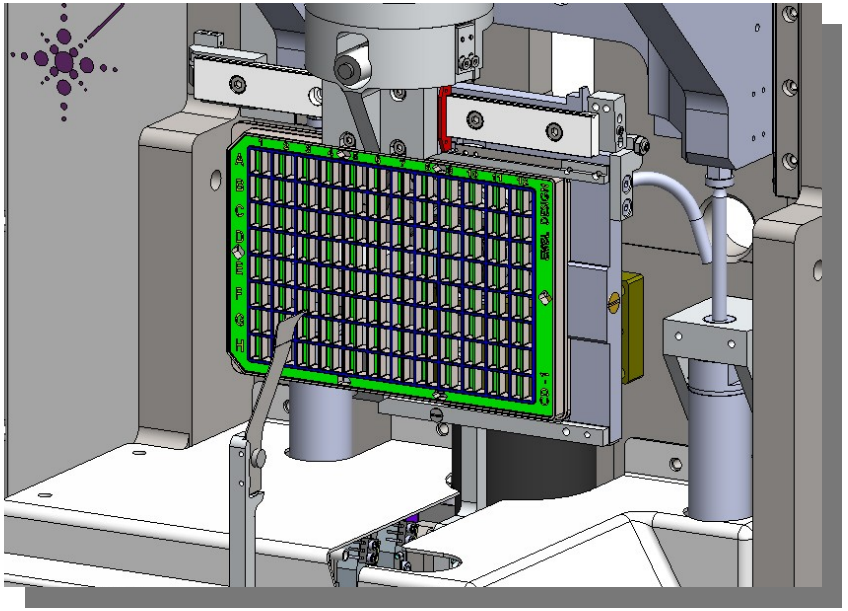
BioMAX experimental station

Goniometry

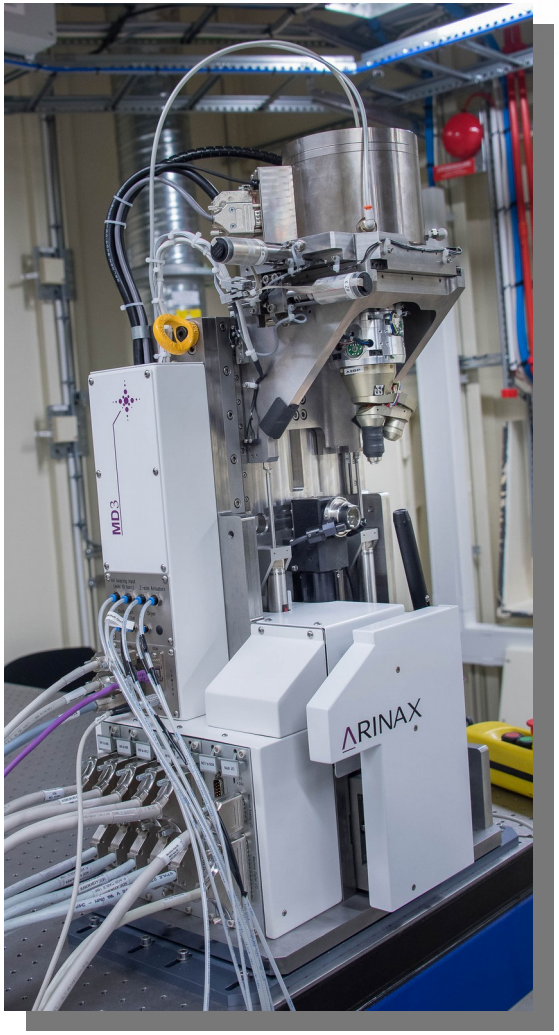


MD3 diffractometer:

- Ultra precise Omega-axis
  - Sphere-of-confusion r=100 nm
  - Max. speed 800 deg/sec
- MK3 Mini-kappa goniometer
- Improved on-axis-microscope
- Crystallization plate holder

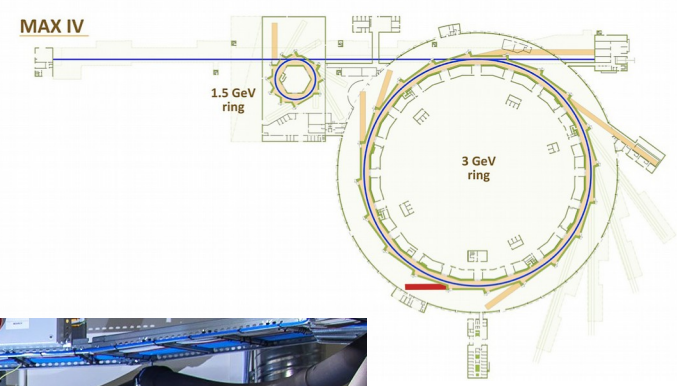


MD3 plate holder



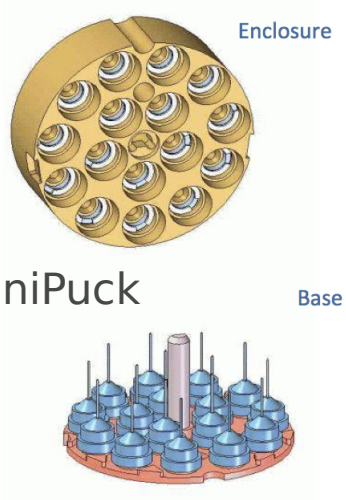
MD3 at BioMAX experimental hutch

Sample changer



ISARA sample changer:

- Dewar capacity
  - 100 samples in SPINE pucks
  - 304 samples in UniPuck
- 4 crystallization plates
- 18 sec sample transfer time



UniPuck

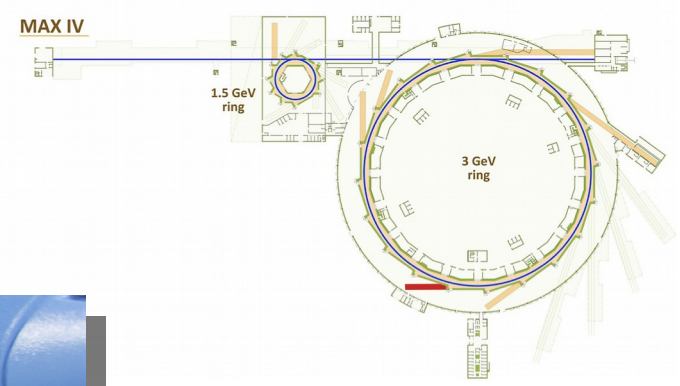
SPINEPuck

ISARA sample changer (IRELEC)

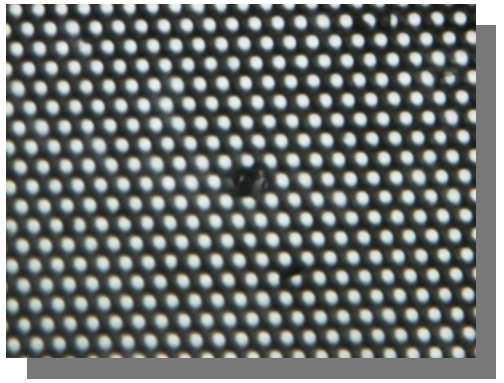
Status

- Ice formation issues with new design
- Currently Unipuck is working
- Integrated into mxcube3, operation, maintenance page and hwobj

HCLab – Room temperature



HClab facility operational

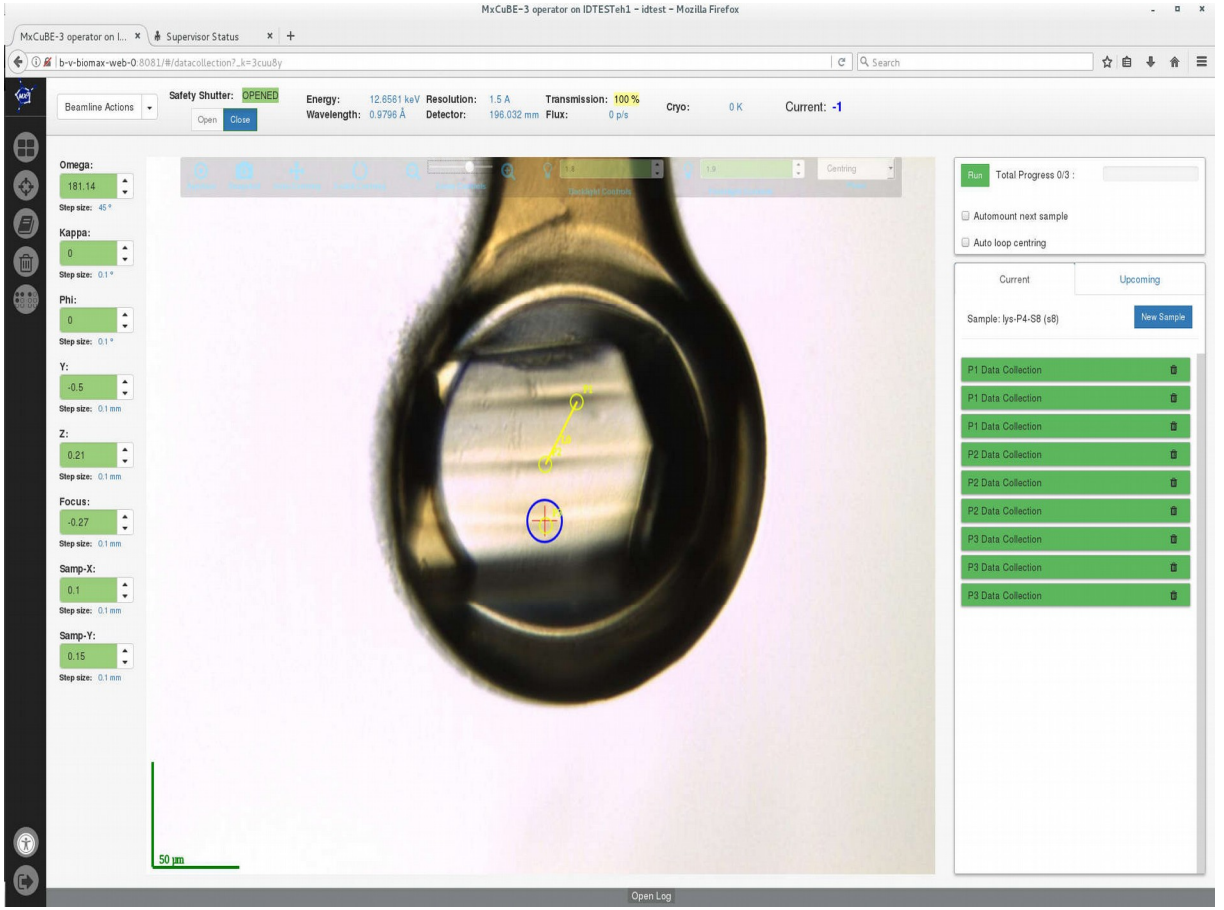


First Si chip operation at BioMAX, (B. Vestergaard, UC)

MXCuBE3

- *Current Status, major features*
  - Sample Centering
  - Standard Oscillation
  - Characterization
  - Helical Scan
  - Sample Changer
    - ISARA adaptation for Tango device and HWO
  - Mesh Scan
  - In Situ
- *In progress and todo*
  - Stability maturation
  - XRF, XANES
  - Parallel processing for spot finding for MESH scan
  - ISPyB and SDM integration

MXCuBE3 data collection view



- *Advantage*

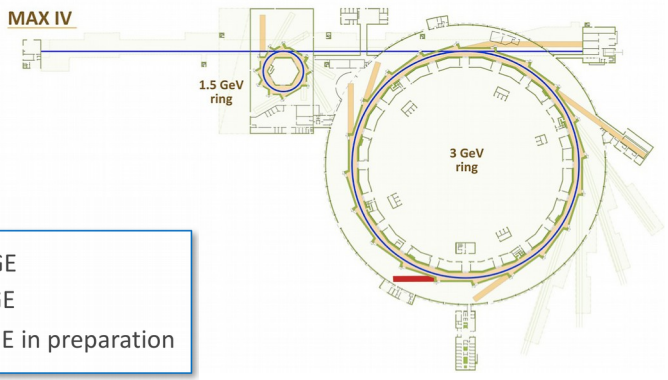
  Joint collaboration with ESRF

- *Challenges*

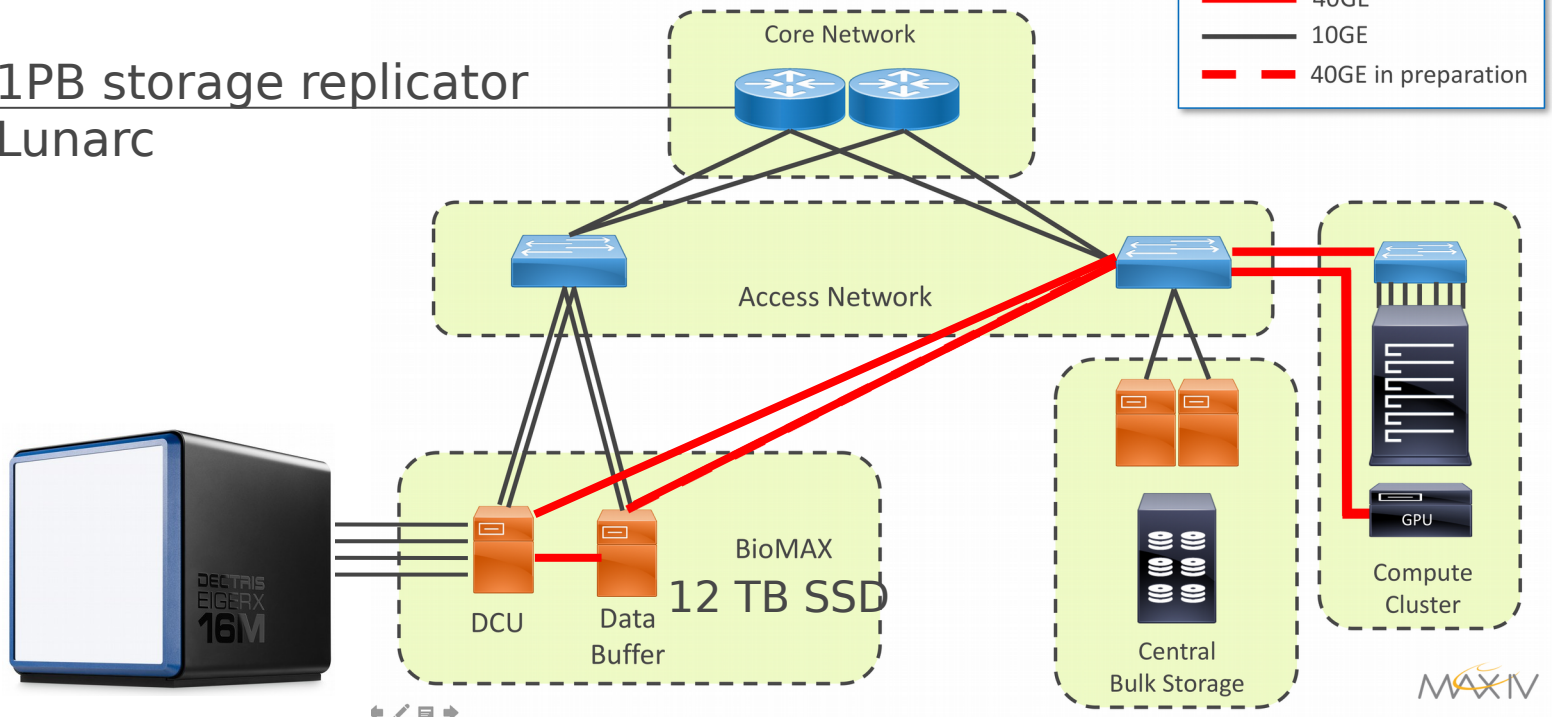
Software stability, user-friendliness and integration with of various hardware + software

IT environment

Eiger 16M IT-environment



1PB storage replicator
Lunarc



Courtesy of Artur Barczyk

~ 1100 CPU cores

60 nodes 2017
25 dedicated to BioMAX

250 TB installed
GPFS file system

- Alternative data retrieval via Globus (www.globus.org)
- DUO (proposal management) in place and will be used soon
- Account and data management system (SDM) → talk by Fredrik

Data reduction and performance

- Three pipelines currently used
  - fast_dp, autoPROC, BioMAX_Pipeline
- System to install all MX software on cluster, PreSTO, collaboration with National Supercomputer Centre and Lunarc.
  - Thinlinc to create simple interface to cluster
  - XDS and central GPFS file system? XDS makes many small I/O operations...testing alternatives

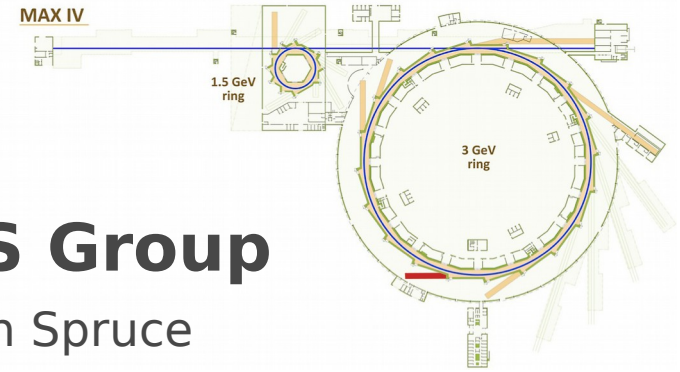
MAX IV, GPFS system (1)	Lunarc, Same blades type (1)	4 Nodes, NFS mount 8 XDS-jobs 24 processes (2)	8 Nodes NFS mount 16 XDS-jobs 24 processes (2)
134.0 sec	52 sec	56.2 sec	45.6 sec

(1) 900 images, thaumatin, 0.1 deg/image, (2) 900 images, Dectris data

Outlook

- Remote operation using web based MXCuBE. This will be critical during 2018. Involves MAXIV IT systems.
- ISARA sample changer: all functionalities and a lot of testing -> ready to users!
- Remaining equipment to integrate…
- Extend beamline capabilities (energy tuneability, beam stability feedback systems, MESH scan, XRF, minikappa…

Acknowledgement



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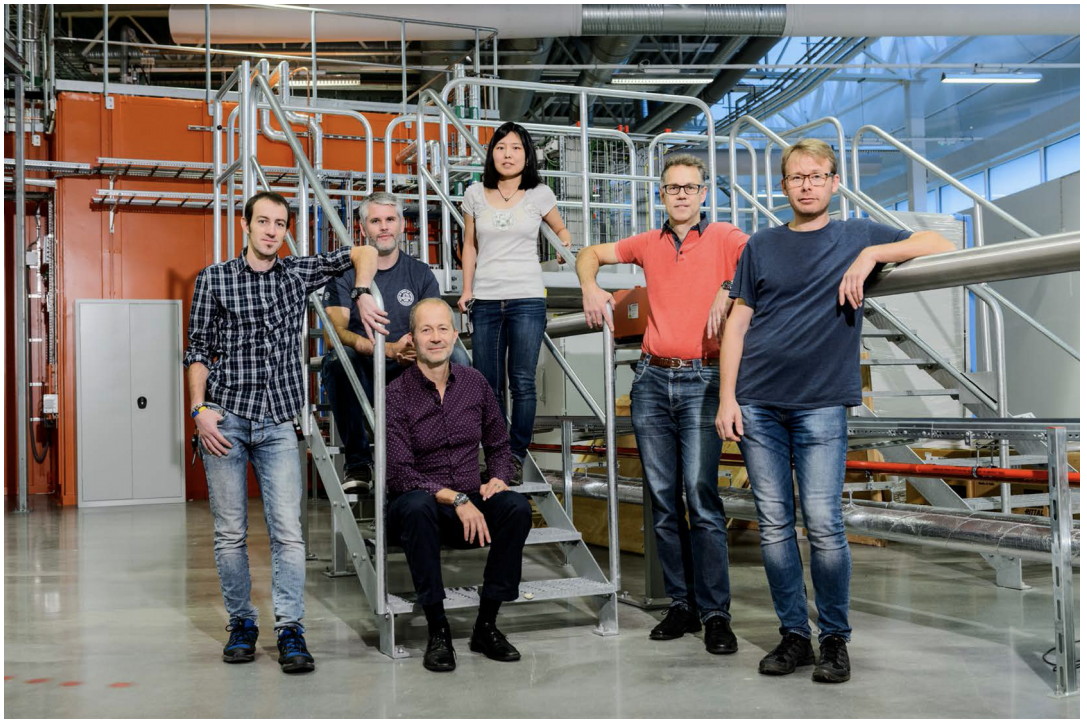

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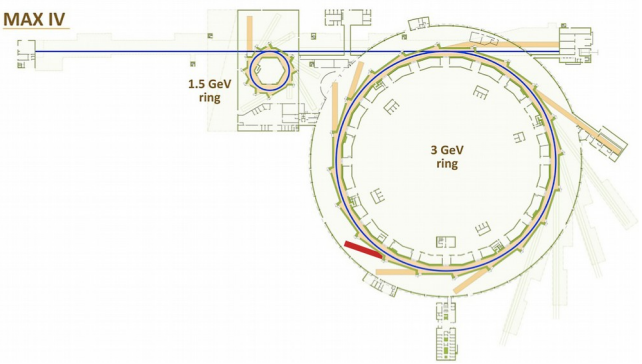
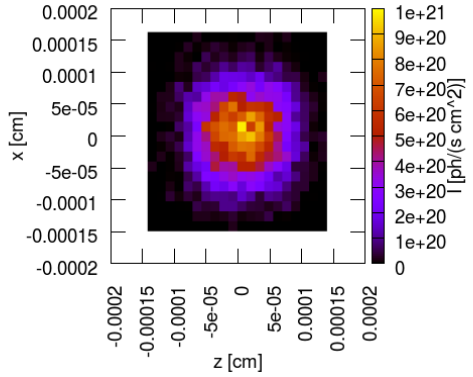
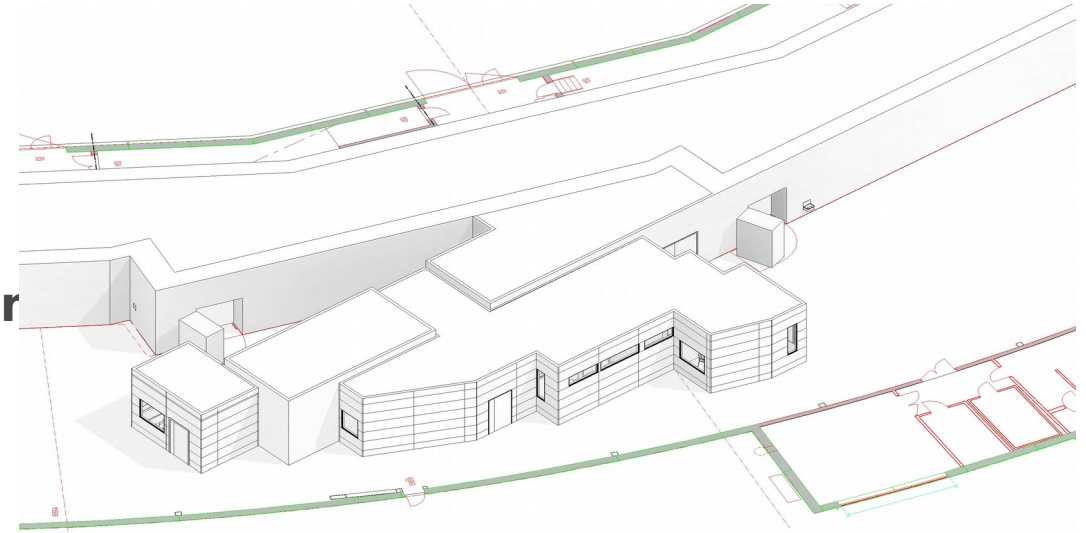




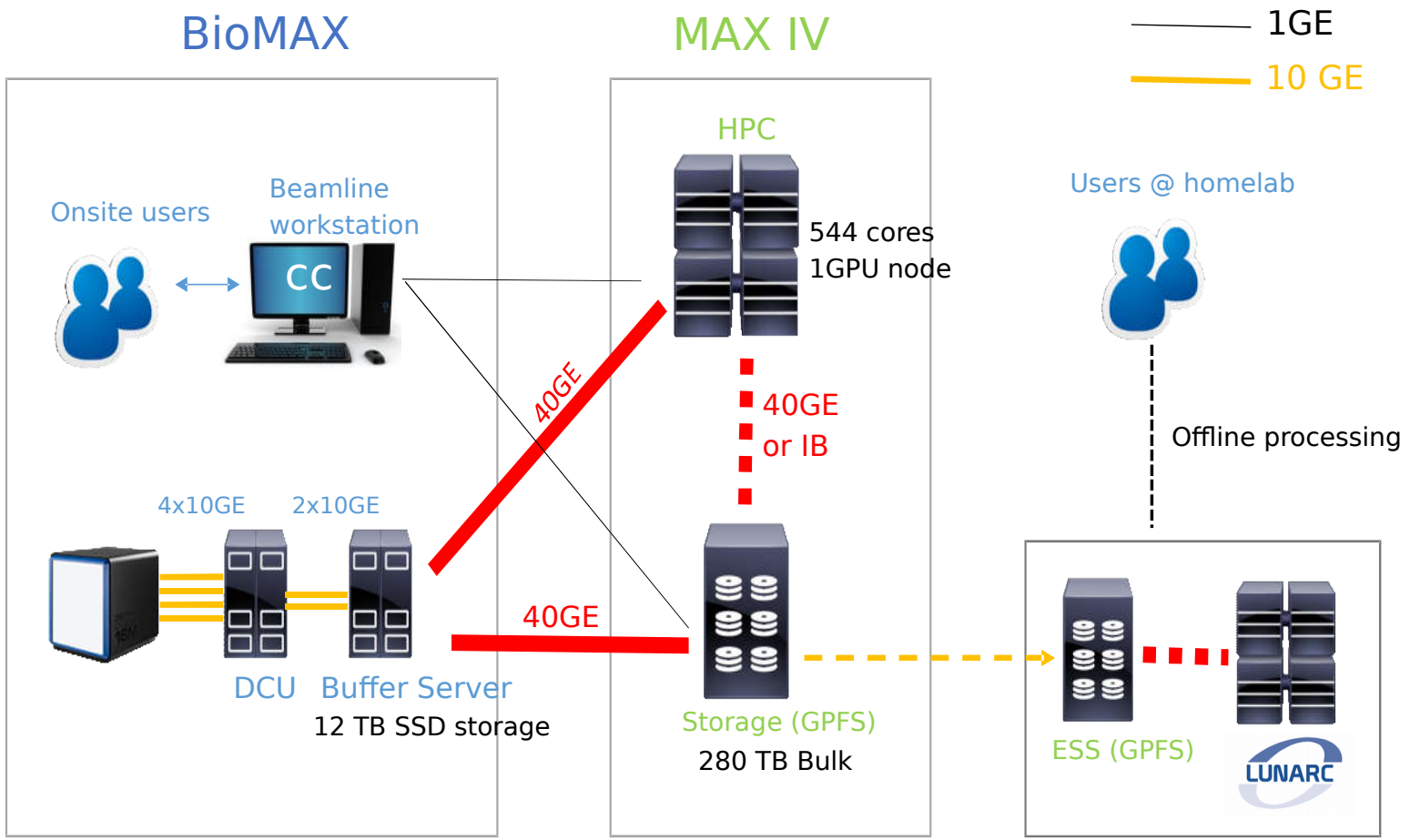


Plans for the second MX bear

- Microfocus beamline
- **1 x 0.7** μm^2 beam at sample
- Photon flux **10^{13} - 10^{15}**phot/sec
- Traditional setup (goniometry, sample environment)
- Exploratory setup (serial crystallography, fixed target single shot)
- Optimal source for most demanding projects (large complexes, membrane proteins)

Status: funded by Novo Nordisk Foundation

BioMAX – IT Infrastructure



Data reduction and performance

- Automatic processing
  - Fast_dp
  - autoPROC
  - Biomax_pipeline

	HPC – 4 nodes (24 cores, CPU E5-2650 v4 @ 2.20GHz)	HPC - 8 nodes (16 cores, CPU E5-2650 v4 @ 2.20GHz)	BufferServer (24 cores, CPU E5-2643 v4 @3.4GHz)	Kay (2 cpus, HT)	SLS - 4 nodes (16 cores, E5-2690 @2.70 GHz)
Time*	53s	36s	136s	120 s	76.6 s

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

- Run XDS with SLURM on HPC

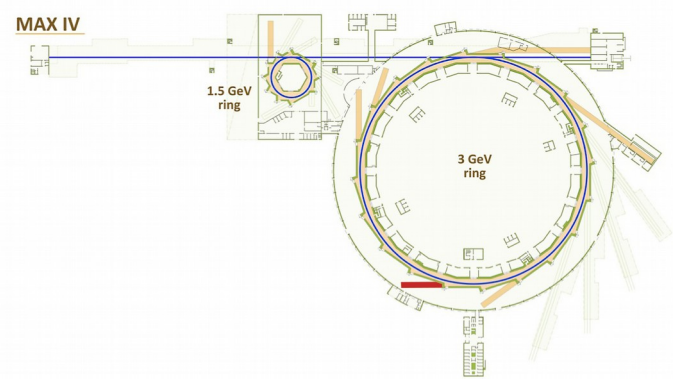
  https://github.com/JieNanMAXIV/xds_slurm

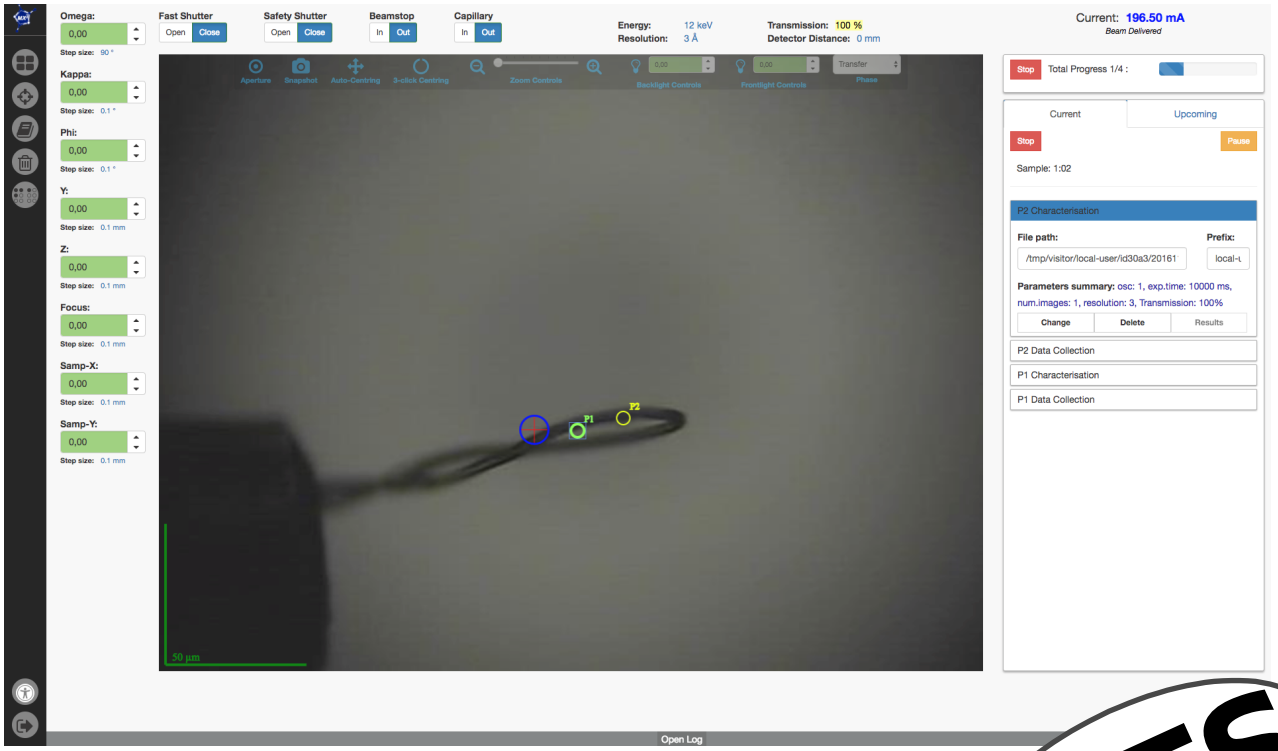
MXCuBE3

- *Current Status, major features*
  - Sample Centering
  - Standard Oscillation
  - Characterization
  - Helical Scan
  - Sample Changer
  - Mesh Scan
- *Todo*
  - Stability maturation
  - XRF, XANES
- *Advantage*

  Joint collaboration with ESRF
- *Challenges*

  Integration with of various hardware, software, Software stability and user-friendliness



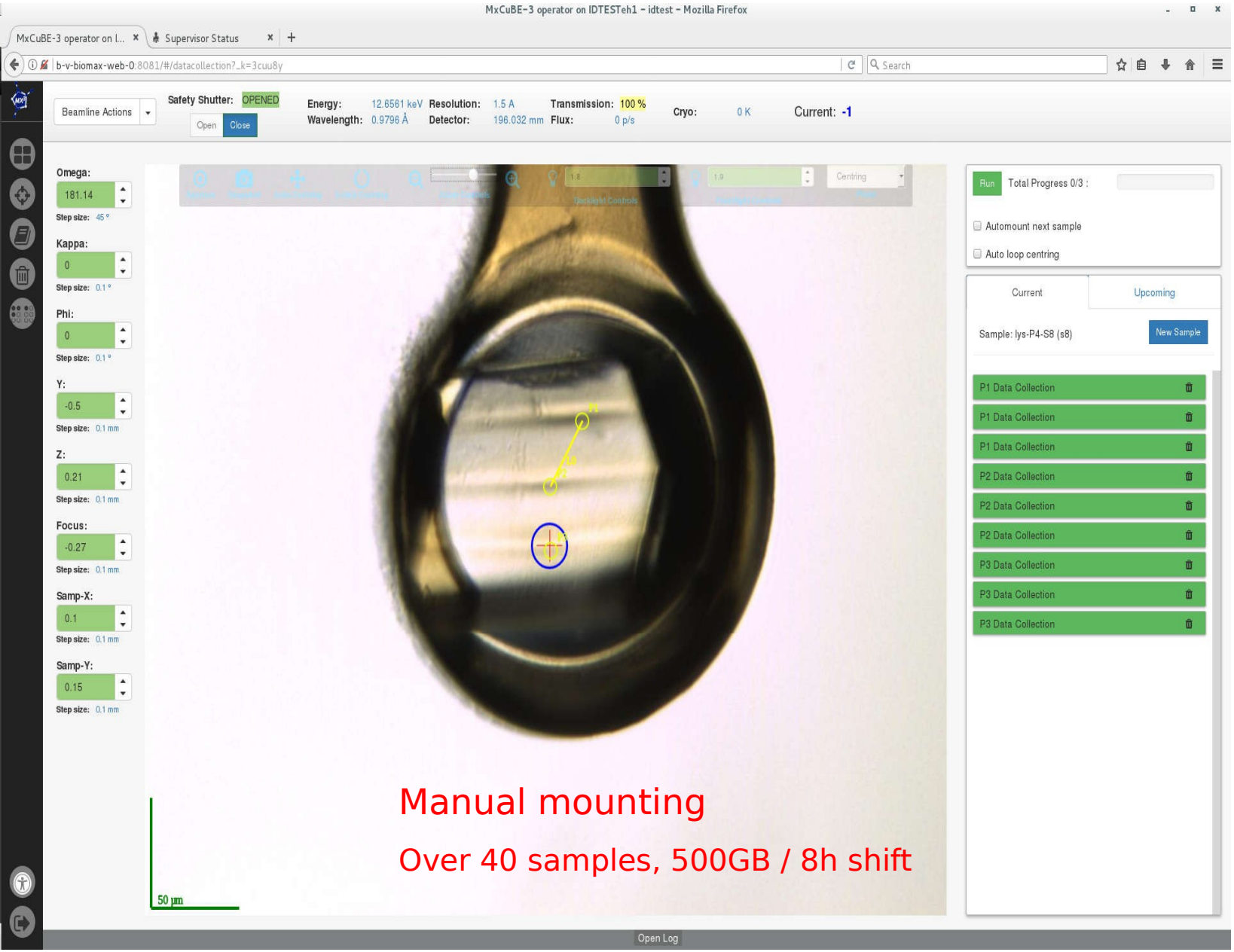


MXCuBE3 data collection view

KITS

MAX IV

MXCuBE3 at BioMAX



Main features

- Sample Video
  - 3 click Centering
  - 2D Centring
  - Auto-Loop Centri
- MD3 controls
  - Motors
  - Zoom
  - Light
  - phase
- Data Collection
  - Standard collecti
  - Characterization
  - Helical Scan
- Processing
  - Launched on HPC
- Queue