Deploying a PILATUS 6M for Protein Crystallography at IMCA-CAT

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OVERVIEW

Control

1

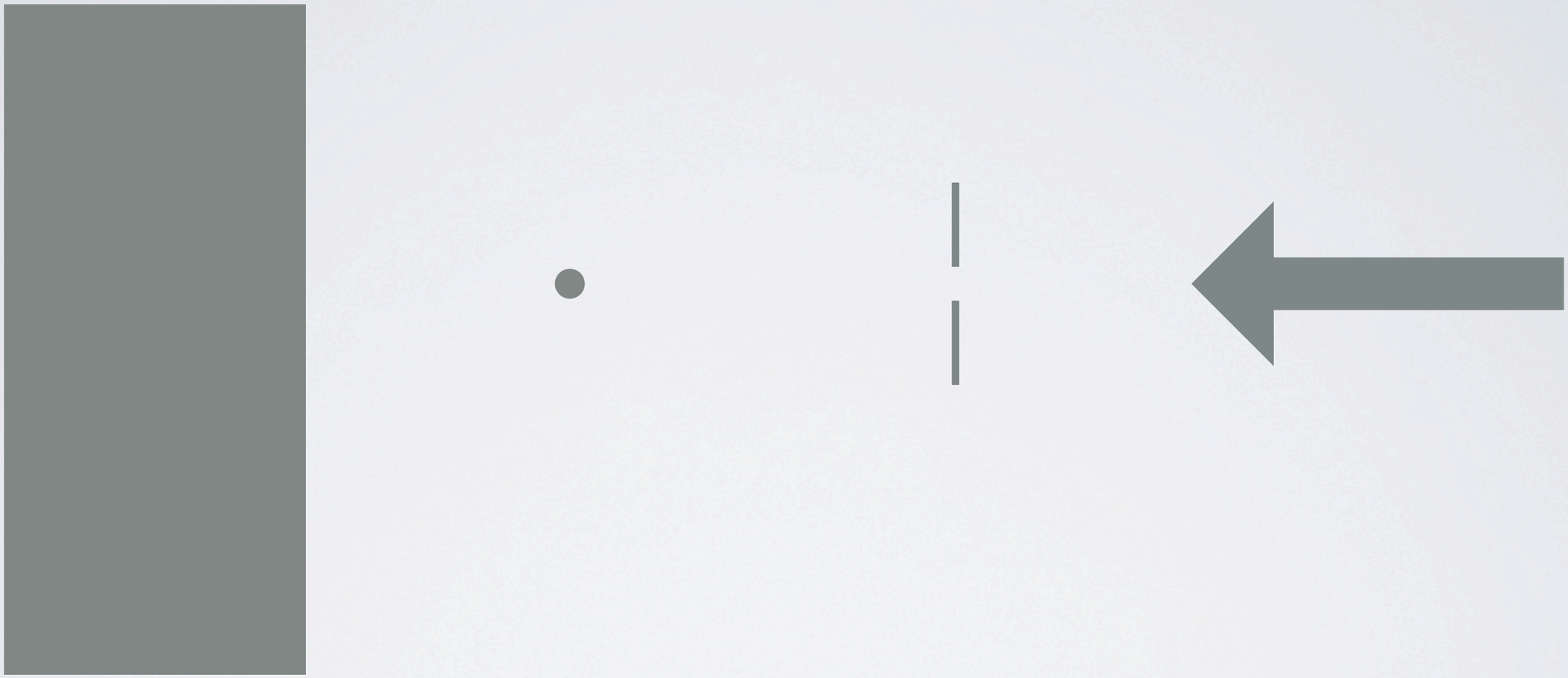
Crystallography

2

Storage

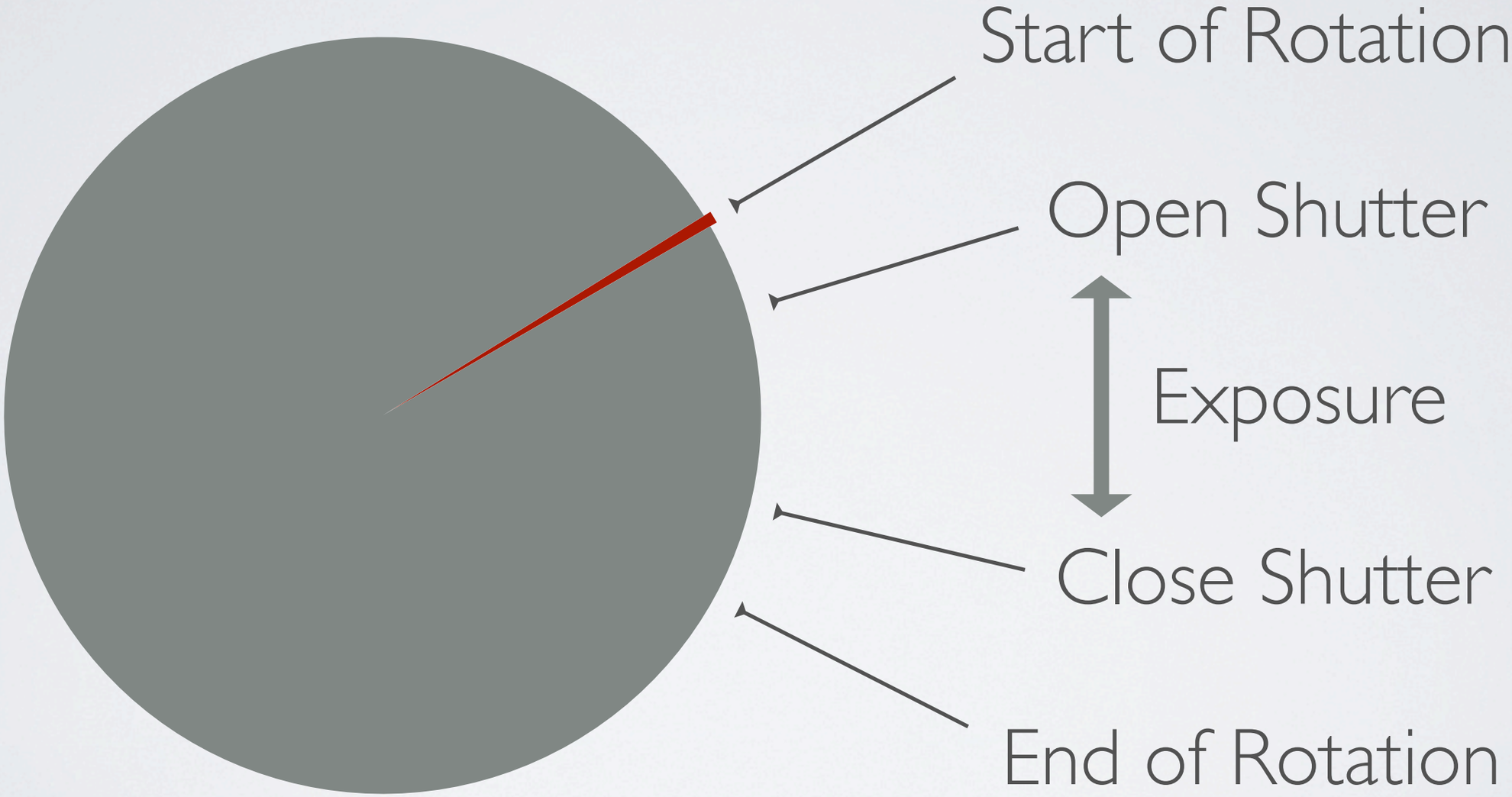
3

EXPERIMENT BASICS

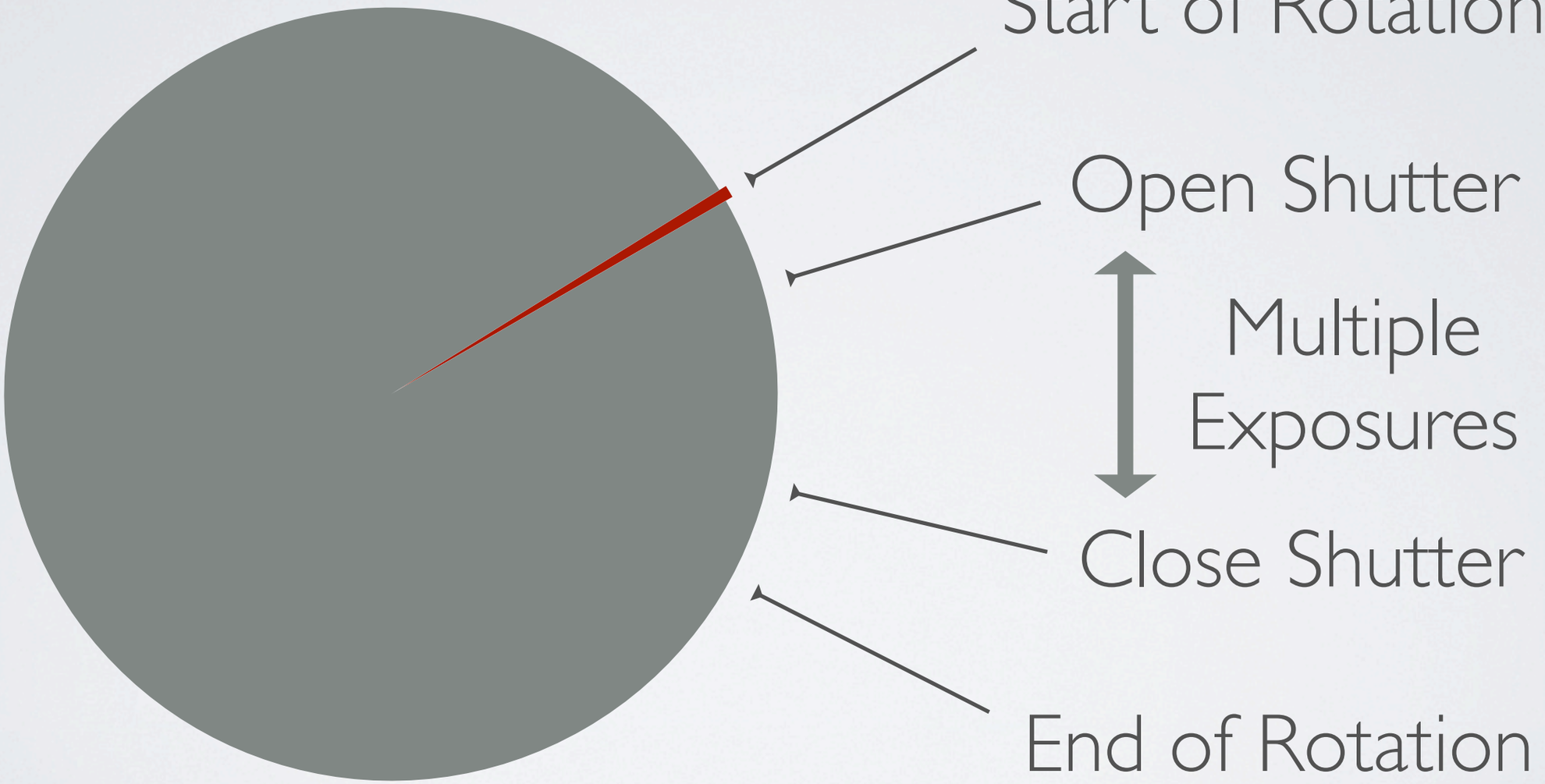


Detector Sample Shutter X-rays

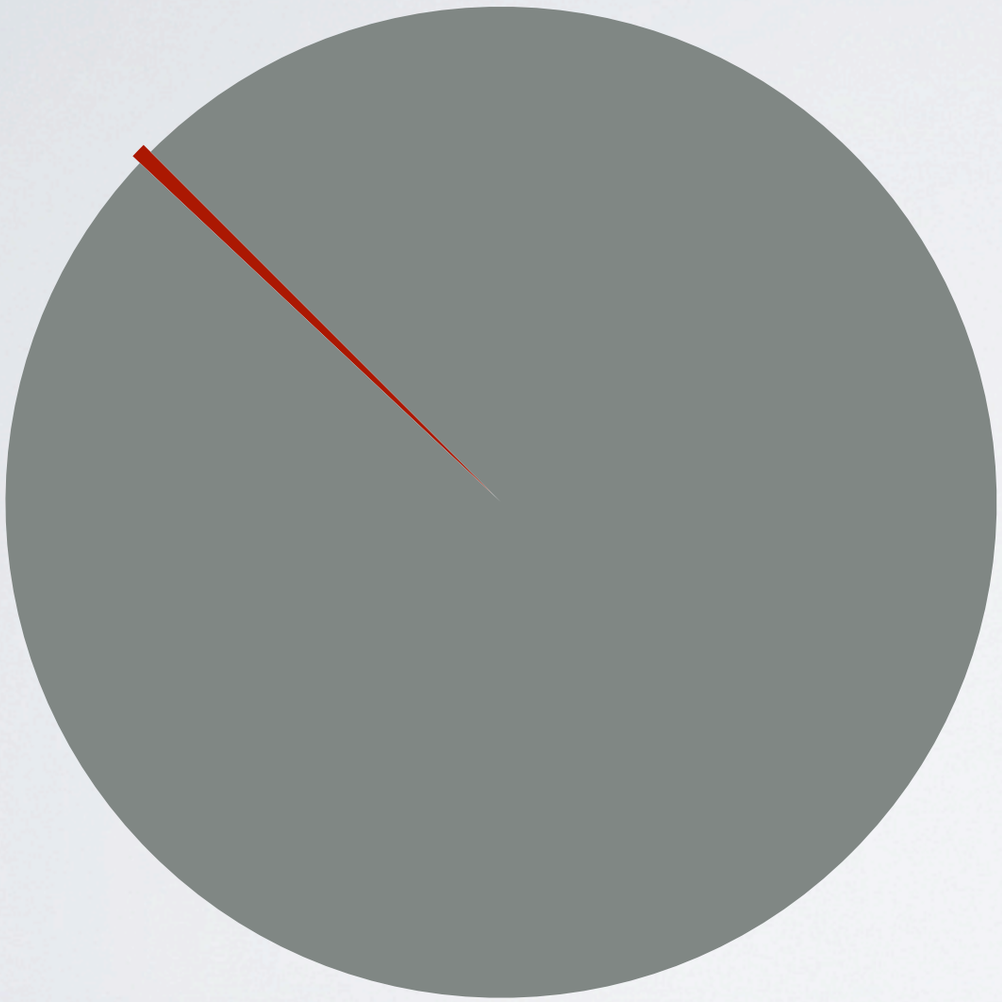
STEP-ROTATION



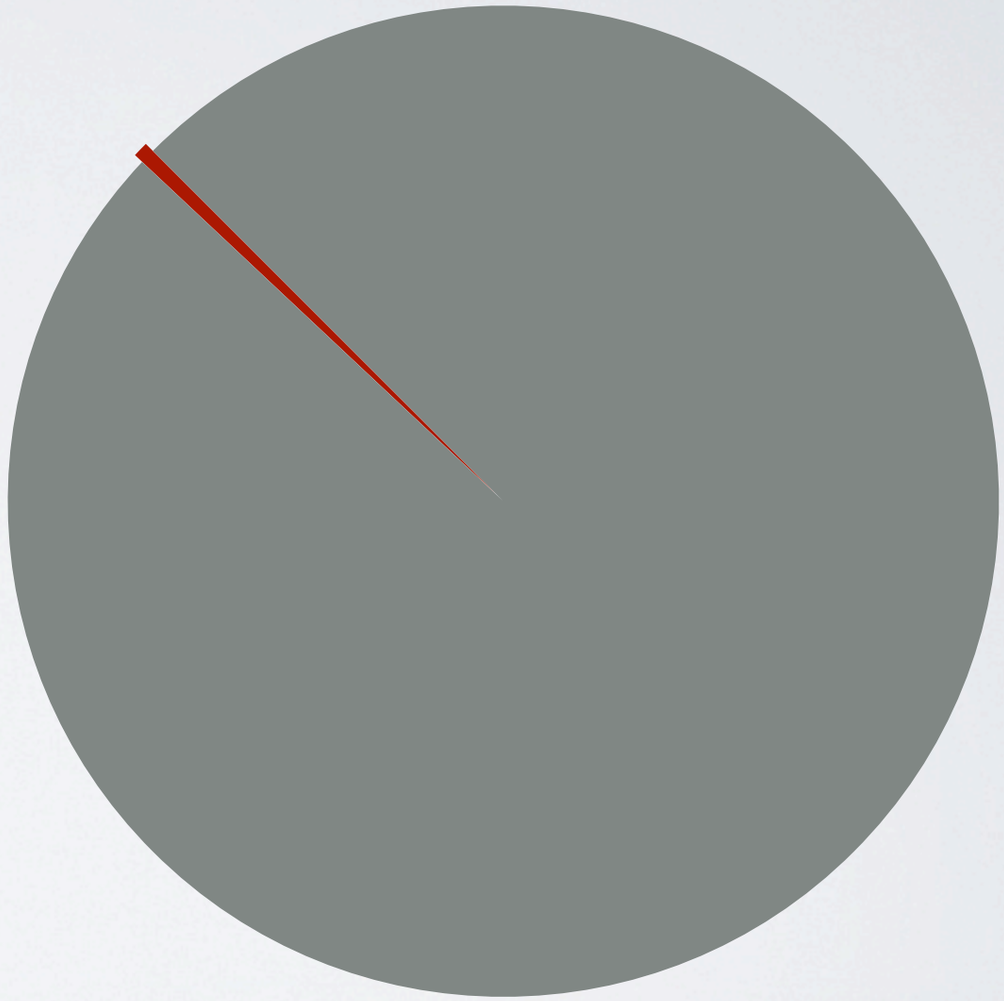
CONTINUOUS-ROTATION



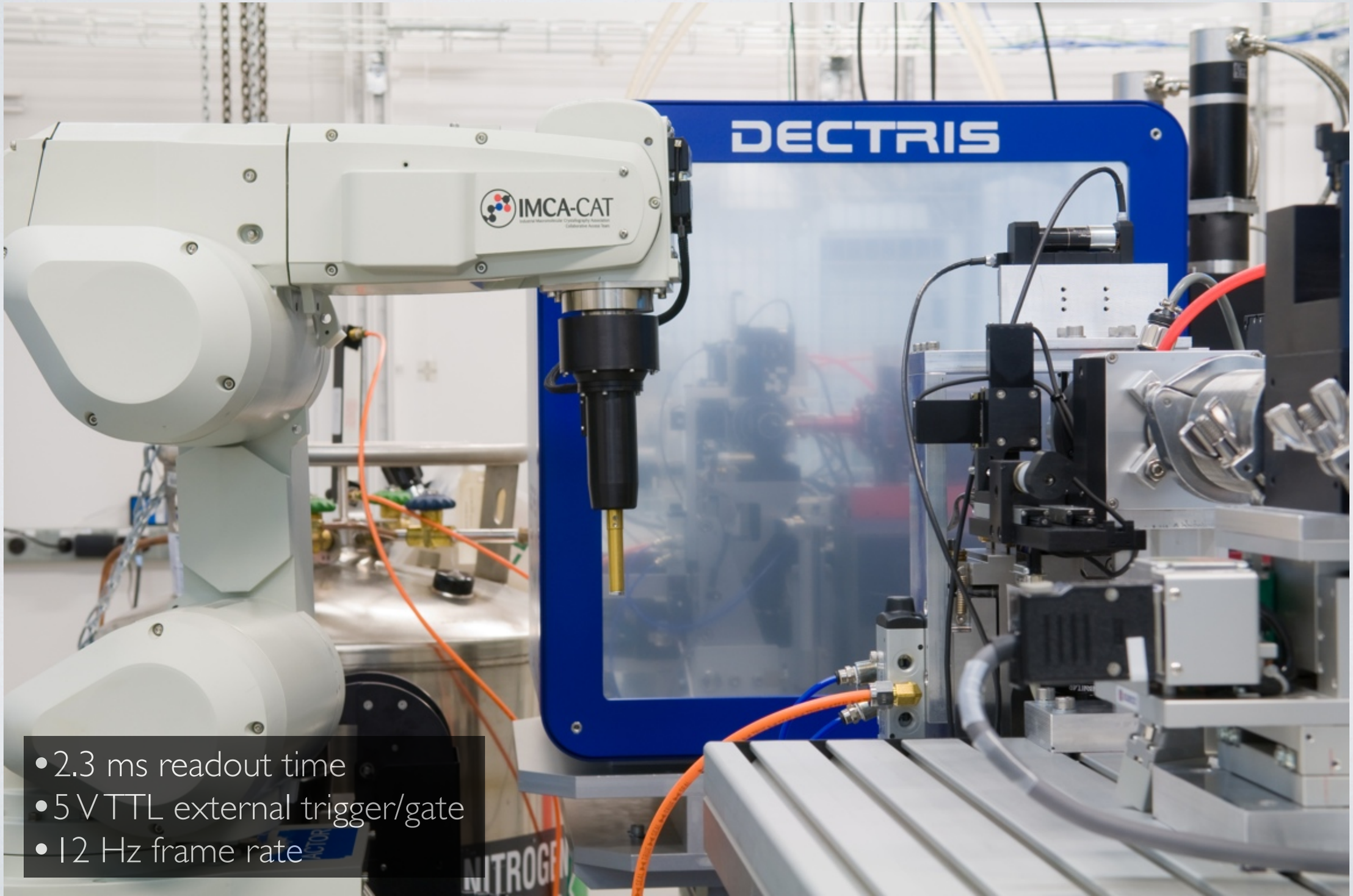
STEP



CONTINUOUS

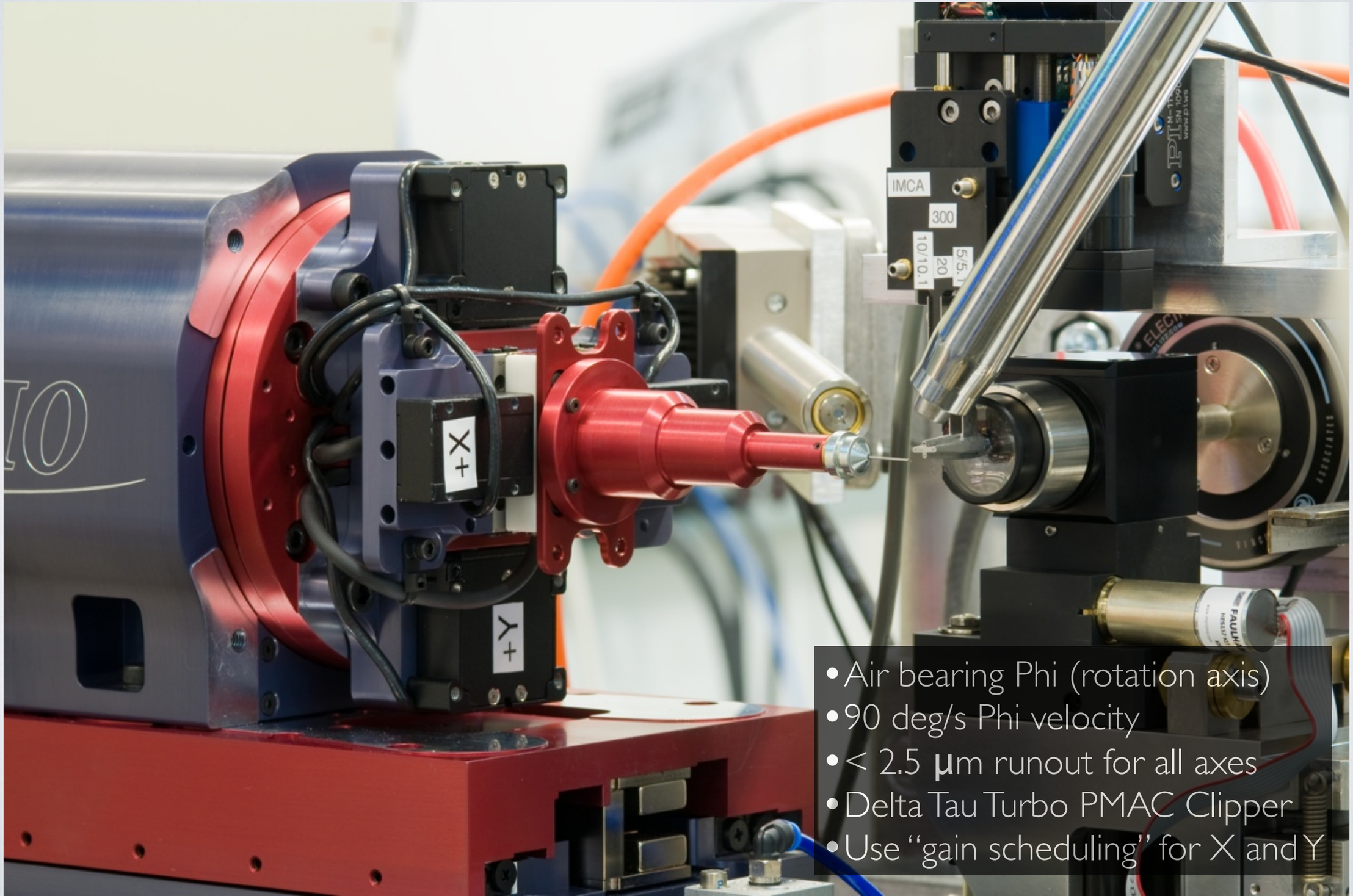


DECTRIS PILATUS 6M

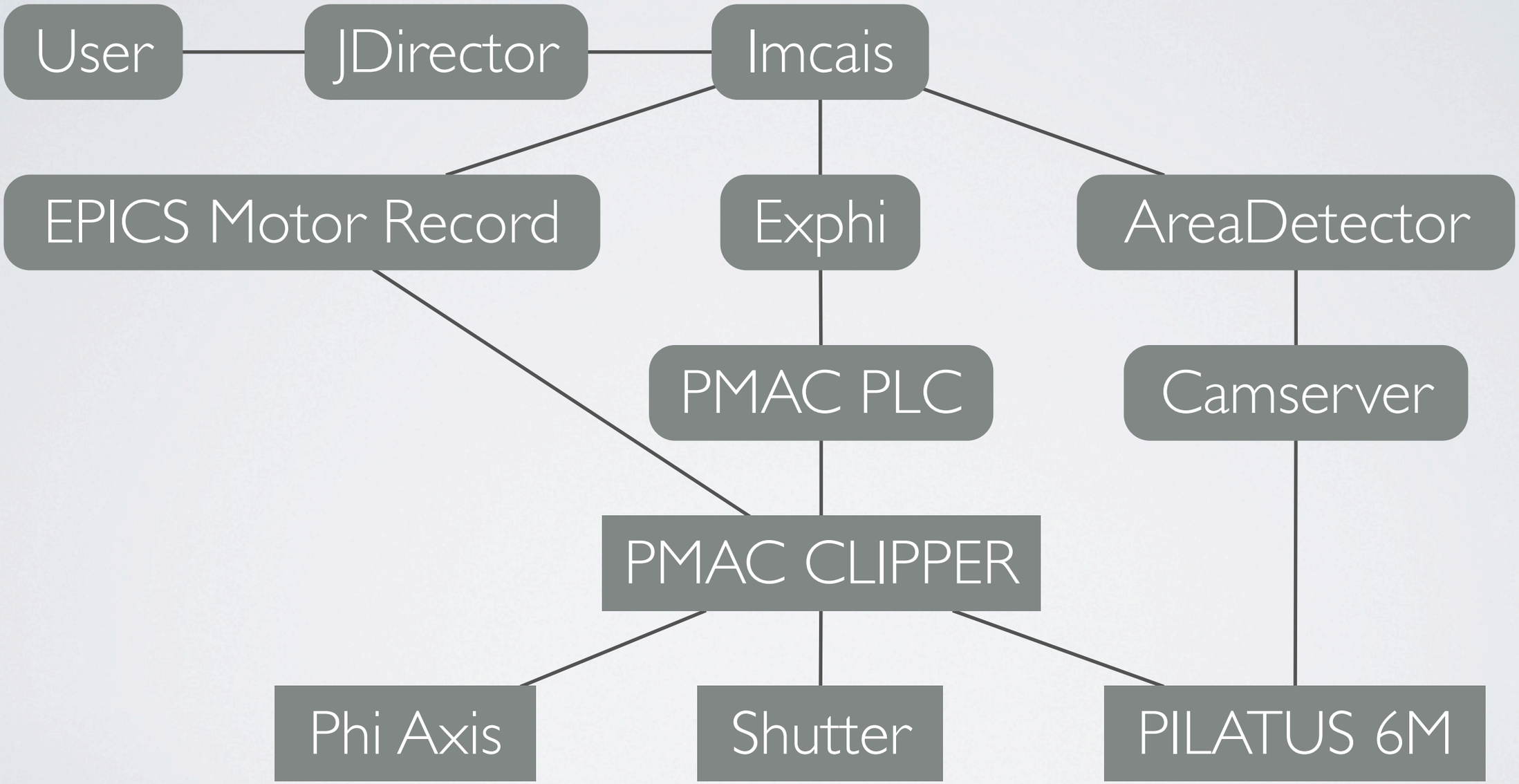


- 2.3 ms readout time
- 5 V TTL external trigger/gate
- 12 Hz frame rate

ALIO GONIOMETER

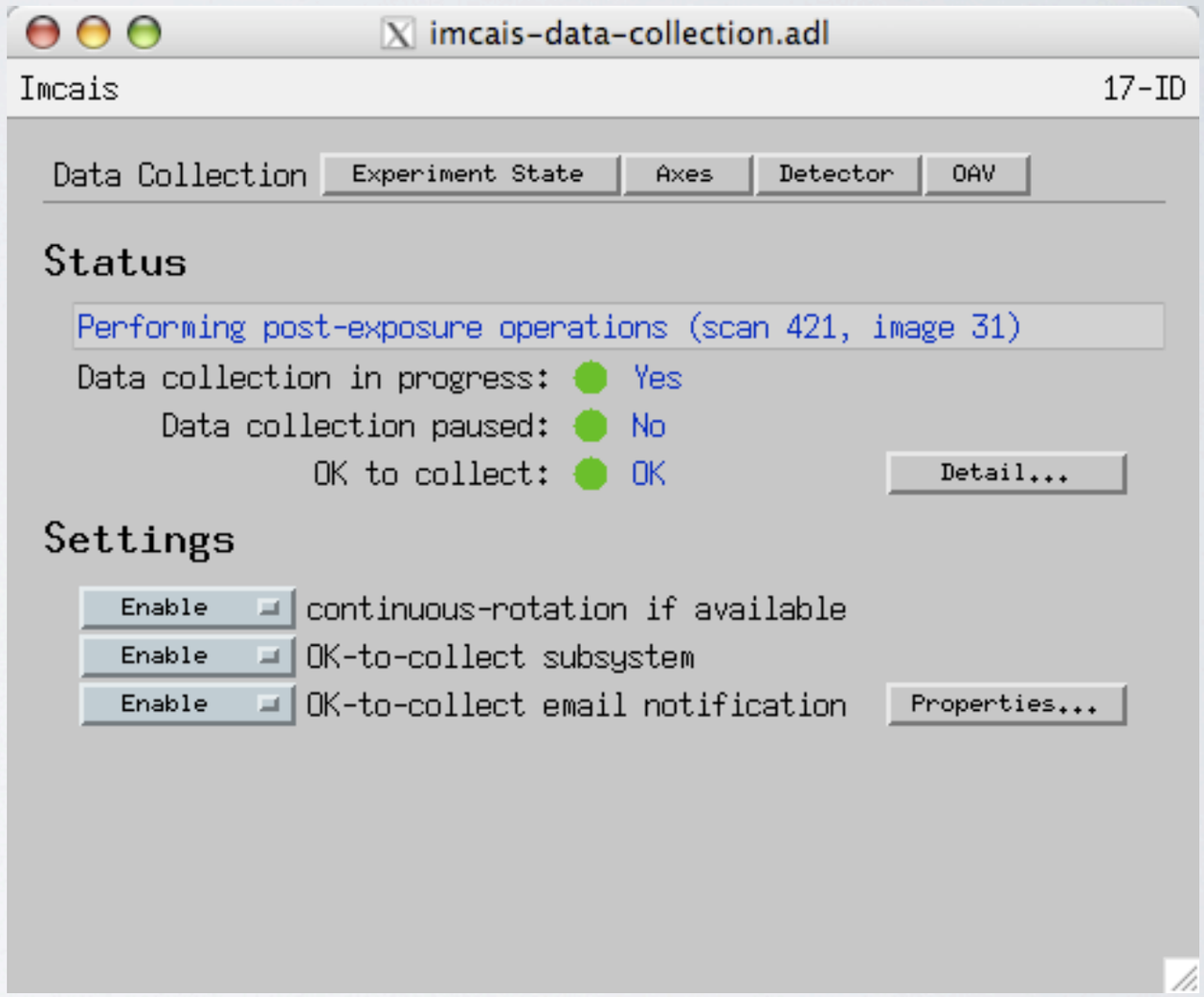


IMPLEMENTATION

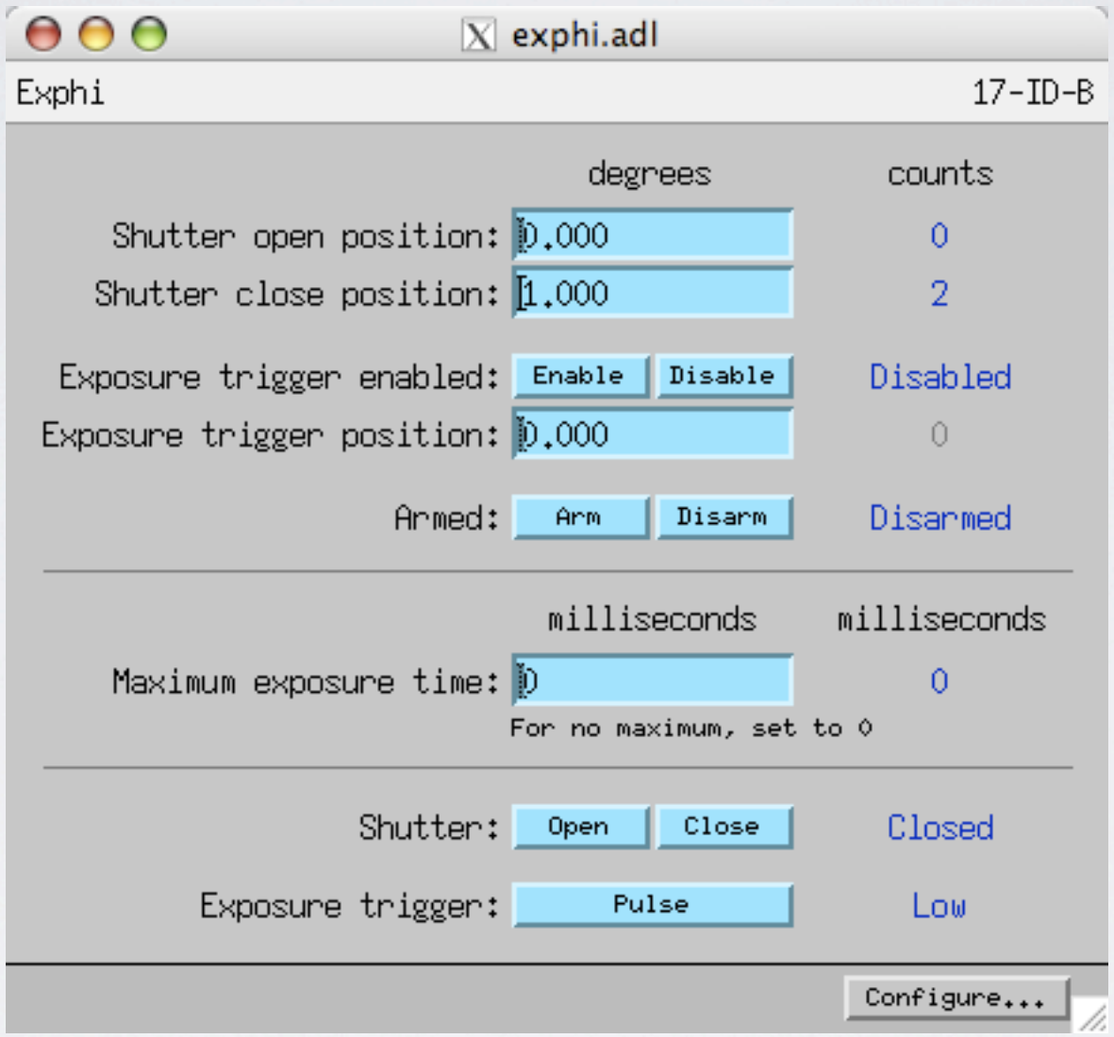


Imcais

1. Sets up Exphi
2. Sets up areaDetector
3. Moves Phi

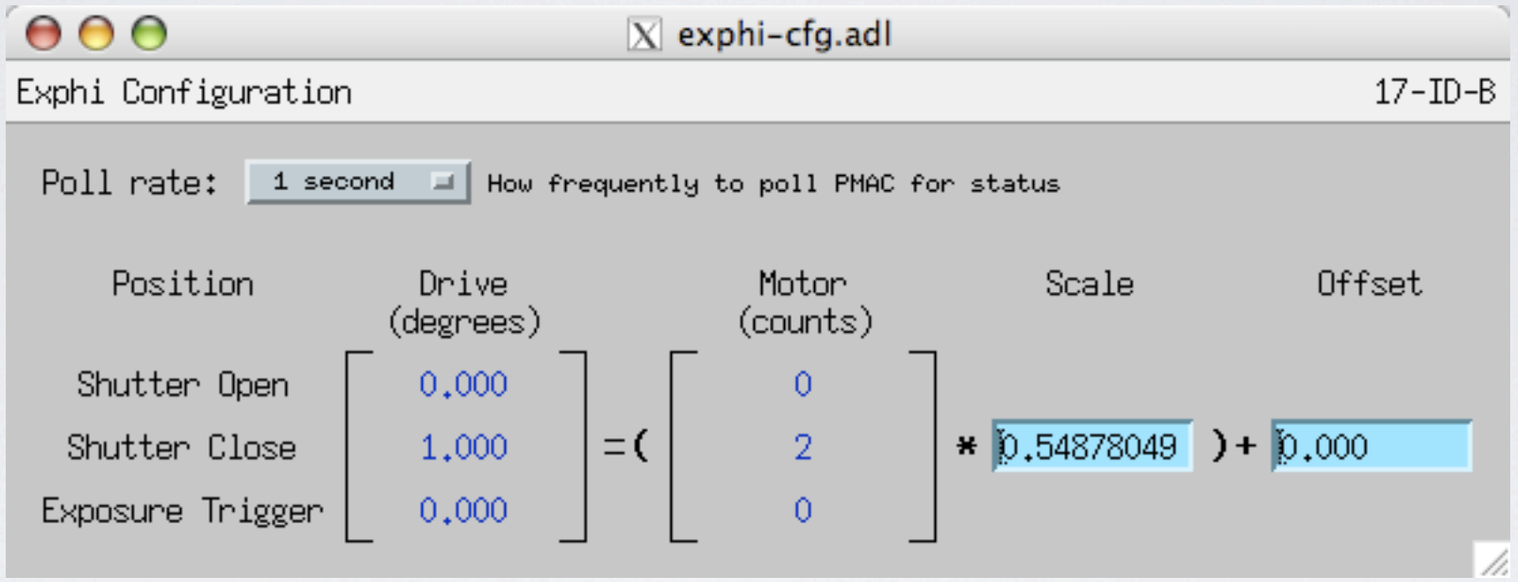


Exphi



- Shutter controlled via Turbo PMAC Clipper digital output point
- Exposure trigger controlled via Turbo PMAC Clipper digital output point

Exphi


exphi-cfg.adl
Exphi Configuration
17-ID-B
Poll rate:
1 second
How frequently to poll PMAC for status
Position (degrees)
Drive (counts)
Motor
Scale
Offset
Shutter Open
Shutter Close
Exposure Trigger
0.000
1.000
0.000
=(
0
2
0
* 0.54878049)+ 0.000

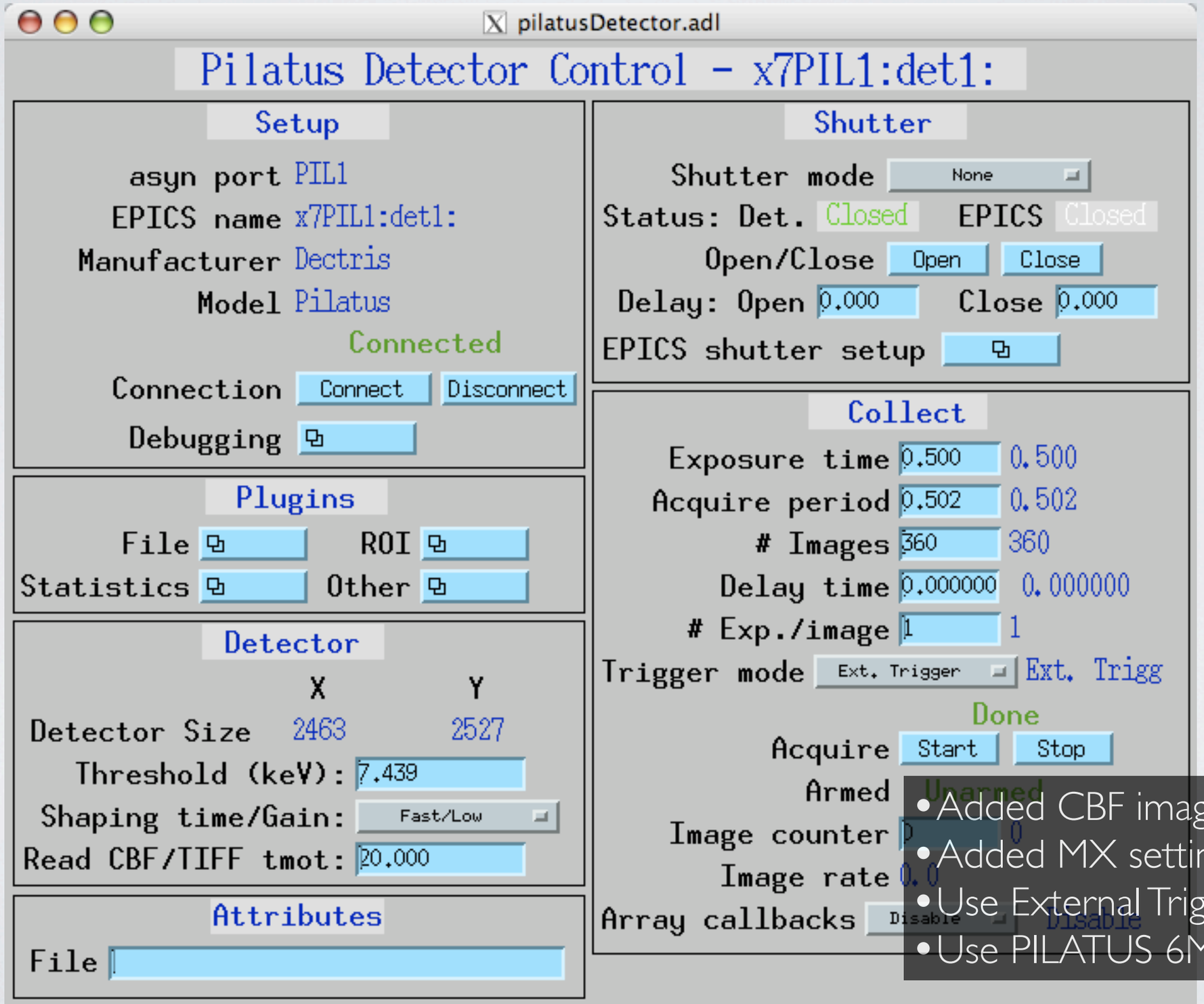
PMAC PLC Program

- Runs as regular PLC
- Not compiled
- M-variable for position

Possible optimizations:
- Run PLC at servo priority
- Use position-compare function

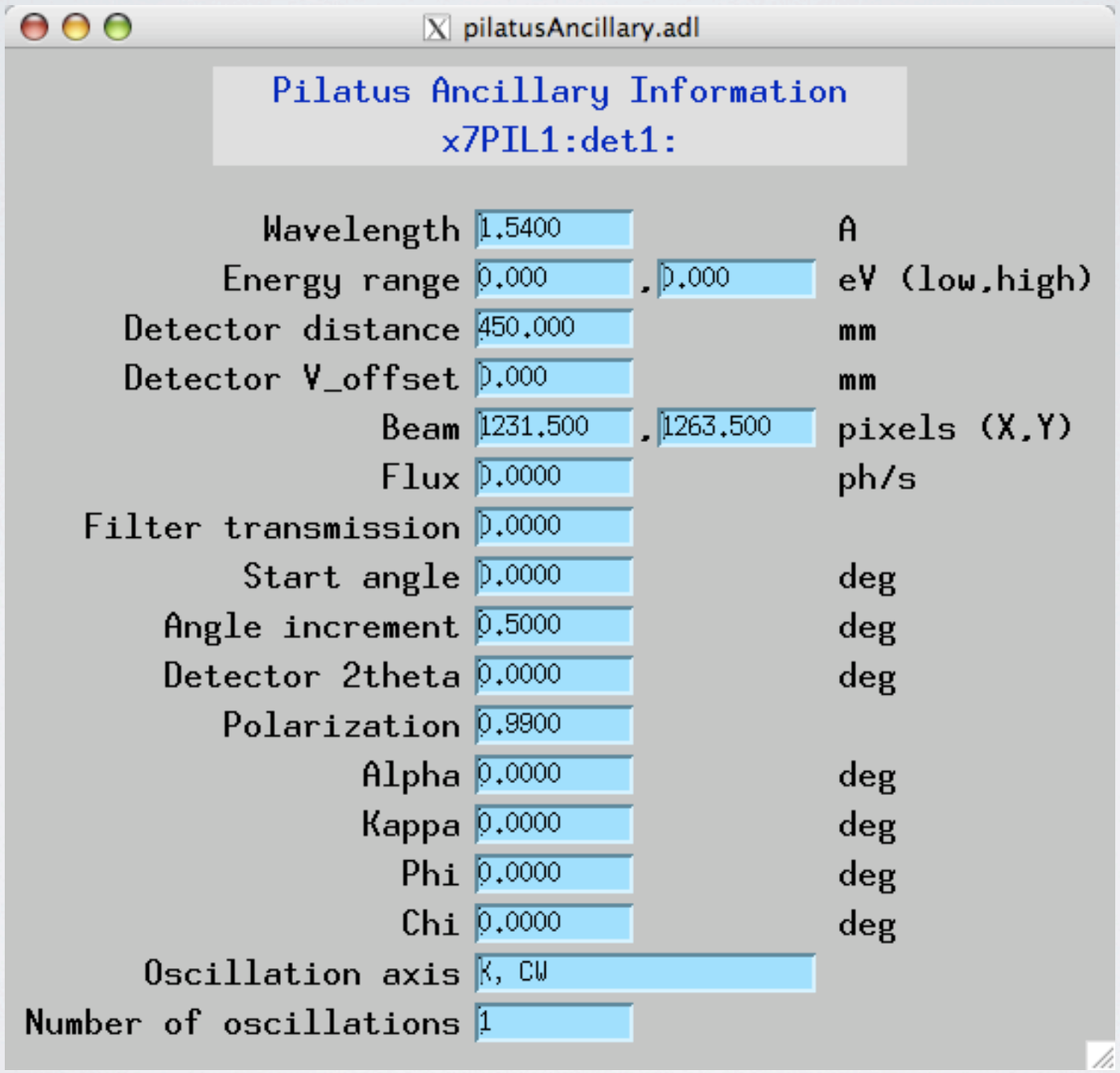
```
CLOSE
END GATHER
DELETE GATHER
DELETE TRACE

P1=0
P4=0
P7=M0
P8=M2
P10=0
P11=0
P12=0

OPEN PLC 3 CLEAR

; Open exposure shutter if requested, and start timer
IF (M0!=P7)
  M0=P7
  IF (M0=1)
    I5111=P6*8388608/I10
  ENDIF
ENDIF

; Close exposure shutter if maximum exposure time reached
IF (M0=1 AND P6!=0 AND I5111!>0)
  P7=0
  M0=0
  P1=0
  P12=0
ENDIF

; Start exposure trigger pulse if requested, and start timer
IF (M2!=P8)
  M2=P8
  IF (M2=1)
    I5112=10*8388608/I10
  ENDIF
ENDIF
...
```

AreaDetector PILATUS Driver

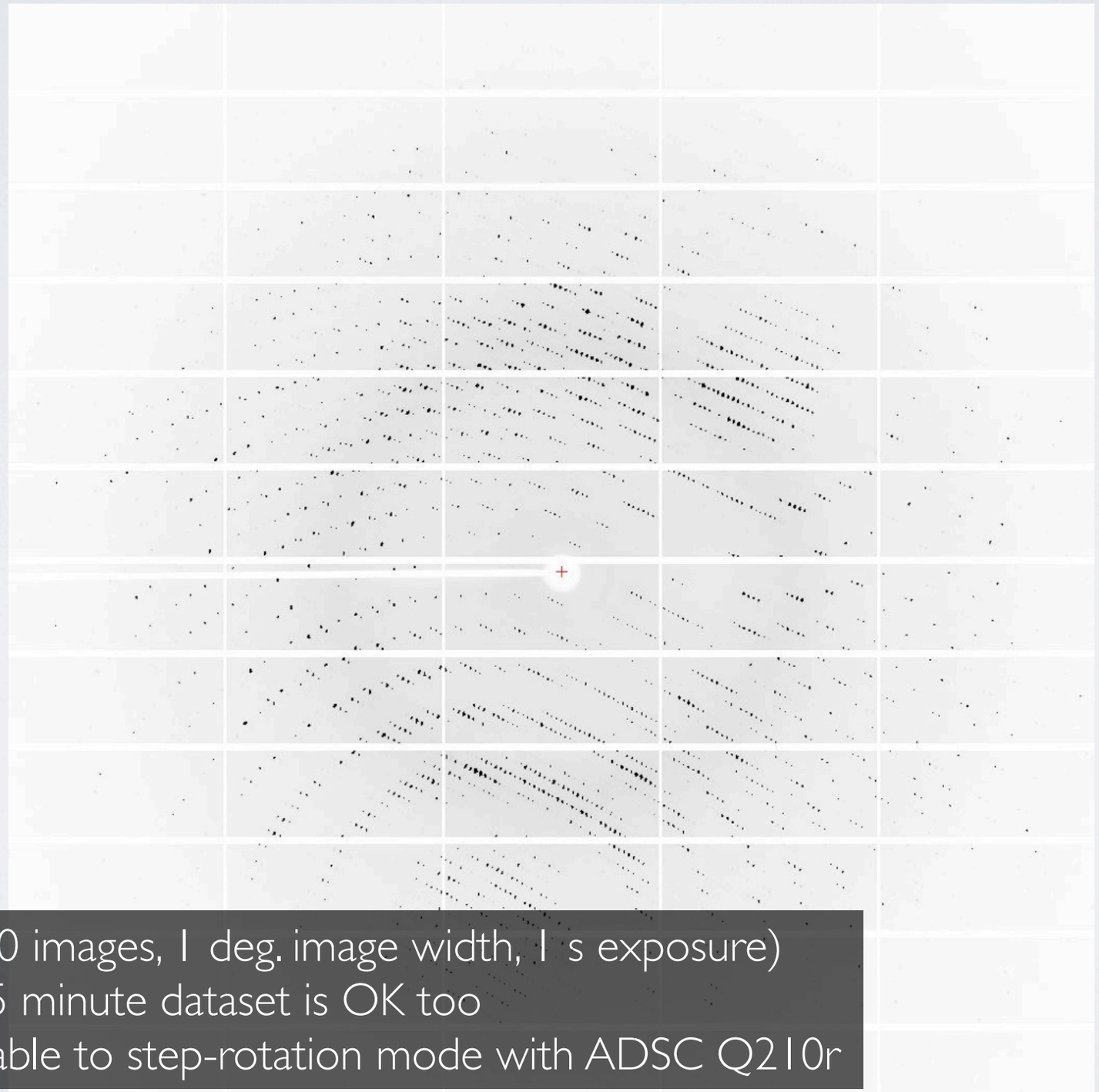


- Added CBF image support
- Added MX settings support
- Use External Trigger mode
- Use PILATUS 6M internal timer

AreaDetector PILATUS Driver



CRYSTALLOGRAPHY



- 3 minute dataset (180 images, 1 deg. image width, 1 s exposure)
- Test data suggests 1.5 minute dataset is OK too
- Data quality comparable to step-rotation mode with ADSC Q210r

PILATUS 6M COMPUTING INFRASTRUCTURE AT 17-ID

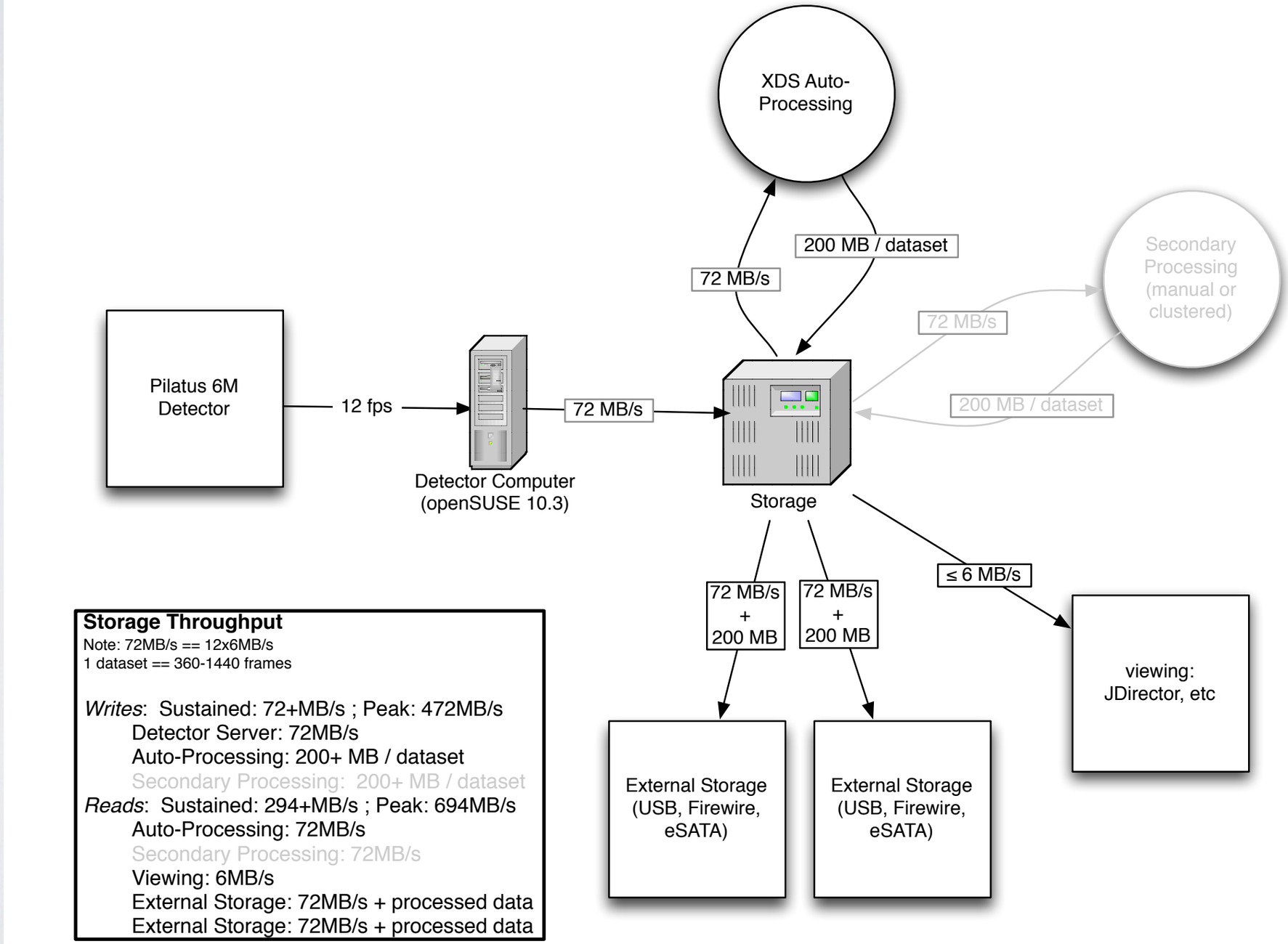
COMPUTING OVERVIEW

- Fast and Reliable Storage
- Fast Network
- Fast Workstations

STORAGE REQUIREMENTS

- Aggregate Throughput: 500-700MB per second
- Approximately 50TB
- Highly Available
- Scalable (size and performance)
- Avoid vendor lock-in
- Compatible with detector server (openSUSE 10.3)
- POSIX Compliant
- Modular (reconfigurable to another solution)

DATA FLOW



Storage Throughput

Note: 72MB/s == 12x6MB/s
1 dataset == 360-1440 frames

Writes: Sustained: 72+MB/s ; Peak: 472MB/s
- Detector Server: 72MB/s
- Auto-Processing: 200+ MB / dataset
- Secondary Processing: 200+ MB / dataset

Reads: Sustained: 294+MB/s ; Peak: 694MB/s
- Auto-Processing: 72MB/s
- Secondary Processing: 72MB/s
- Viewing: 6MB/s
- External Storage: 72MB/s + processed data
- External Storage: 72MB/s + processed data

LUSTRE FILE SYSTEM

- High-Availability
- Scalable
  - Size: up to 64PB
  - Performance: scales nearly linearly to the number of OSTs
- Server Read Caching: reduces load on storage backend
- Used in similar environments (eg, LS-CAT)
- Open Source
- Thriving community (even after Oracle's acquisition of Sun)

LUSTRE CONFIGURATION

Lustre

- Two MetaData Servers (MDS) - Active/Passive Failover
- Two Object Storage Servers (OSS) - Active/Active Failover
- On-site installation by DataDirect Networks

High Availability: Heartbeat and Pacemaker

MDS/OSS Servers

- Dual Quad-Core Xeons
- 12 - 24GB RAM

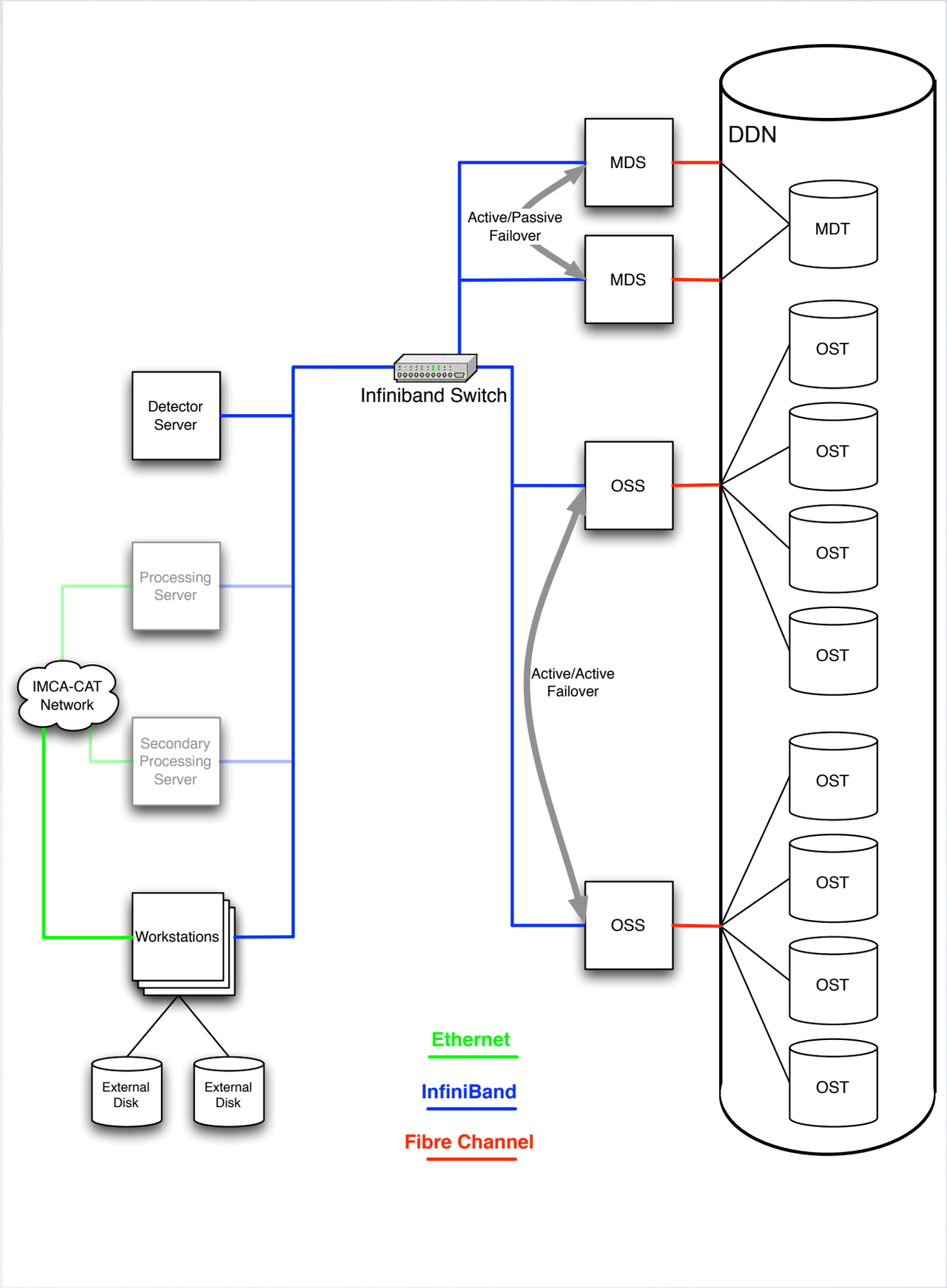
STORAGE HARDWARE

DataDirect Networks S2A6620

- Four 8x Fibre Channel Connections
- 80TB Raw Storage (File Data)
    - 80x 1TB SATA drives
    - 8x 10 drive RAID6 arrays (~7.5TB each)
    - ~60TB usable
- 3TB Raw Storage (MetaData)
    - 10x 300GB 10k RPM SAS drives

STORAGE NETWORK

- Primary: InfiniBand DDR (20Gb/s)
- Backup: Gigabit Ethernet



WORKSTATIONS

- Data Collection
- Data Backup
- Data Processing (x2)
- Specs
  - Dual Quad-Core Xeons
  - 24GB RAM
- Process datasets in 5-15 minutes

OVERALL PERFORMANCE

Greater than 500MB/s aggregate

FUTURE

- Tweak settings on DDN S2A6620
- Tweak Lustre parameters
- Improve data processing times
- Evaluate automated data processing

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