



PILATUS: A 2-Dimensional X-Ray Detector For Macromolecular Crystallography

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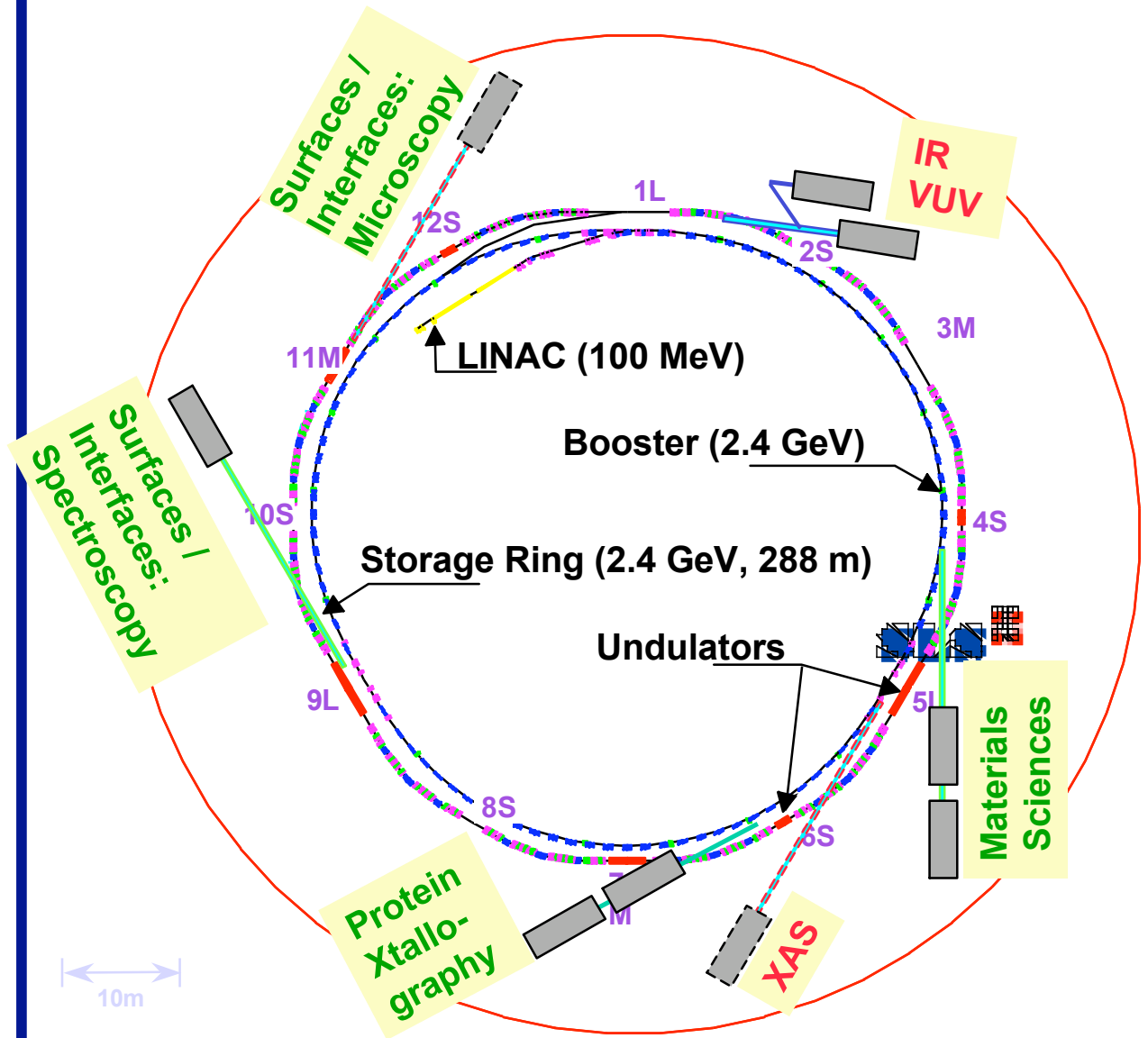
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³ *CMS-Project, Paul Scherrer Institut, CH-5232 Villigen-PSI*



SLS Layout



Green: first phase beamlines

Red: proposed beamlines

Data collection in protein crystallography

Spot size:

- Beam divergence
- Mosaicity of the crystal
- Distance sample-detector
- Point spread function of detector

Crystal rotation

- 30-180 degree for complete data set
- Currently: Discrete rotation, integration over certain rotation angle
- Future: Continuous rotation, integration determined by detector frame rate (**Fine phi slicing**)

Crystallized Protein

Beam

Beam

Energy: 5-17.5 keV
Intensity: ~10/s
Focal spot size: Adjustable to 25 x 15 μm
Divergency: 150 μrad x 28 μrad (FWHM)

Diffraction data

- reflect crystal symmetry group
- orientation of the crystal \rightarrow orientation matrix
- High dynamic range: >10 between strong and weak reflections
- Intensities need to be determined accurately (1%)
- Determination of amplitudes and phases leads to electron density maps

Resolution:

$$2d \cdot \sin(\theta) = \lambda$$

For $d=1\text{\AA}$ and $\theta=60^\circ$

Diffacted beam

X-ray Detector

Diffraction pattern

Detector requirements;

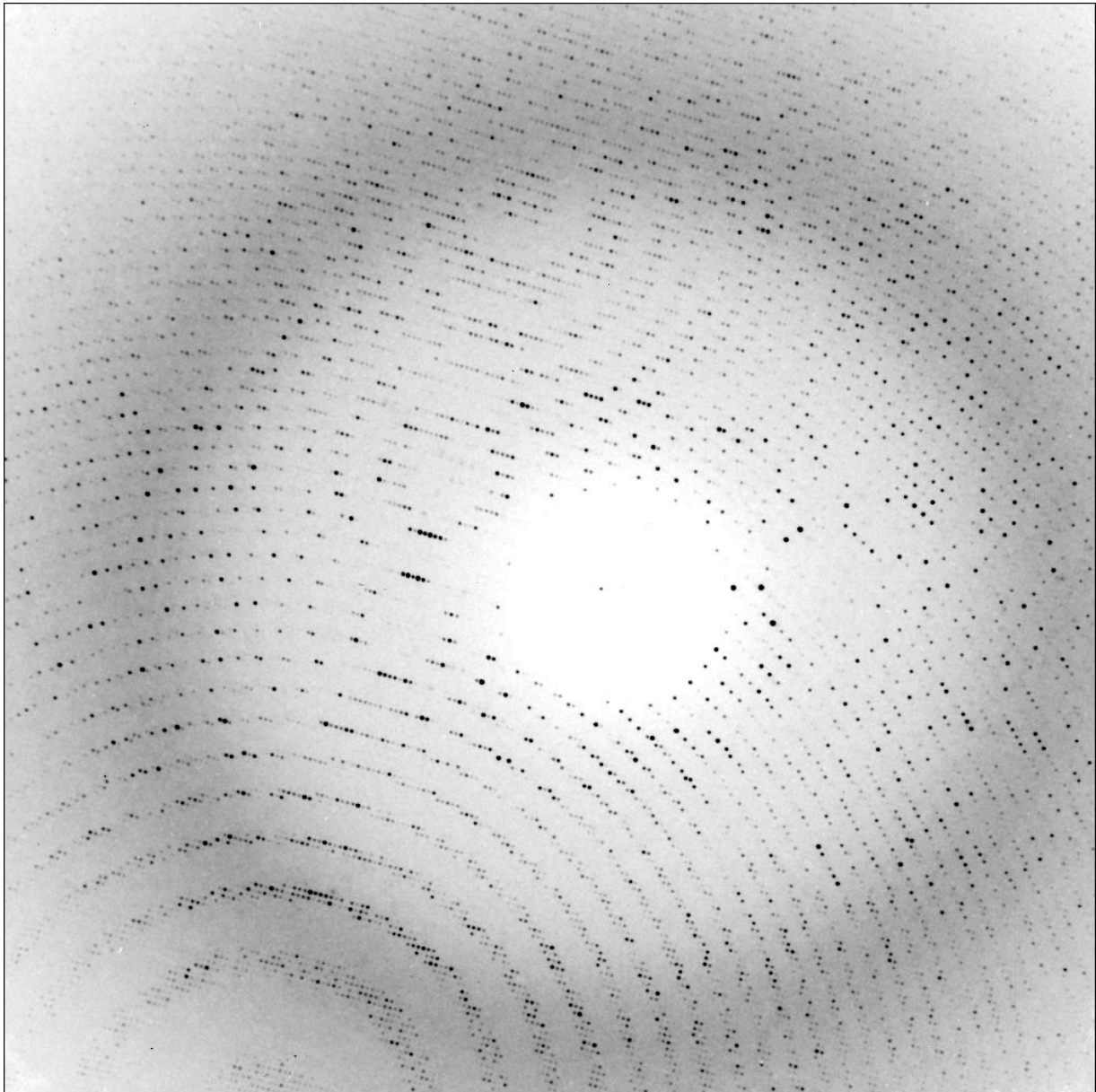
- Large area (40 x 40 cm) and/or large number of pixels
- Detect a high number of reflection orders (>500)
- Accurate determination of integrated intensities
- Wide dynamic range (>16 bit, i.e. single photon counting detector)
- Fast readout (<0.1s)



Pixel Detectors



X-Ray Diffraction From A \square X-174 Virus Crystal





Macromolecular Crystallography

Determine the structure of highly complex molecules to atomic resolution

Molecular Weight > 1 MDa
(> 50,000 atoms)

Applications:

Enzymes

Viruses

Catalytic mechanisms

Electron transport

Energy transduction

Motility

Drug Design

Structural genomics



The SLS Pixel Detector

& Size: 40 x 40 cm² (0.16m²)

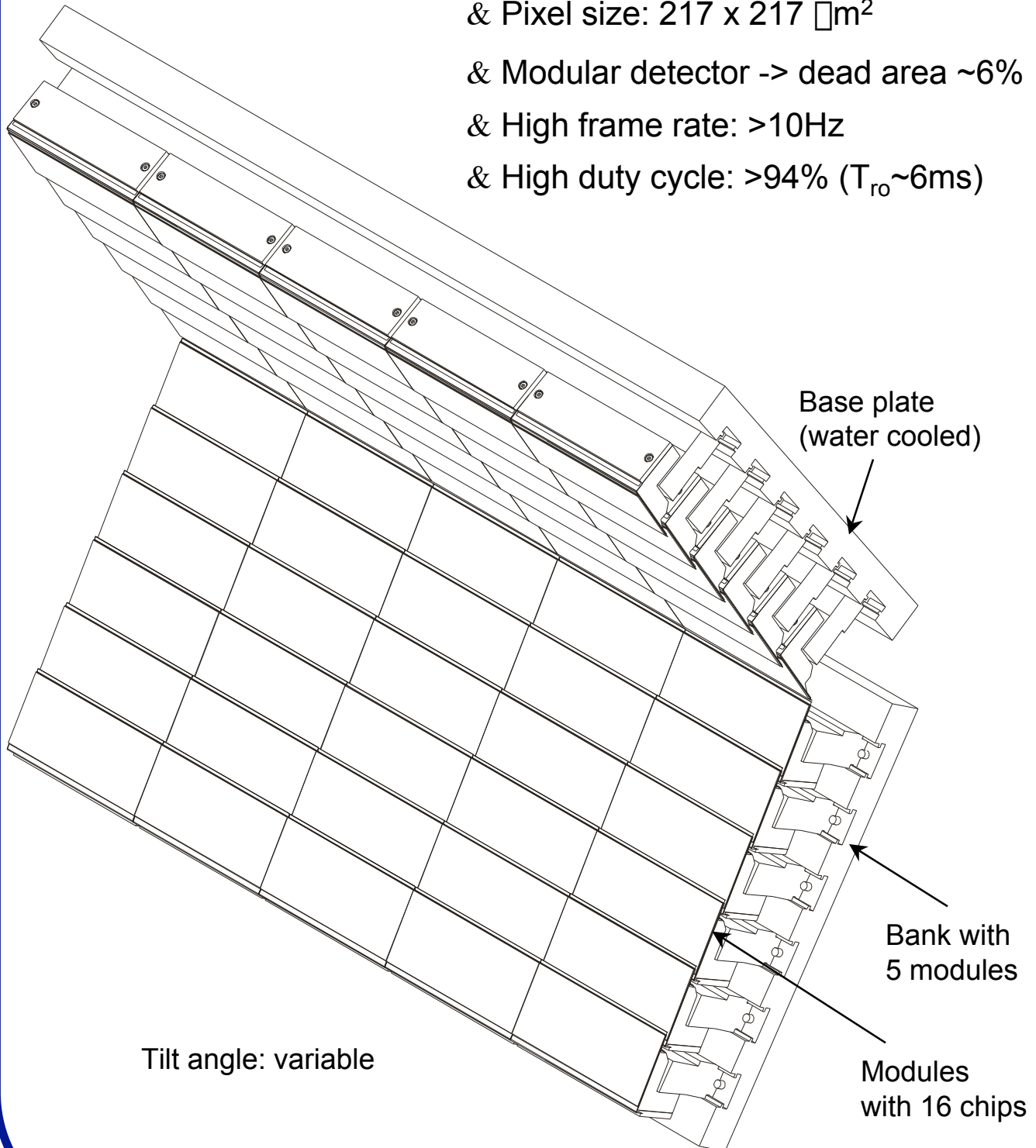
& 2000 x 2000 pixels

& Pixel size: 217 x 217 μ m²

& Modular detector -> dead area ~6%

& High frame rate: >10Hz

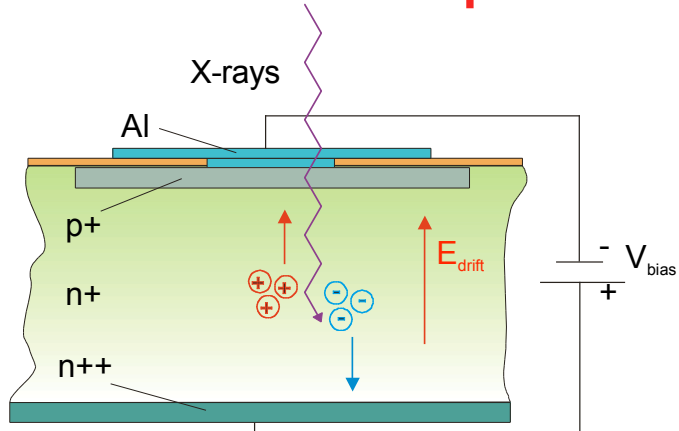
& High duty cycle: >94% (T_{ro} ~6ms)



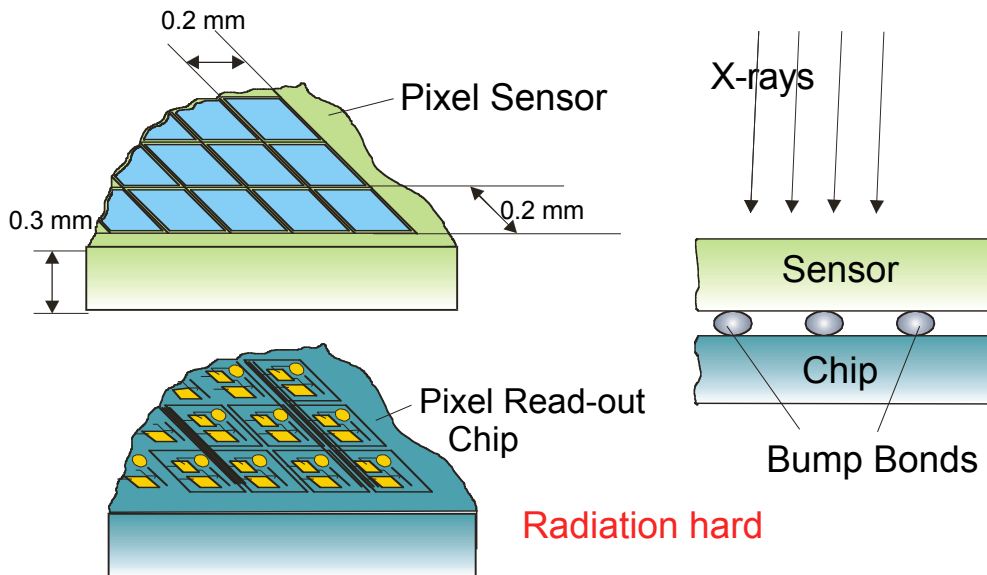
Pixel Detectors: Principle

Si pn-junction

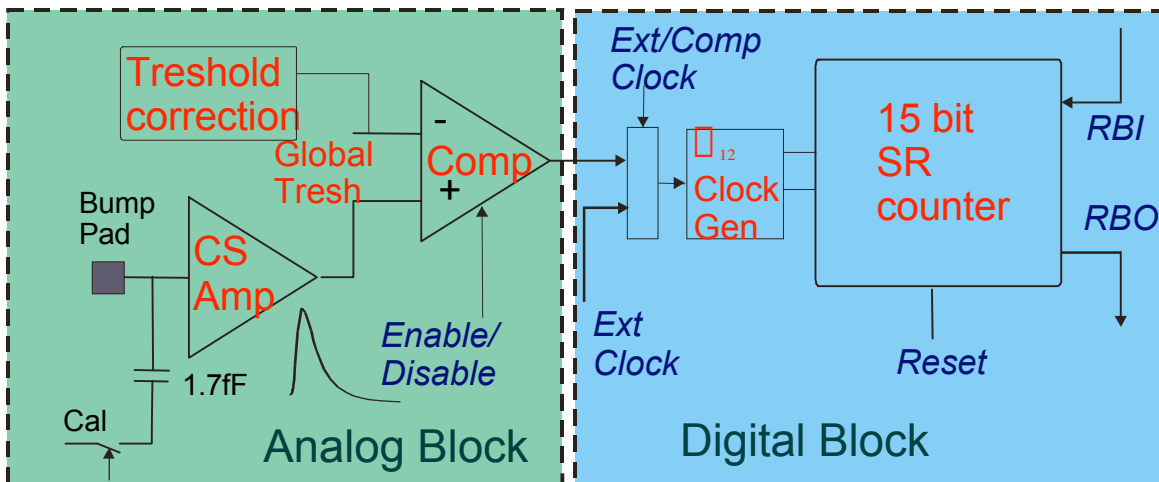
3.6 eV to create
1 eh-pair



Detector



Pixel electronics



Please see landscape-oriented supplement:

Slide 8: Bump-bonded Module

Slide 9: PILATUS Module

Slide 10: Final Module Assembly

Slide 11: Bank With 3 Modules

Slide 12: Module Fabrication

Slide 15: Flat-field Correction

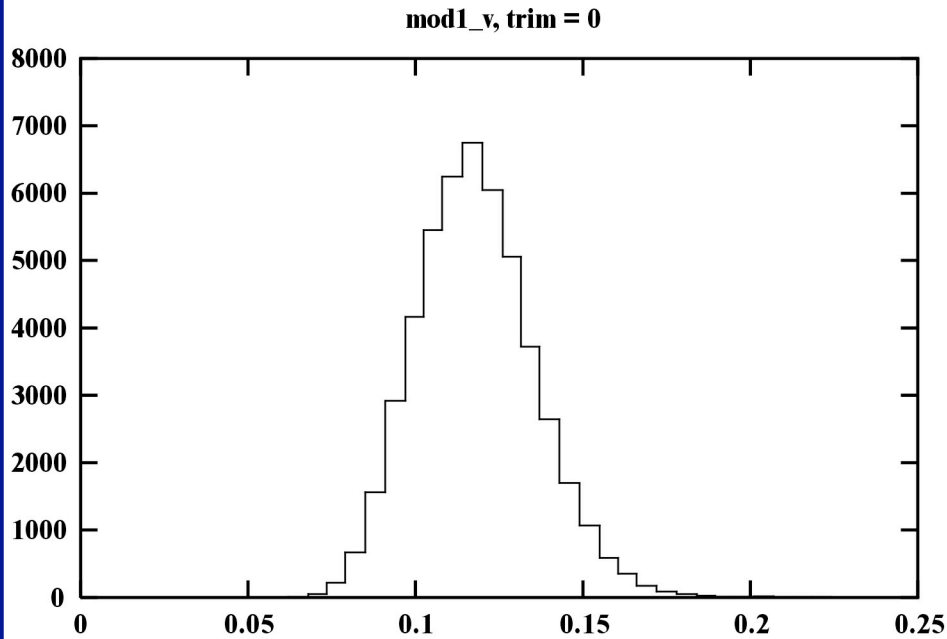
Slide 18: Continuous Fine μ -Slicing

Slide 19: Lysozyme: MOSFLM Autoindex

Slide 20: Lysozyme: MOSFLM Refined Cell



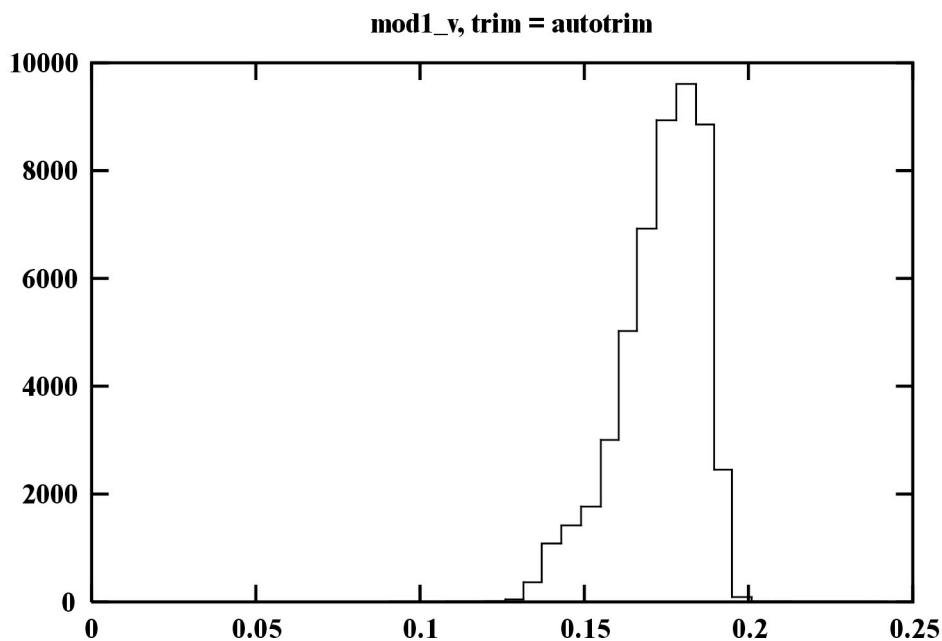
Trimming A Module With A Global Vcmp



N pixels = 49641

Avg. threshold = 1120 e-

RMS = 181 e-



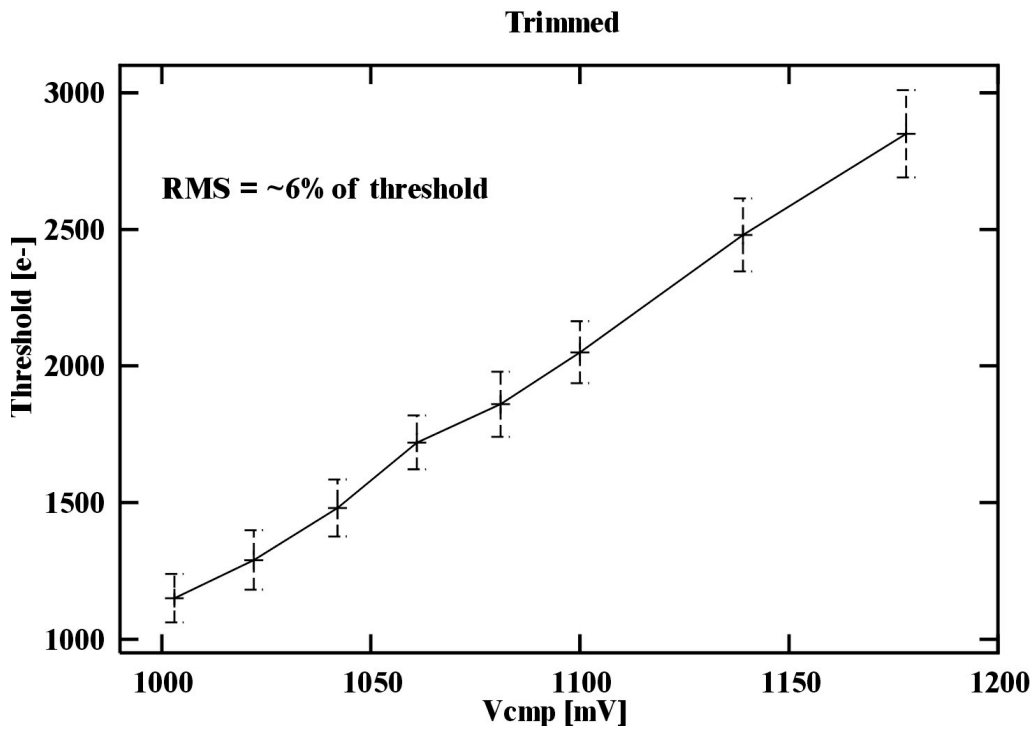
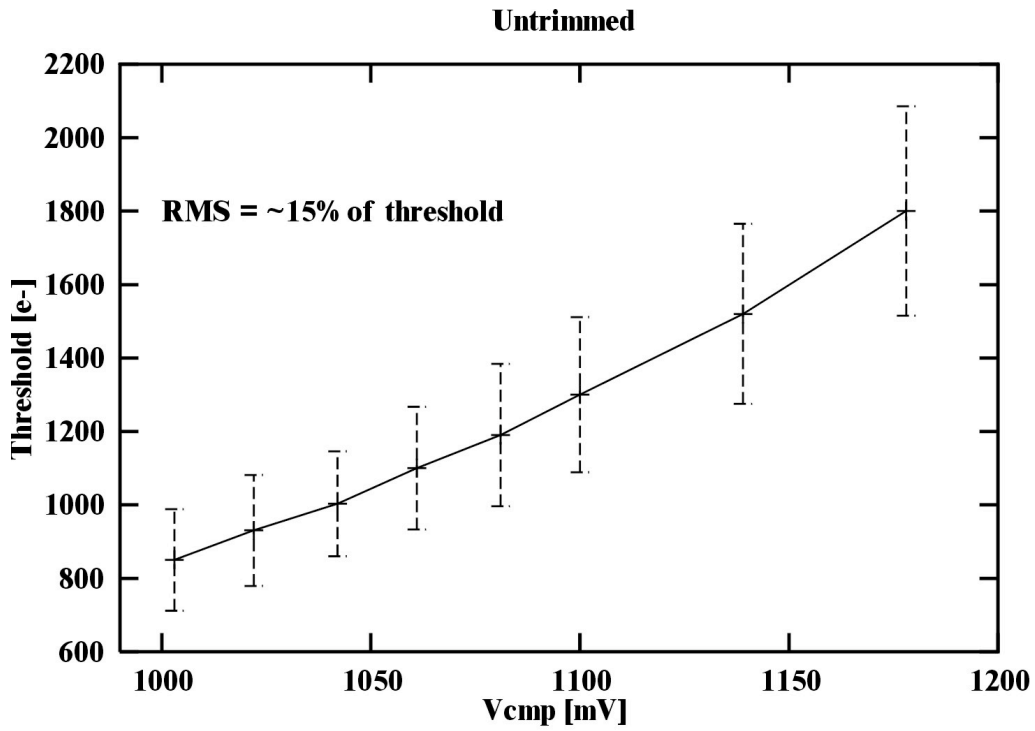
Trim target = 1800 e-

Avg. threshold = 1680 e-

RMS = 132 e-

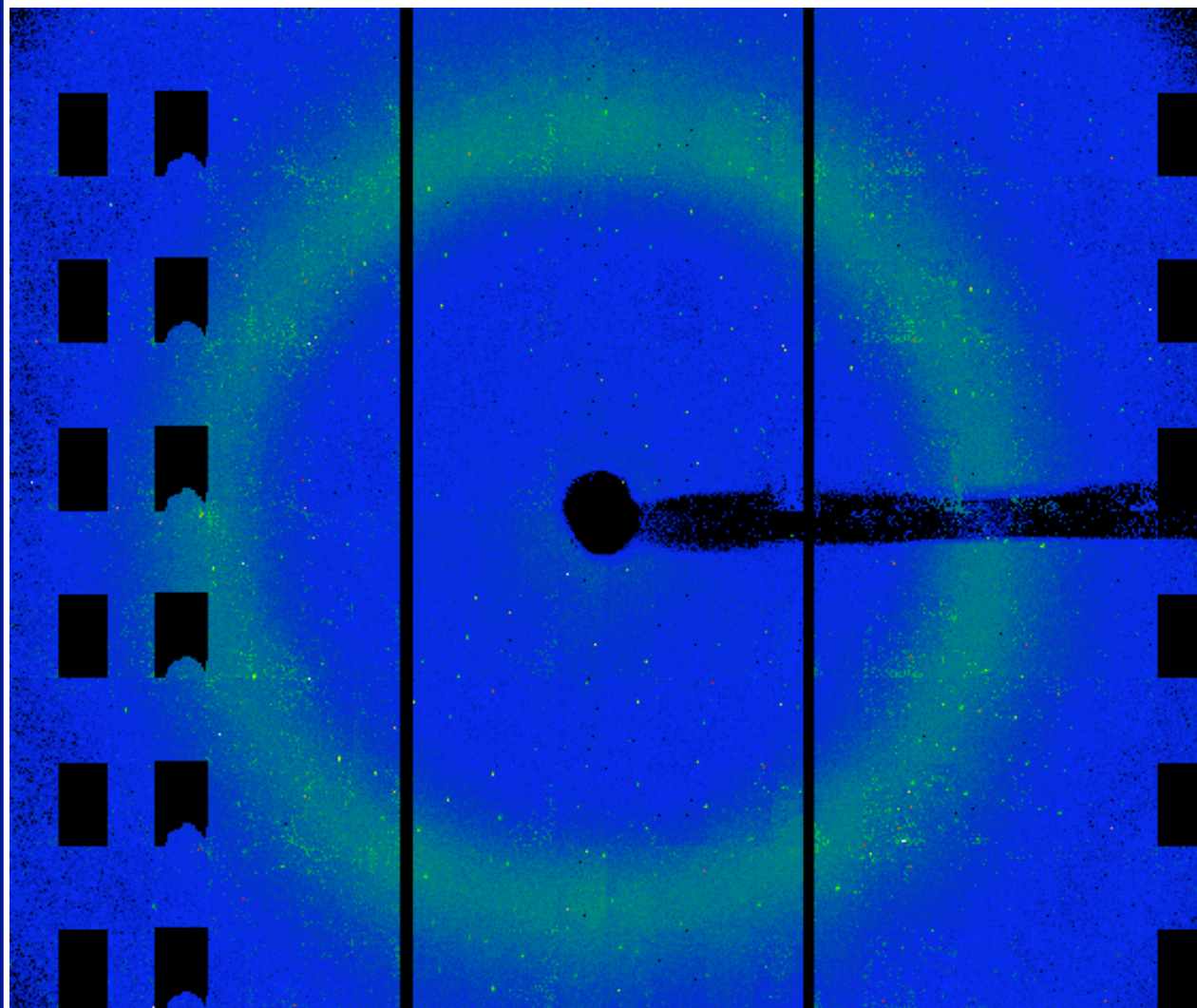


Threshold vs. V_{cmp}





PILATUS Detector Crystallography



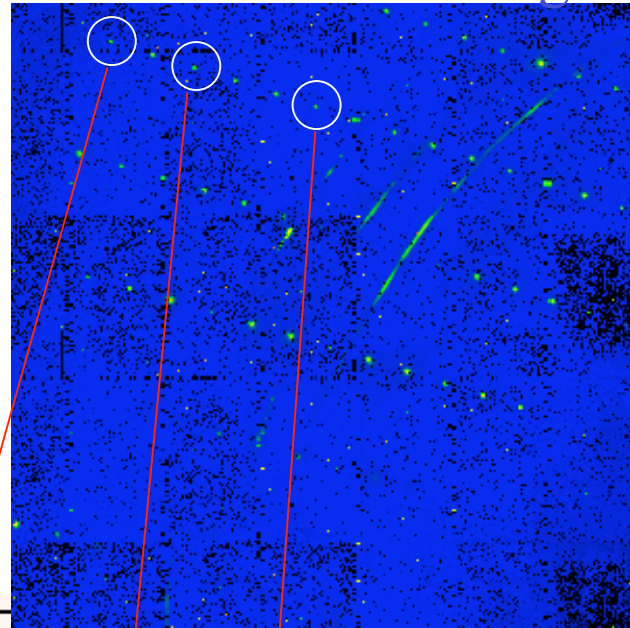
Lysozyme
1° rotation
2 s exposure



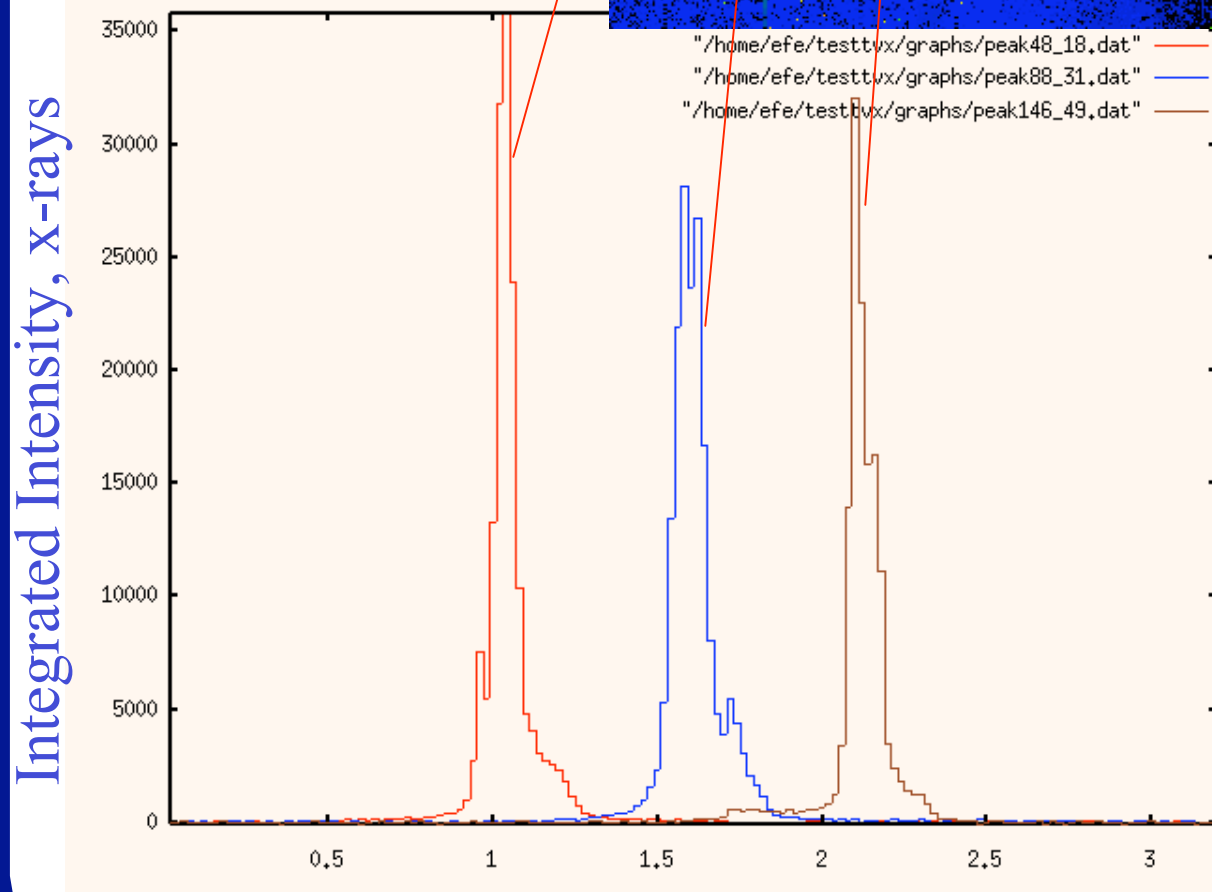
Fine Δ -Slicing with PILATUS



1.5° Rotation Image



Lysozyme:
0.02° steps
0.5 s exposure
FWHM:
0.06° - 0.10°





SLS 2k 2k Pixel Detector

PIXEL:

217 \times 217 μm^2

Preamplifier and shaper

Threshold discriminator with 4-bit trim

15-bit counter

$>10^5$ x-ray/s

CHIP:

CMOS 0.8 μm DMILL rad-hard

Designed at PSI

44 \times 78 pixels, 9.9 \times 18.3 mm²

Read out at 10 MHz

MODULE:

Fully depleted diode array



81 \times 36.6 mm² \times 300 μm , 57,462 pixels

Indium bump-bonded to 16 chips

Chips read out in parallel (5 ms)

Module control board

BANK:

5 modules

Bank control board caches data

DETECTOR:

12 banks

Adjustable V-shape

With fine-slicing, a 180° rotation may produce
2000 8 MB images (16 GB) in ~3 min.