MXCuBE at MAX IV

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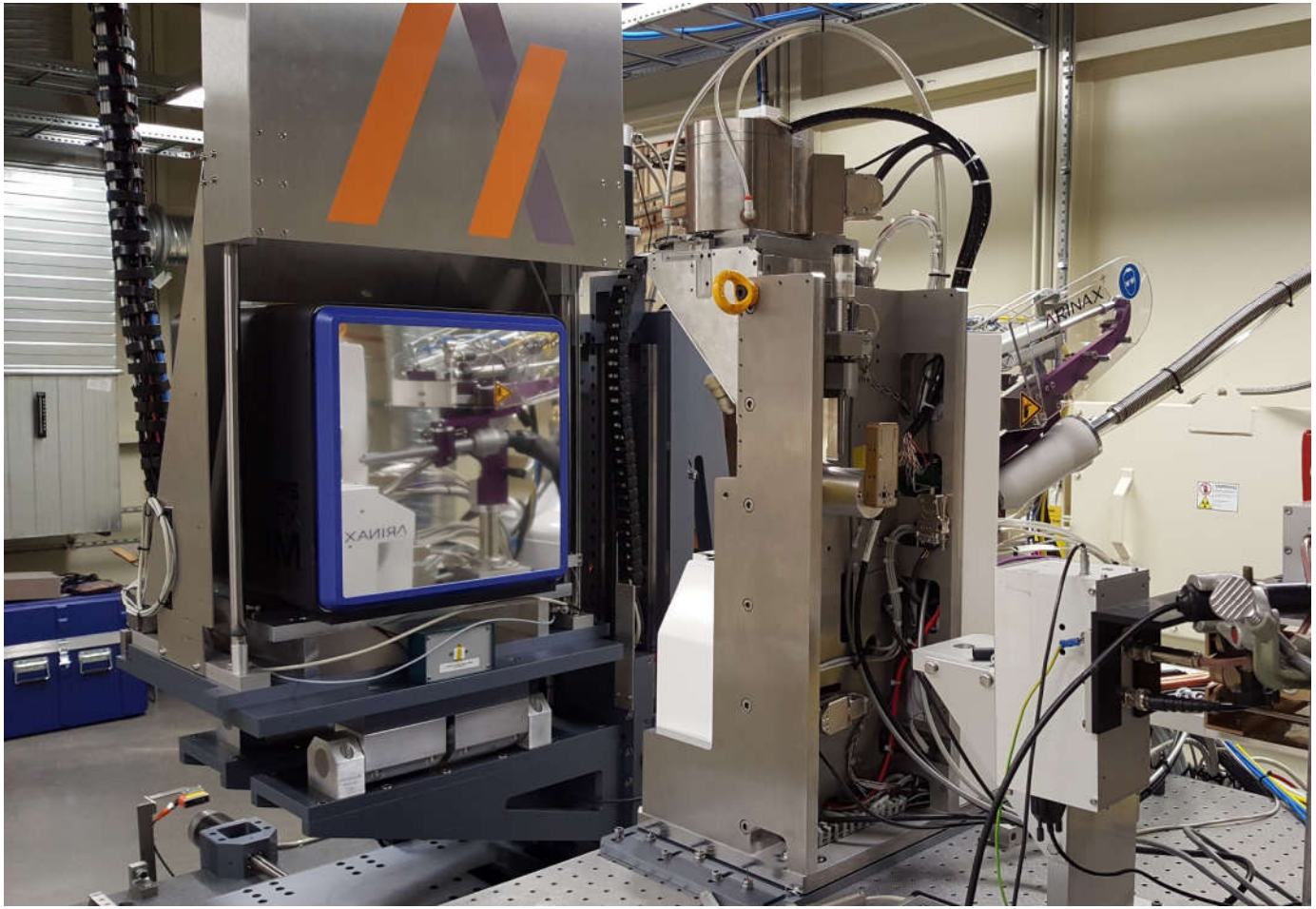
Jan. 16th, 2017

MX Beamline at MAX IV - BioMAX

- MAD Station, 5 – 25 keV
- In-vacuum undulator
- MD3 Micro-Diffractometer
  - Mini-kappa
  - Crystallization Plate holder
- Detector, Eiger 16M
- Cryojet5, HClab and REX
- Amptek fluorescence detector
- BCU
- ISARA, Sample Changer

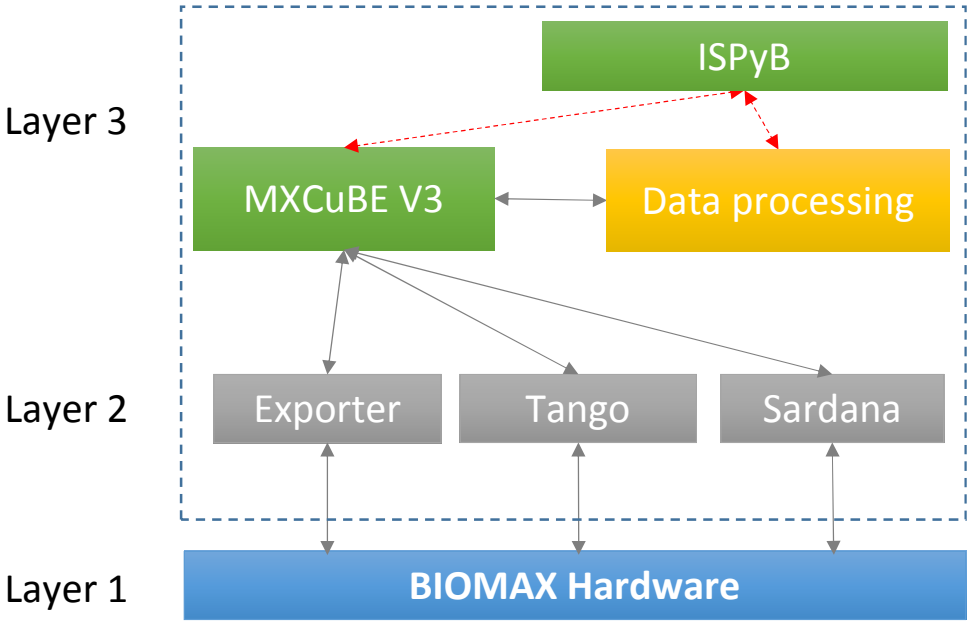


ISARA – Sample Changer

Four grippers

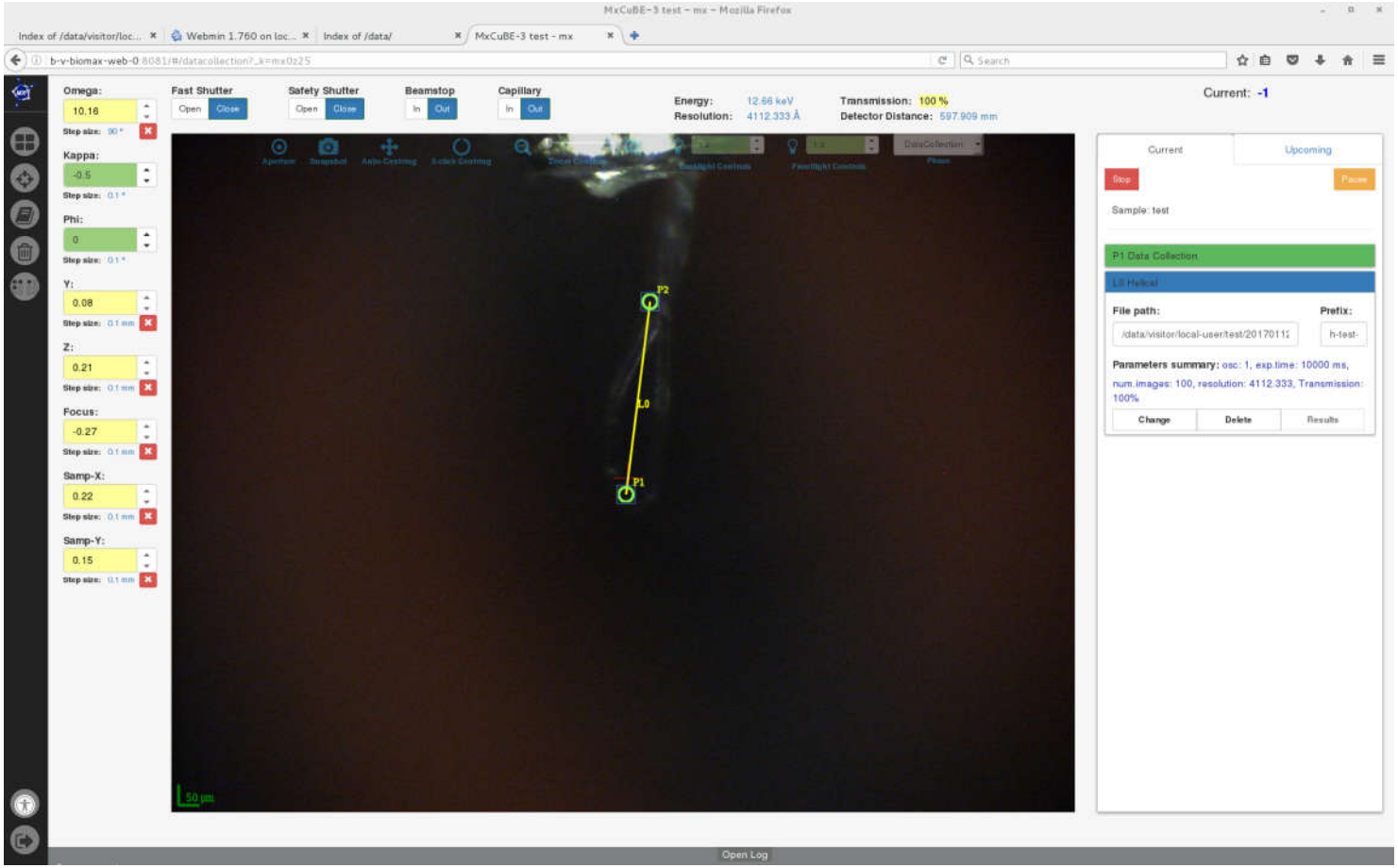
- Unipuck (Double)
- Unipuck (Single)
- SPINE (Single)
- Plate

BioMAX Software Overview



MXCuBE3 at BioMAX

- Sample View
  - 3-click centering,
  - Loop Centering
  - 2D Centring
- Data Collection
  - Std. Data collection
  - Characterization
  - Helical scan
  - Support queue
- Beamline/machine info.
- Processing



HardwareObjects

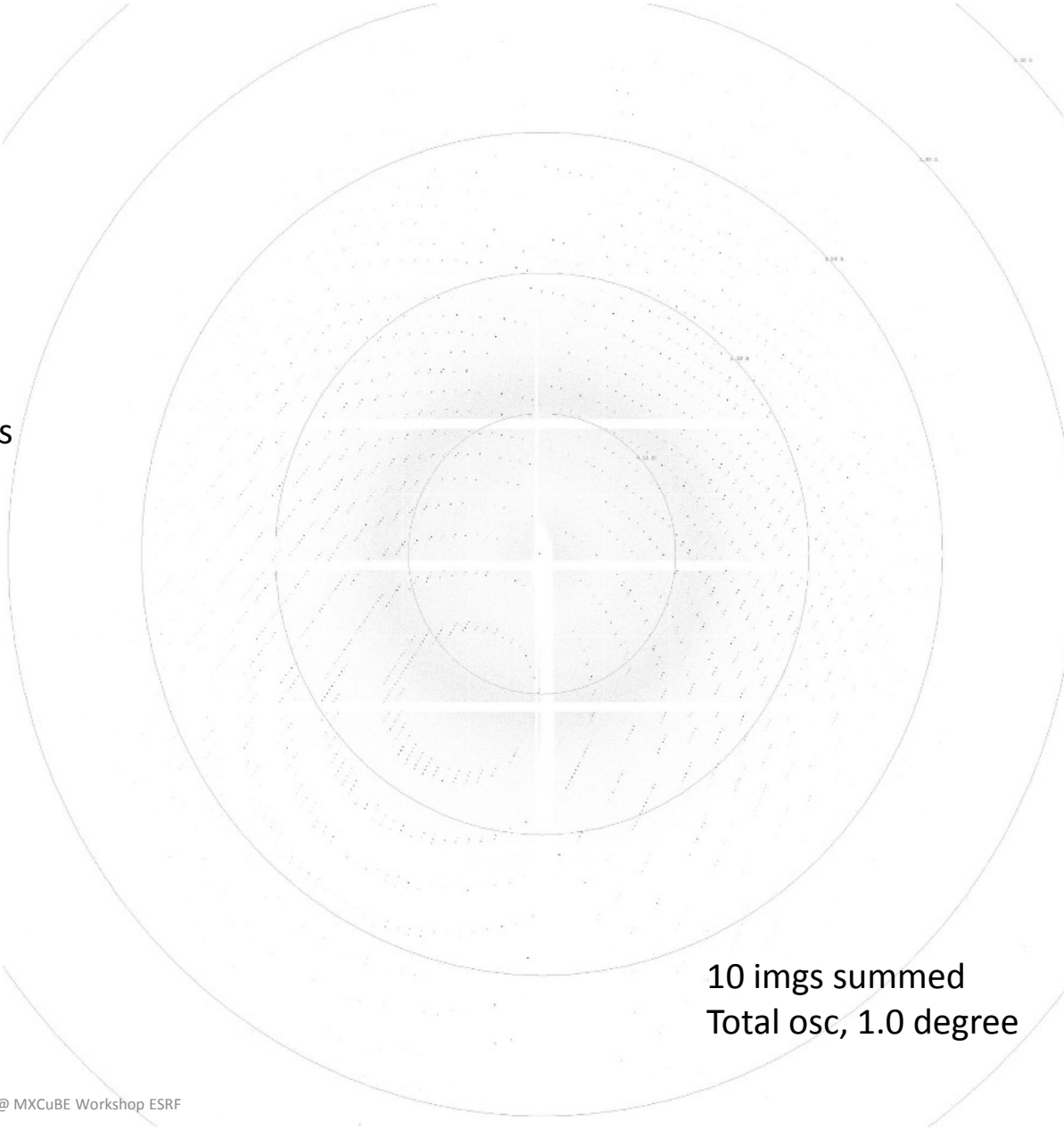
- 2.2 branch
- new hwobjs
  - BIOMAXEiger.py and BIOMAXEigerMockup.py
  - BIOMAXCollect.py (AbstractCollect.py)
  - BIOMAXMD3.py (GenericDiffractometer.py)
  - BIOMAXResolution.py
  - BIOMAXBeamInfo.py
  - BIOMAXAperture.py

Data Collection at BioMAX

- Ring Current, 20-50 mA
- Beam size, 20 x 5 um^2 (hor x ver)
- Estimated photon flux (sample): over 10e11 ph/s
- Fixed energy: 12.7 keV
- User operation: Commissioning users
- Sample mount: manual

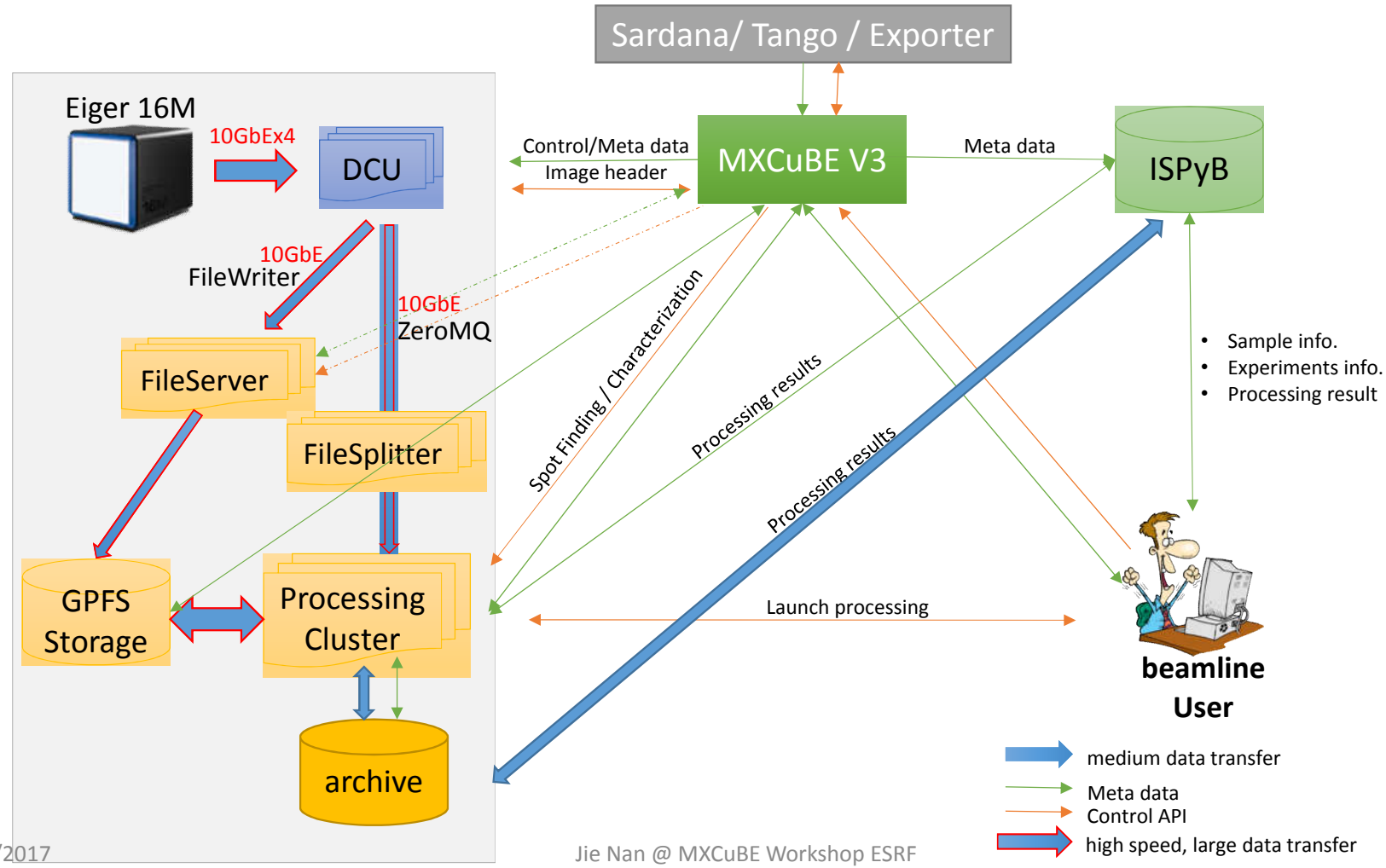
Thaumatin crystal

- Osc. 0.1 degree
- Exposure, 0.1 s
- Helical scan



10 imgs summed
Total osc, 1.0 degree

BioMAX Data Flow Overview



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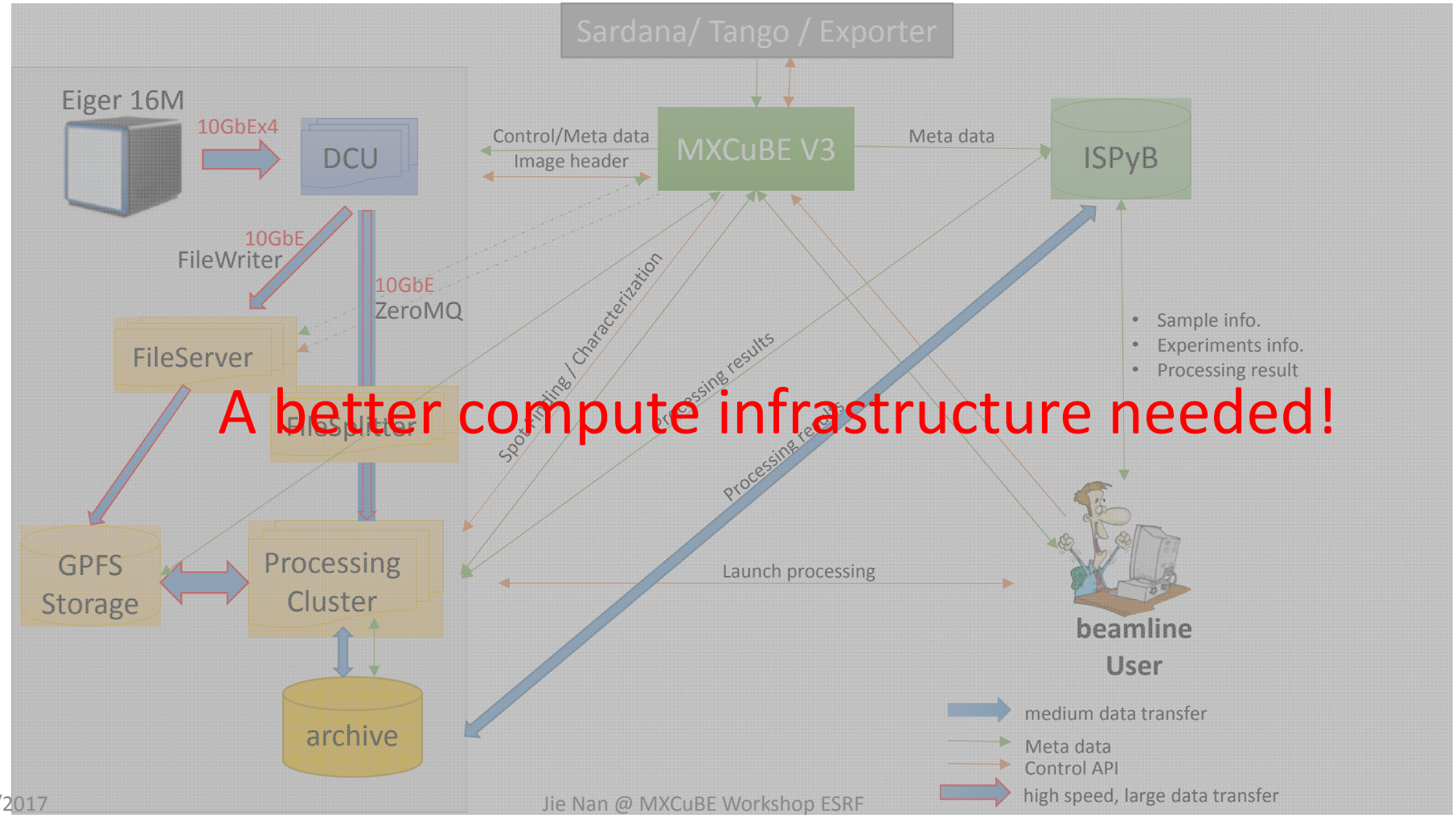


Upgrade of Compute Infrastructure

Current Status

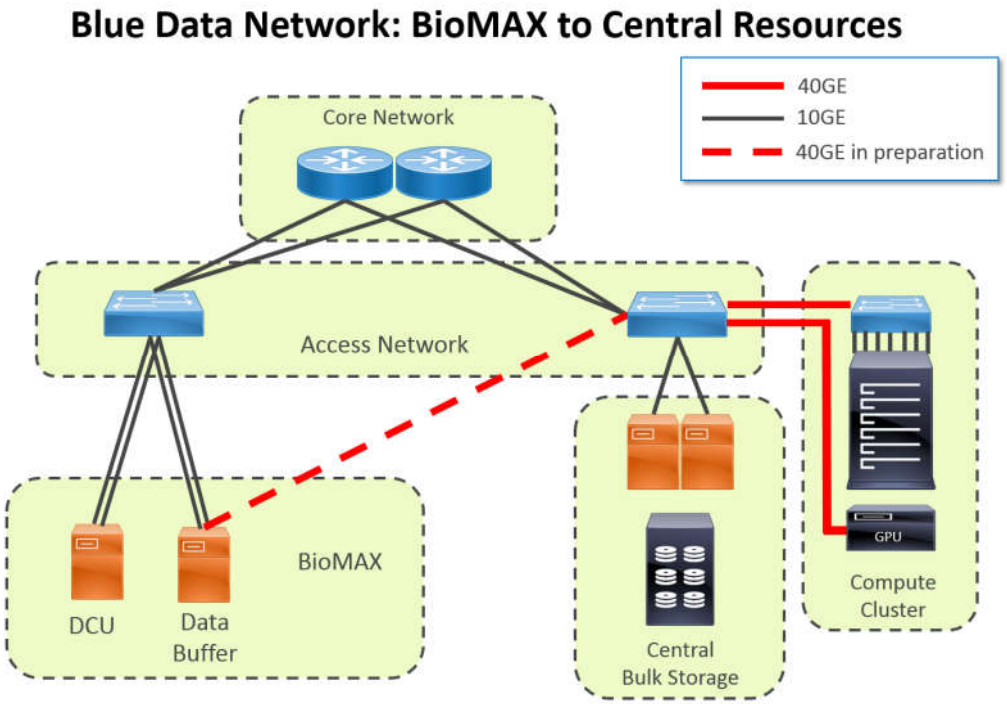
- 1 Gb/s to 10 Gb/s
- Buffer server at BioMAX
- GPFS storage
- HPC Cluster with 8 nodes (shared)

Further upgrade of 40GE based network

- Buffer Server to GPFS storage
- Buffer Server to Cluster

Computation

- New 8 nodes, 128 GB RAM, 20 cores per node
- Continuously grow



Future work

- Hardware integration
  - Sample changer
  - Fluorescence detector
  - Cryojet5, HClab and REX
- Experiments
  - Mesh scan
  - Element analysis & XANES
  - MAD data collection
  - Plate manipulation
  - RT collection (HClab) & crsytal freezing (REX)
  - New collection protocols
- Integration with ISPyB
- Data processing
  - Spot finding
  - Reduction

Acknowledgement

MX Group

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

Marjolein Thunnissen

KITS Group

Darren Spruce
Mikel Eguiraun
Fredrik Bolmsten
Antonio Milán-Otero
Artur Barczyk
Zdenek Matej

many others from MAX IV

ESRF

Matias Guijarro
Marcus Oscarsson
Daniele De Sanctis
Antonia Beteva

Vicente Rey Bakaikoa