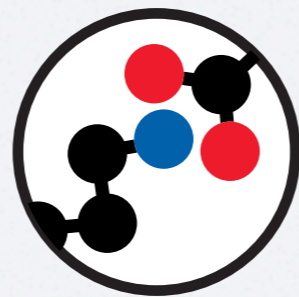


# Deploying a PILATUS 6M for Protein Crystallography at IMCA-CAT

Joe Digilio  
J. Lewis Muir



# OVERVIEW



Control

1



Crystallography

2

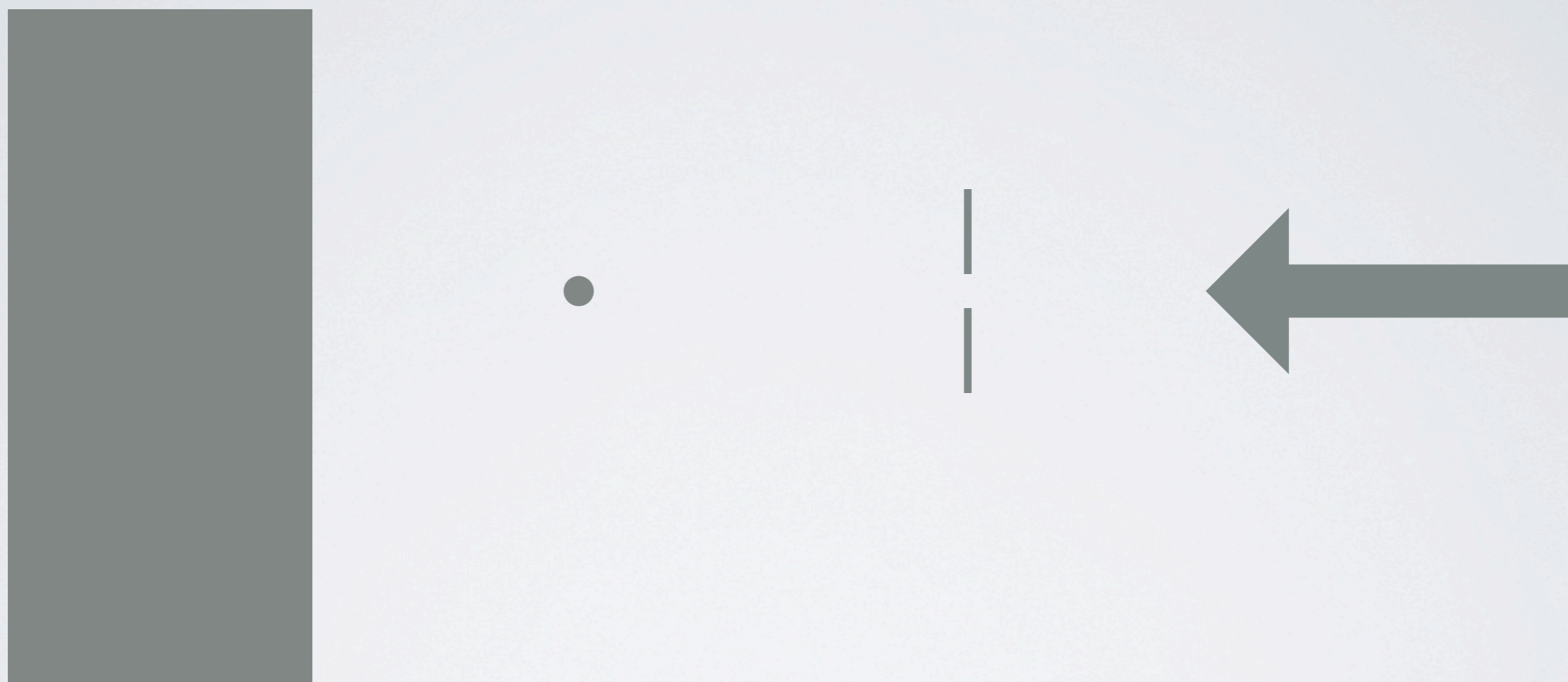


Storage

3



# EXPERIMENT BASICS



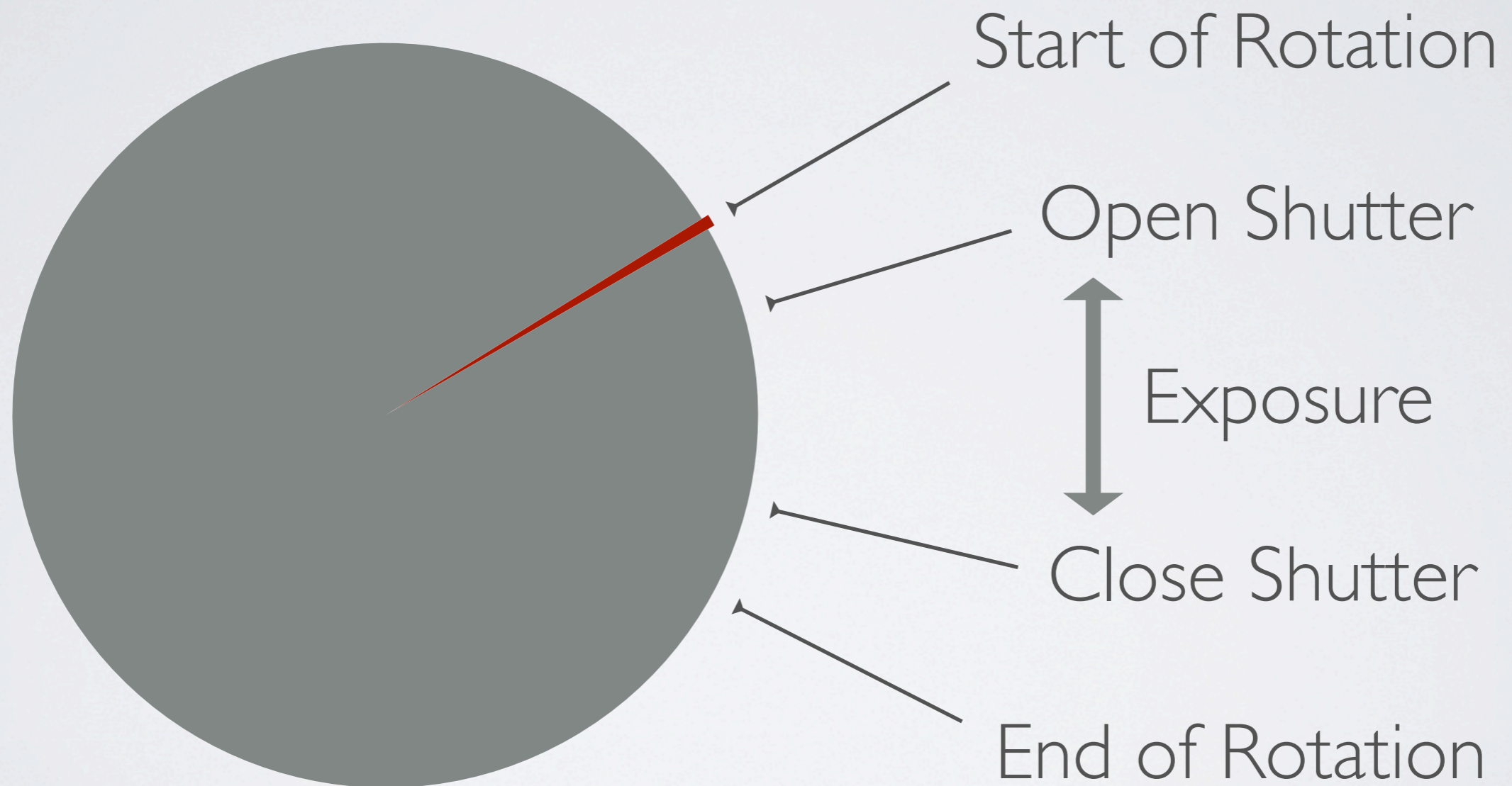
Detector

Sample

Shutter

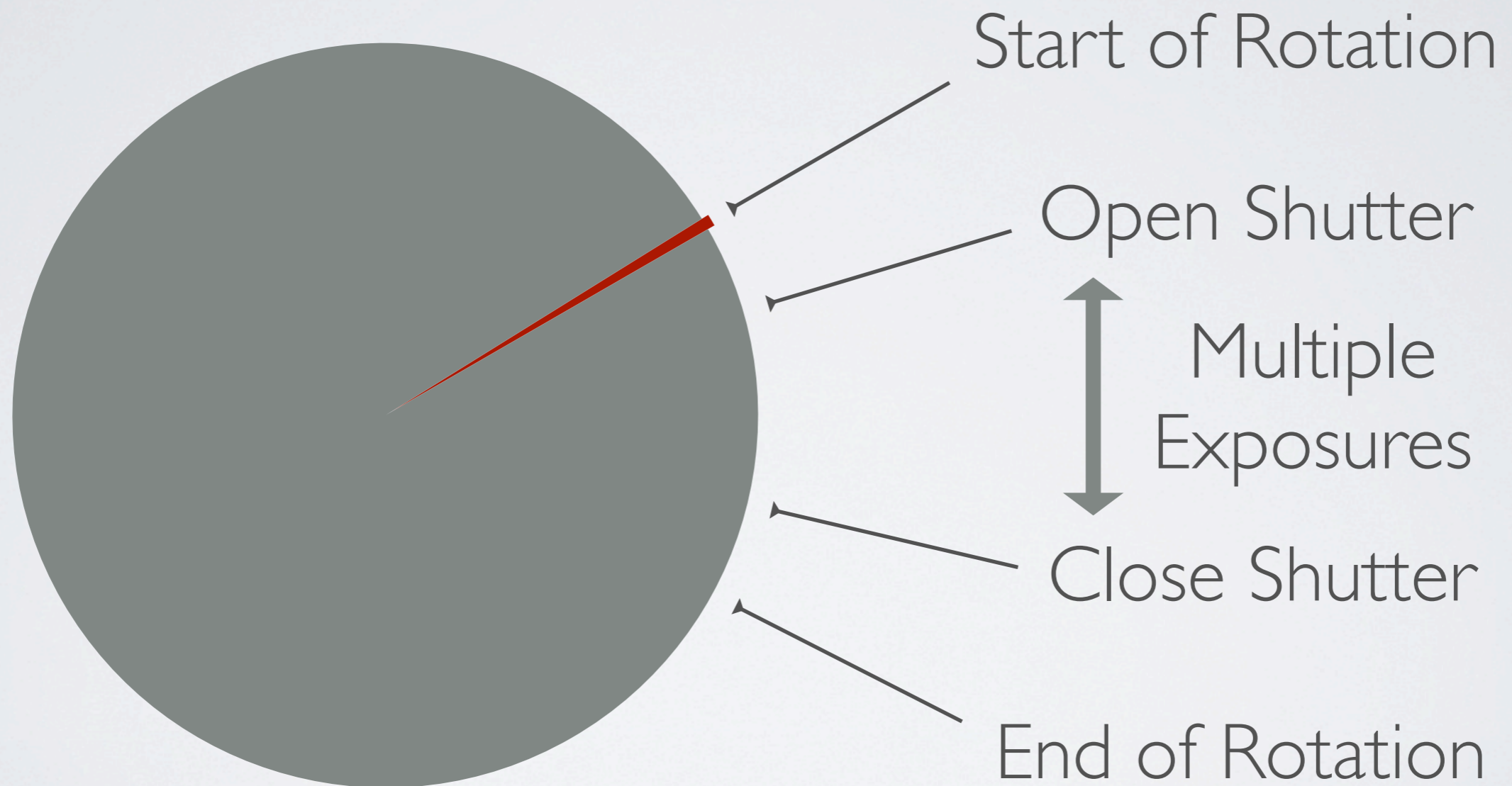
X-rays

# STEP-ROTATION

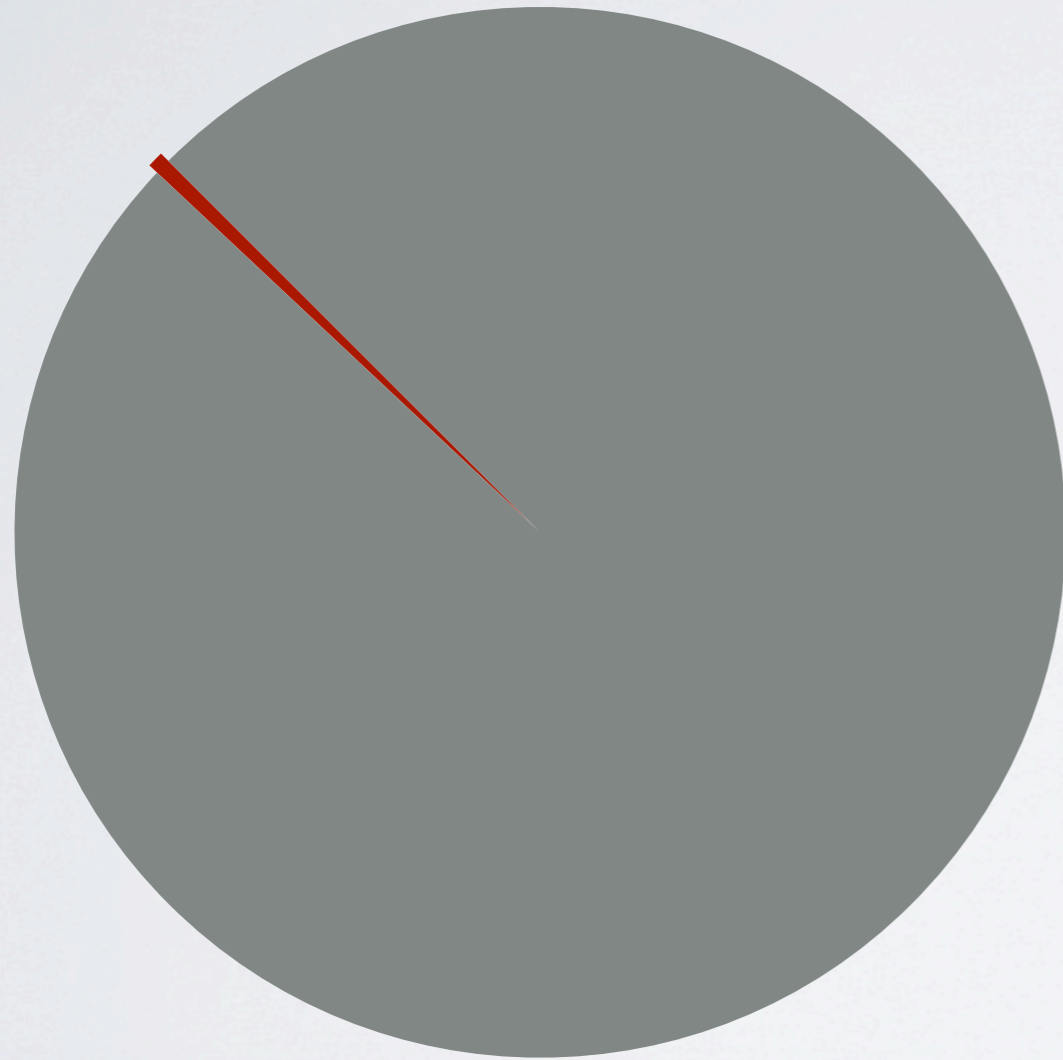




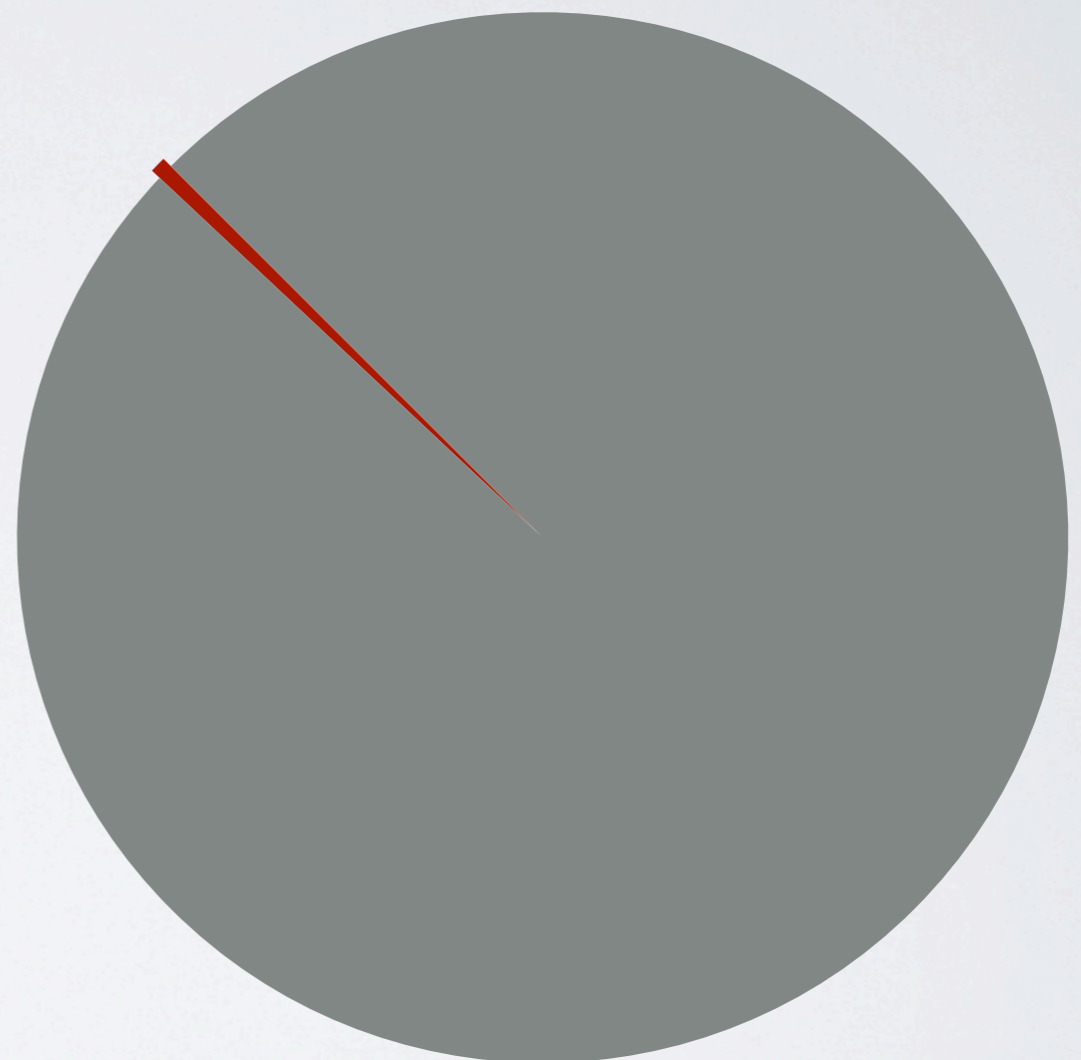
# CONTINUOUS-ROTATION



STEP



CONTINUOUS





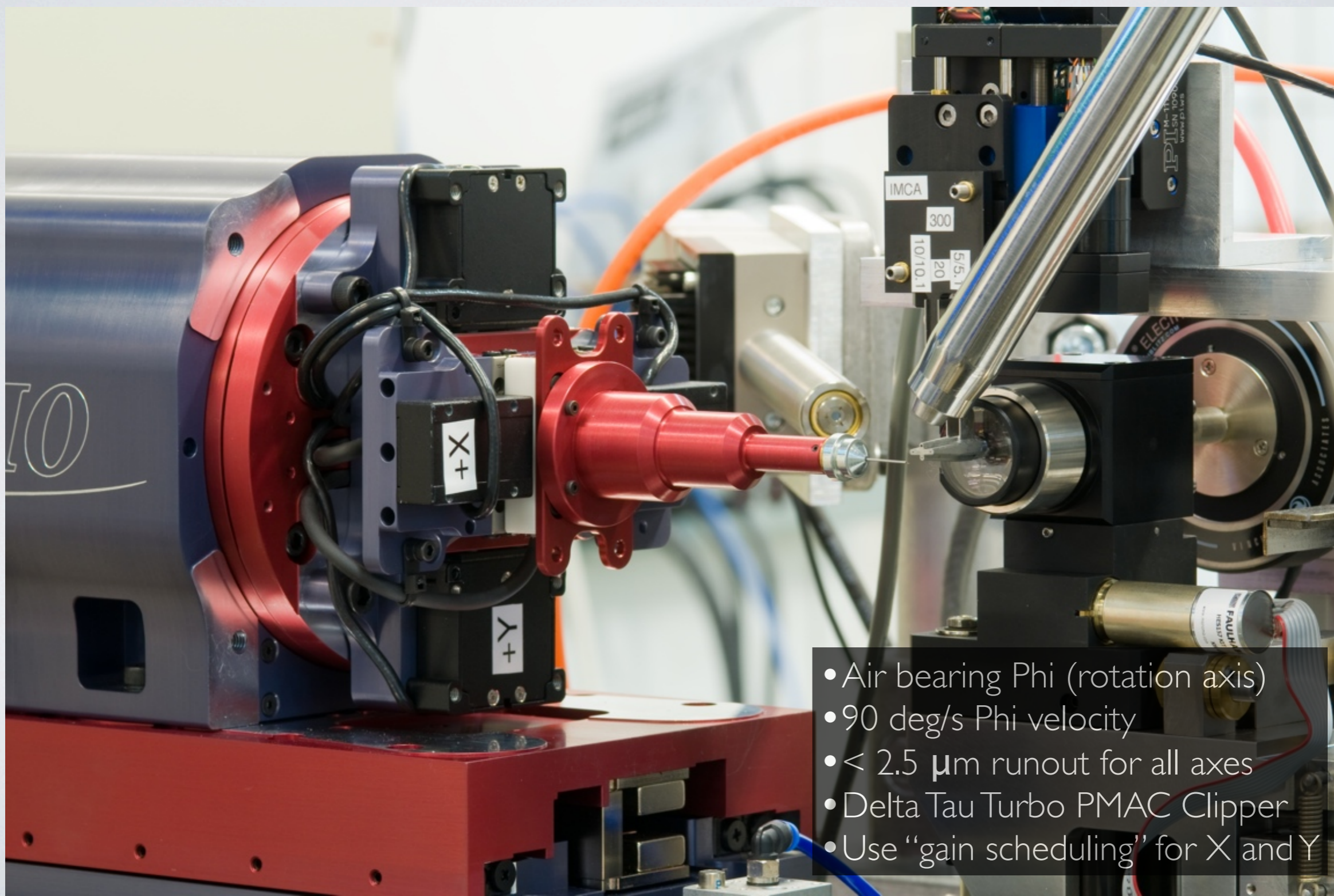
# DECTRIS PILATUS 6M



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



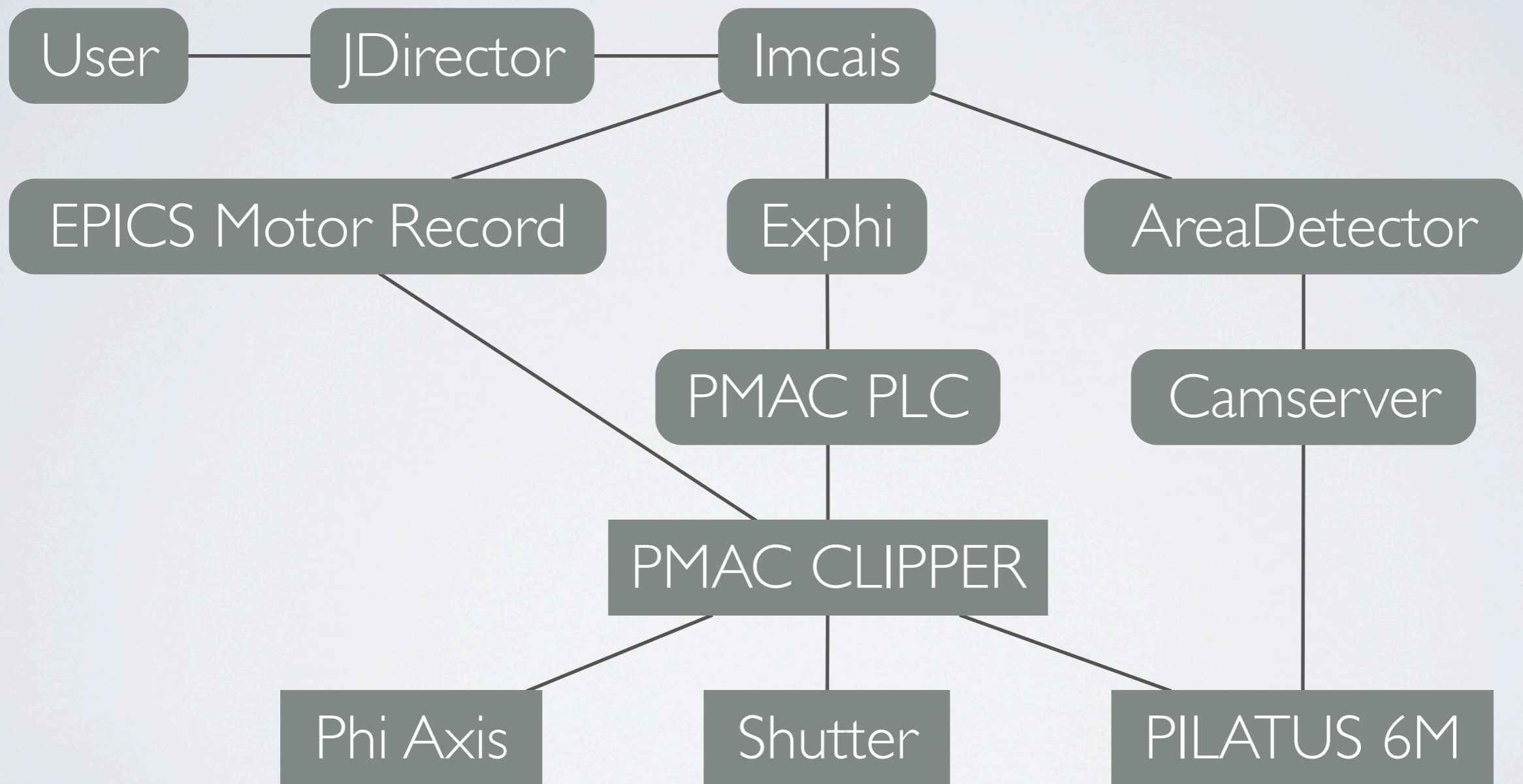
# ALIO GONIOMETER



- Air bearing Phi (rotation axis)
- 90 deg/s Phi velocity
- < 2.5  $\mu\text{m}$  runout for all axes
- Delta Tau Turbo PMAC Clipper
- Use “gain scheduling” for X and Y



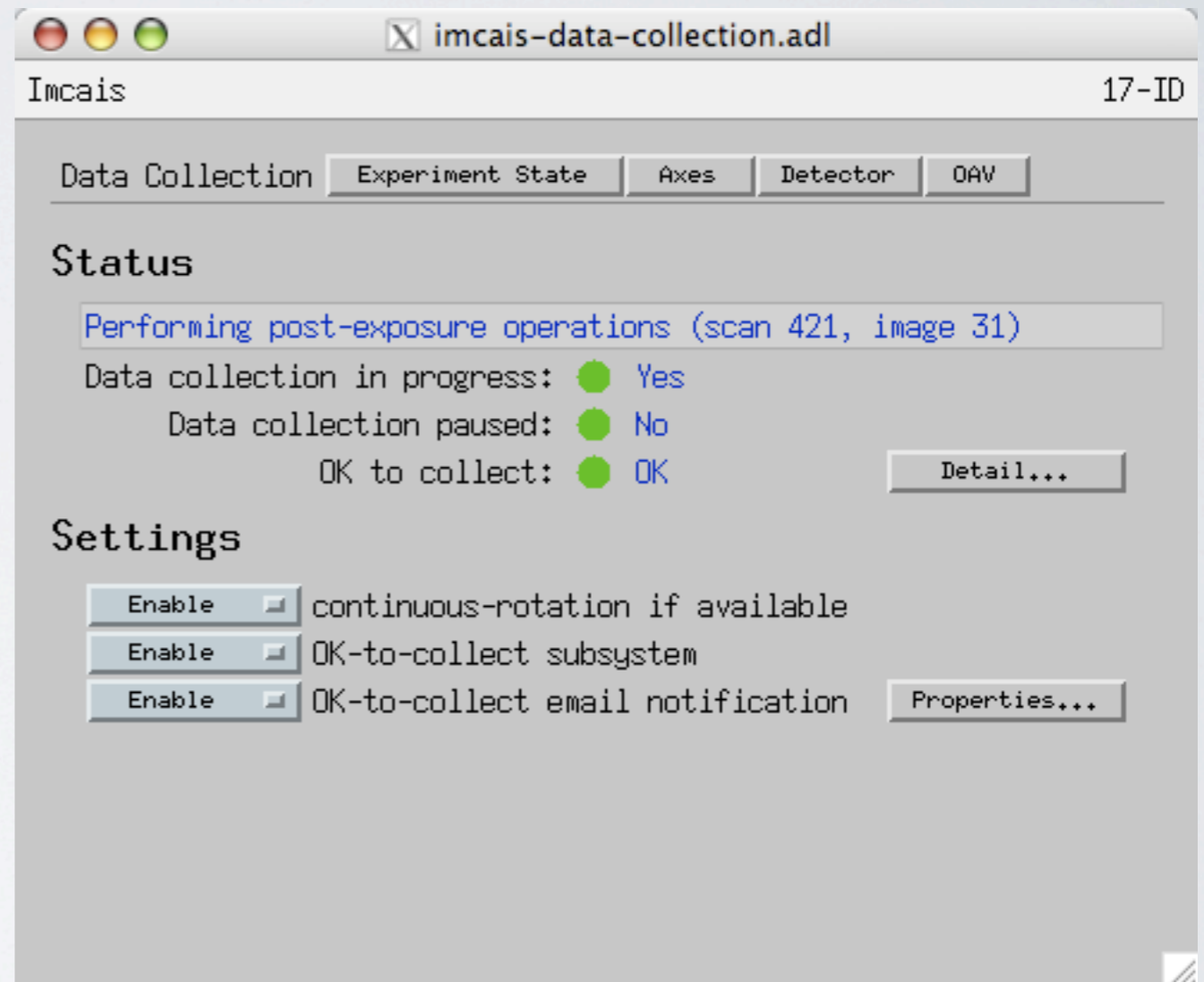
# IMPLEMENTATION





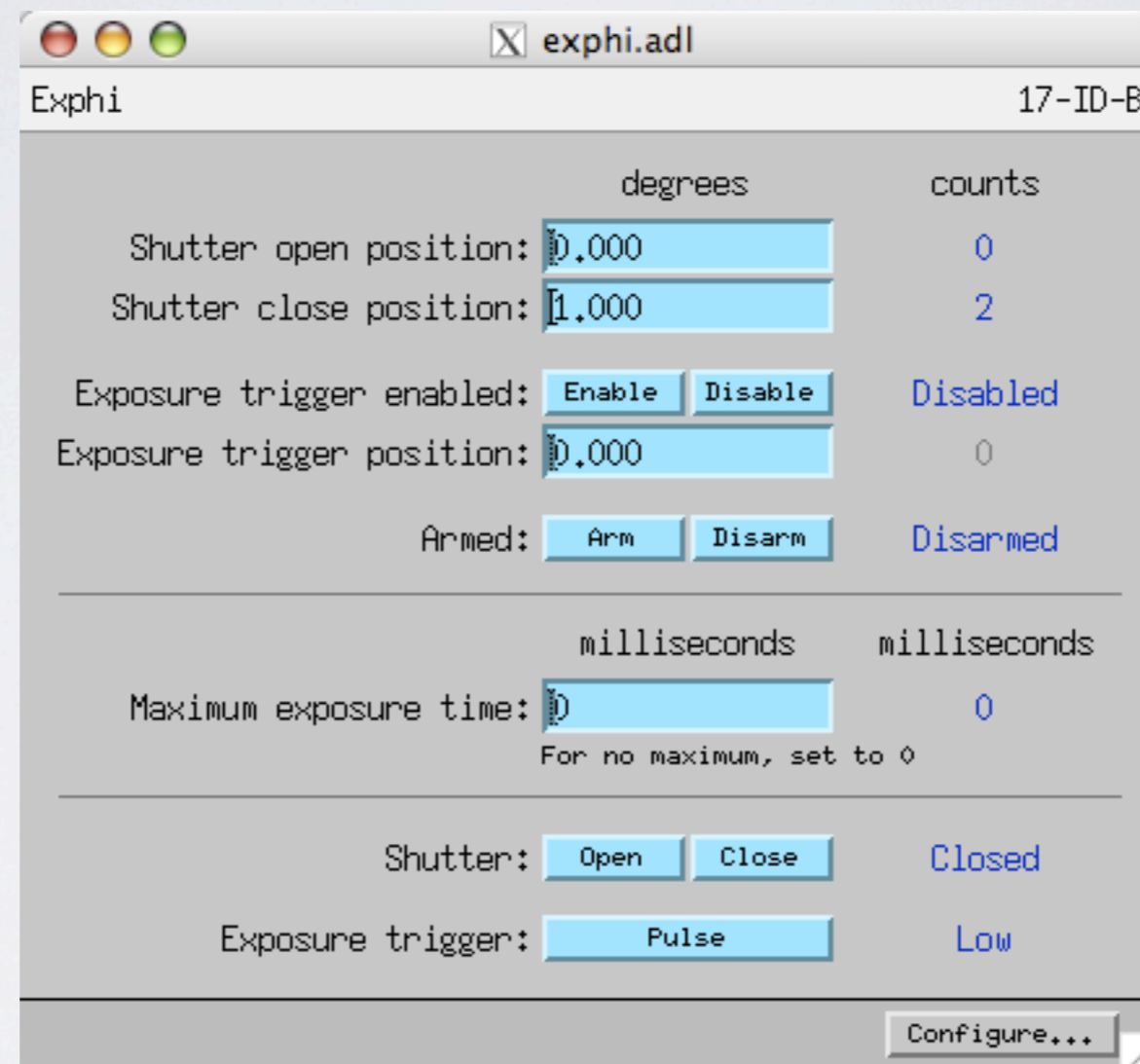
# Imcais

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





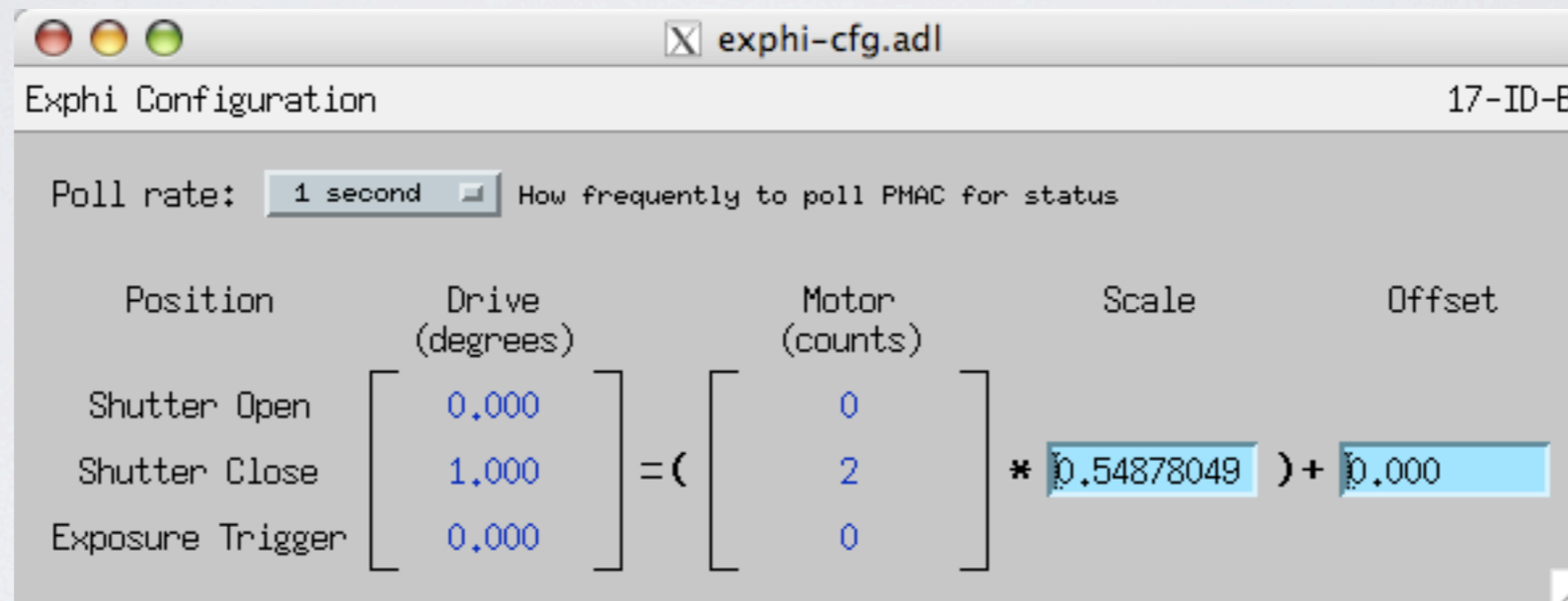
# Exphi



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



# Exphi



The screenshot shows a window titled "exphi-cfg.adl" with the subtitle "Exphi Configuration" and a version identifier "17-ID-B". The window contains a "Poll rate" dropdown menu set to "1 second" with the text "How frequently to poll PMAC for status". Below this is a table with five columns: "Position", "Drive (degrees)", "Motor (counts)", "Scale", and "Offset". The table lists three positions: "Shutter Open", "Shutter Close", and "Exposure Trigger". The "Shutter Close" row is highlighted, showing a drive of 1.000, a motor of 2, a scale of 0.54878049, and an offset of 0.000. The equation  $(2 * 0.54878049) + 0.000$  is displayed next to the motor and scale values.

Position	Drive (degrees)	Motor (counts)	Scale	Offset
Shutter Open	0.000	0		
Shutter Close	1.000	2	0.54878049	0.000
Exposure Trigger	0.000	0		

Equation:  $(2 * 0.54878049) + 0.000$

# 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

The screenshot shows the 'Pilatus Detector Control - x7PIL1:det1:' window. It is divided into several sections:

- Setup:** Shows configuration parameters: asyn port `PIL1`, EPICS name `x7PIL1:det1:`, Manufacturer `Dectris`, Model `Pilatus`. It indicates the device is **Connected** and provides `Connect` and `Disconnect` buttons, along with a `Debugging` checkbox.
- Shutter:** Shows `Shutter mode` set to `None`. Status: `Det. Closed` and `EPICS Closed`. Includes `Open/Close` buttons, `Delay: Open 0.000` and `Close 0.000` input fields, and an `EPICS shutter setup` button.
- Collect:** Shows acquisition parameters: `Exposure time 0.500 0.500`, `Acquire period 0.502 0.502`, `# Images 360 360`, `Delay time 0.000000 0.000000`, `# Exp./image 1 1`. `Trigger mode` is set to `Ext. Trigger`. Includes `Acquire Start` and `Stop` buttons, and an `Armed` status indicator.
- Detector:** Shows physical dimensions: `Detector Size X 2463 Y 2527`. `Threshold (keV): 7.439`. `Shaping time/Gain: Fast/Low`. `Read CBF/TIFF tmot: 20.000`.
- Attributes:** Includes a `File` input field.

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

# AreaDetector PILATUS Driver

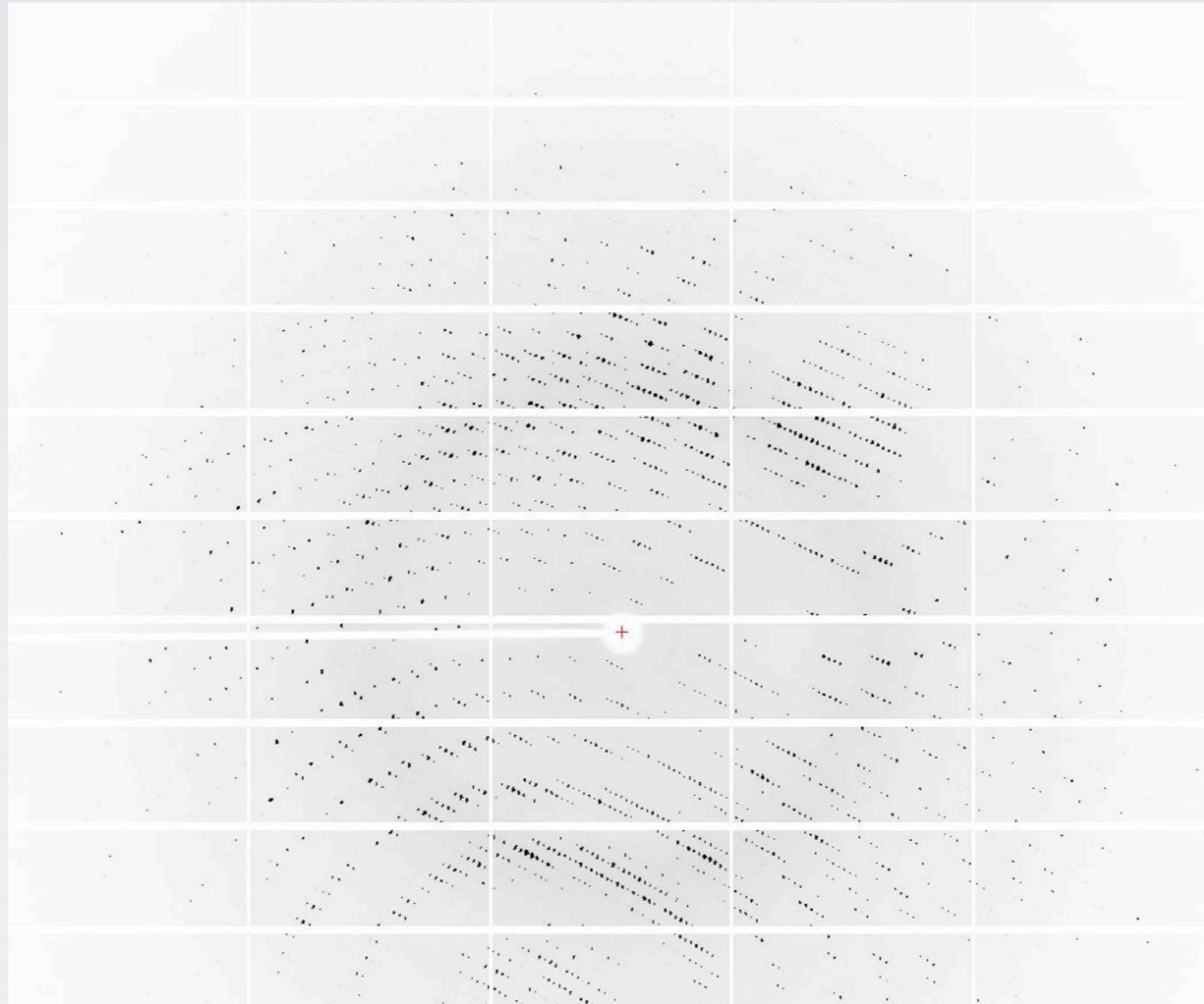
pilatusAncillary.adl

Pilatus Ancillary Information  
x7PIL1:det1:

Wavelength	<input type="text" value="1.5400"/>	Å
Energy range	<input type="text" value="0.000"/> , <input type="text" value="0.000"/>	eV (low,high)
Detector distance	<input type="text" value="450.000"/>	mm
Detector V_offset	<input type="text" value="0.000"/>	mm
Beam	<input type="text" value="1231.500"/> , <input type="text" value="1263.500"/>	pixels (X,Y)
Flux	<input type="text" value="0.0000"/>	ph/s
Filter transmission	<input type="text" value="0.0000"/>	
Start angle	<input type="text" value="0.0000"/>	deg
Angle increment	<input type="text" value="0.5000"/>	deg
Detector 2theta	<input type="text" value="0.0000"/>	deg
Polarization	<input type="text" value="0.9900"/>	
Alpha	<input type="text" value="0.0000"/>	deg
Kappa	<input type="text" value="0.0000"/>	deg
Phi	<input type="text" value="0.0000"/>	deg
Chi	<input type="text" value="0.0000"/>	deg
Oscillation axis	<input type="text" value="K, CW"/>	
Number of oscillations	<input type="text" value="1"/>	



# 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

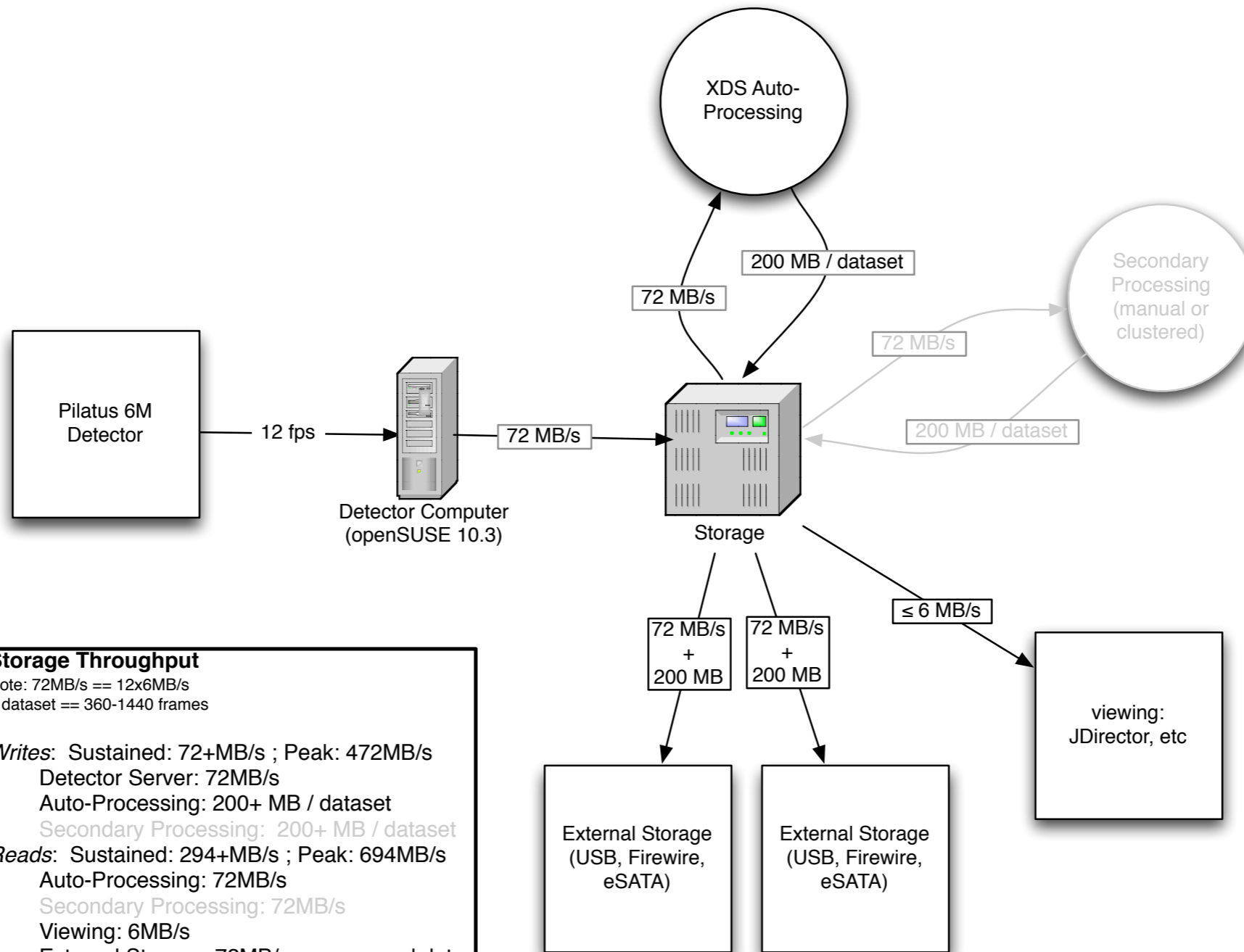
- Fast and Reliable Storage
- Fast Network
- Fast Workstations

# 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

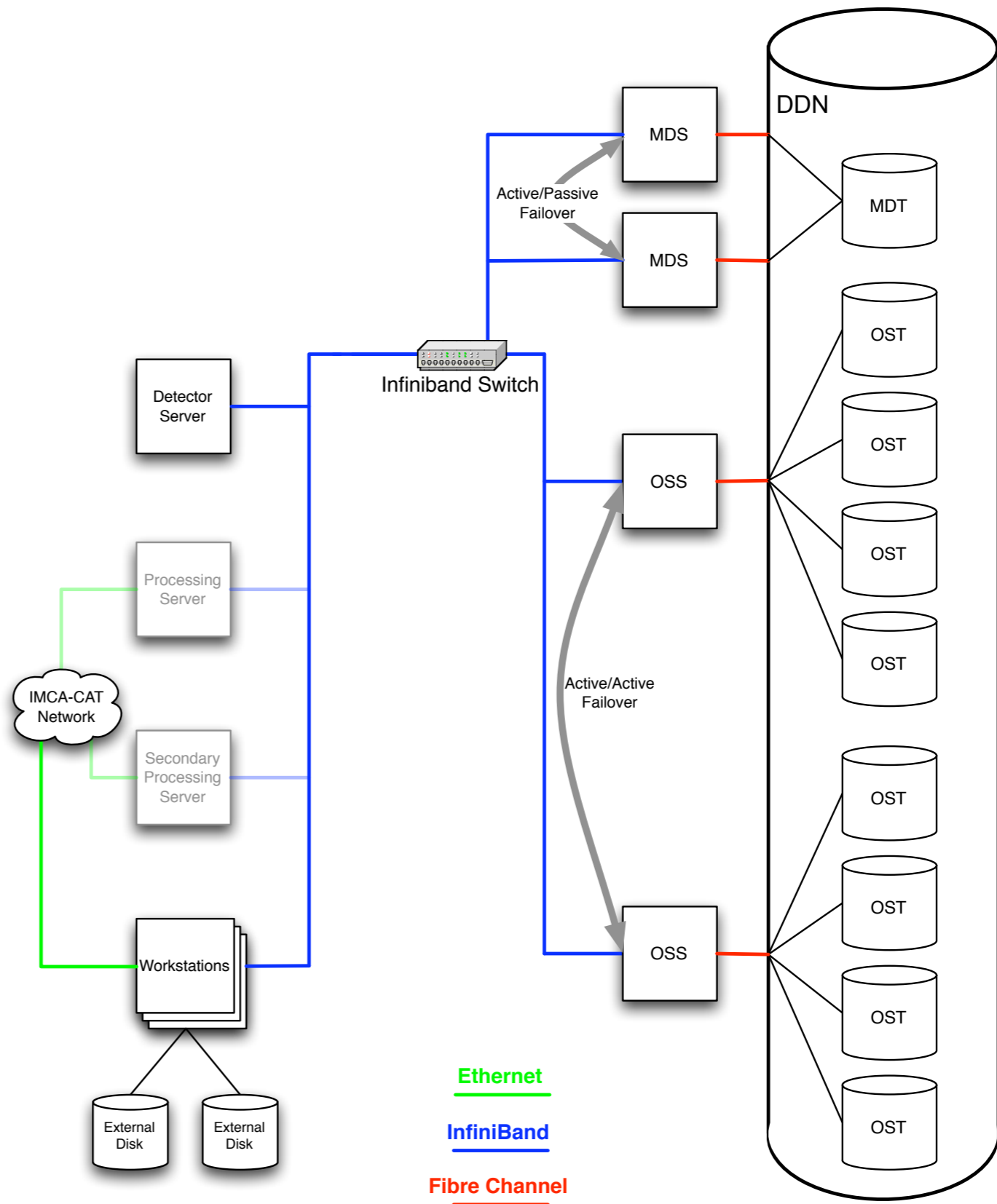
## DataDirect Networks S2A6620

- 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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