DECTRIS

Next Generation X-Ray Detectors

Crystallographic data analysis with single photon counting pixel detectors

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www.dectris.com

Content

- Introduction
- Sensor and module
- Counting-> Pilatus3
- Fine phi slicing
- Other problems
- Conclusions

Mission

DECTRIS develops, produces and delivers outstanding X-ray detectors to industrial and scientific customers all over the world.

Our products enable you to focus on measurements and science.

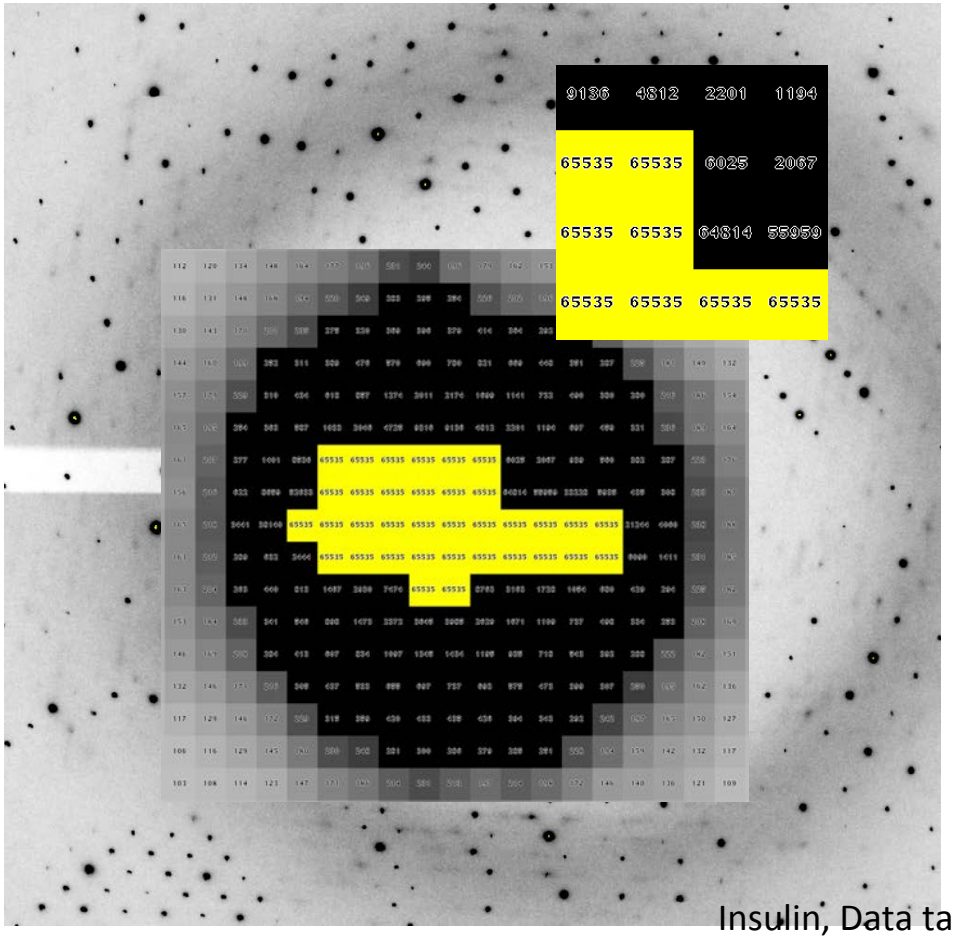
We deliver best possible data

We want our customers to reach the summits!

Dynamic Range and Point Spread Function

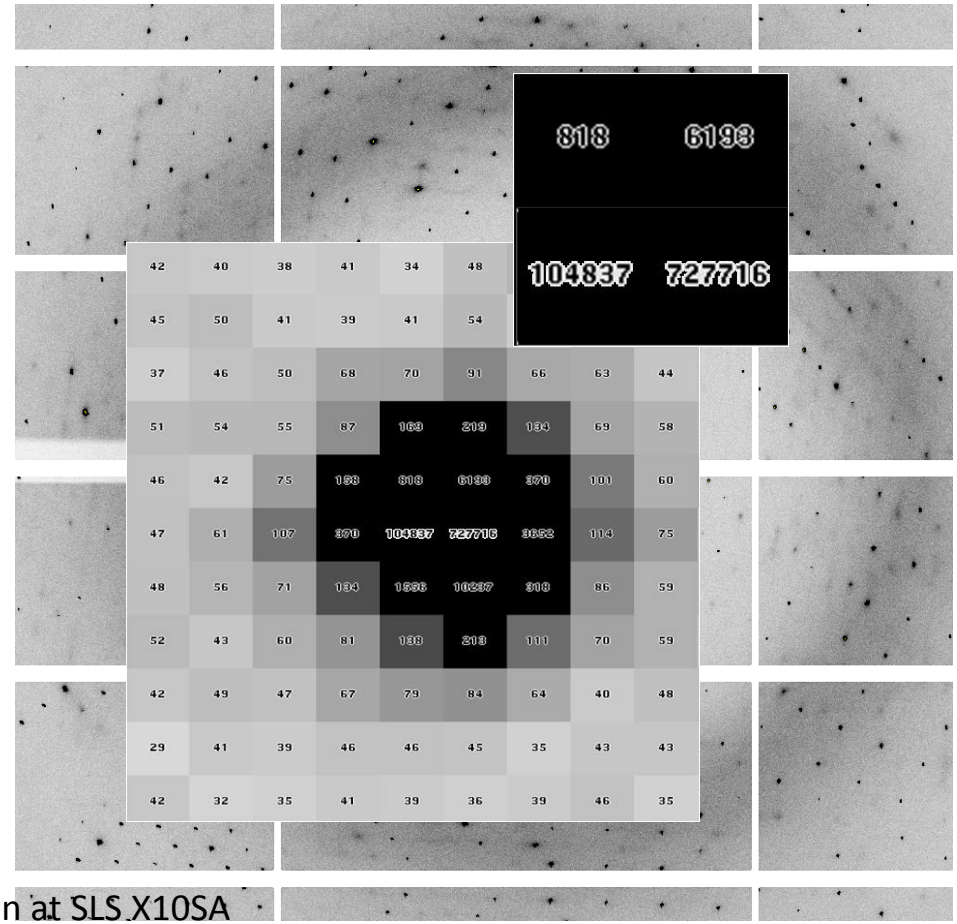
CCD

16 bit (65 535 ADU)



PILATUS

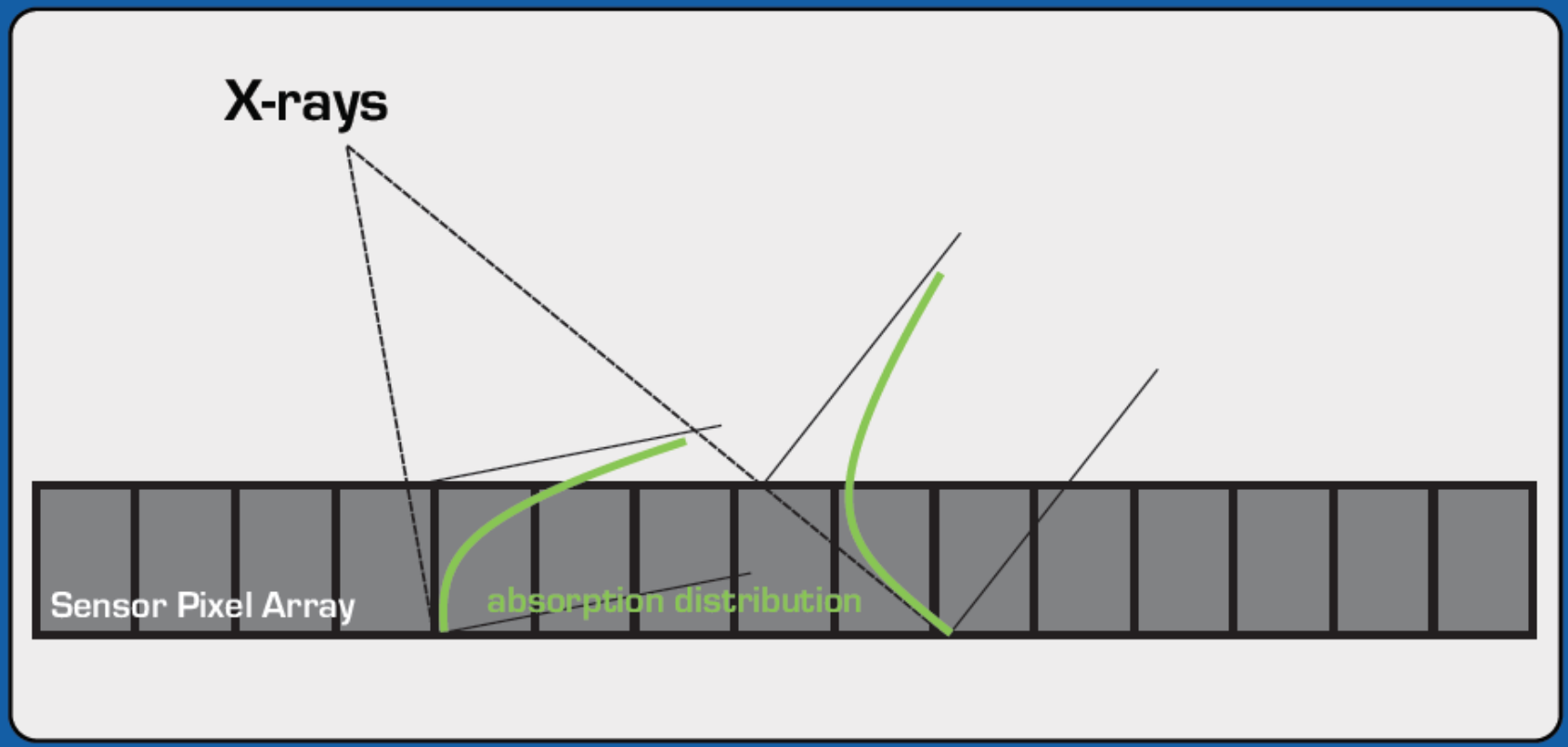
20 bit (1 048 575 counts)



Insulin, Data taken at SLS X10SA

Finite Sensor Thickness

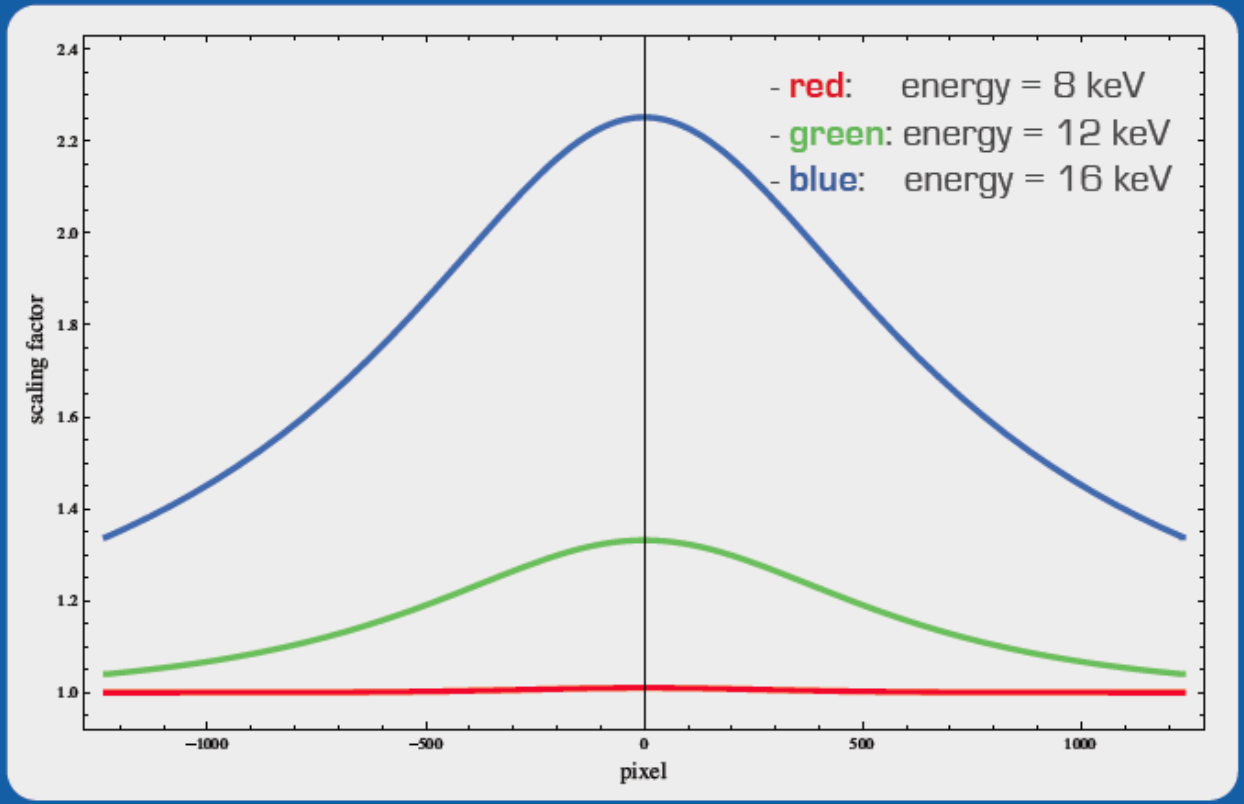
X-rays impacting at oblique angles have different path lengths in the silicon sensor
→ Probability for x-ray absorption increases towards larger 2θ!



Efficiency Correction

$$E_{Si} = \frac{1}{1 - \exp\left[-\mu_{Si} * \frac{t_{Si}}{\cos[2\theta]}\right]}$$

μ_{Si} : linear mass attenuation coefficient of Si [1/mm]
t_{Si}: thickness of the silicon sensor [mm]
2θ: diffraction angle [deg]

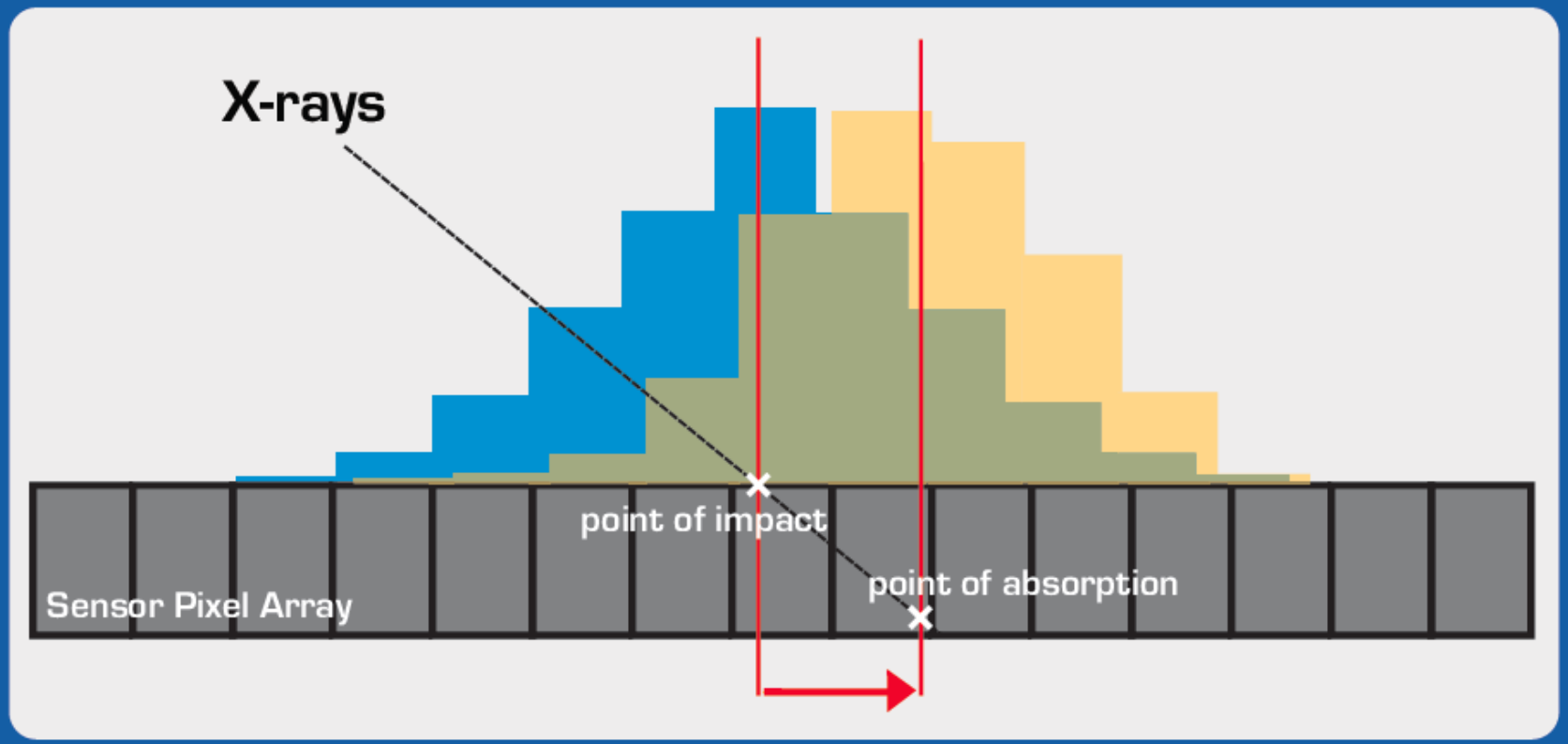


Parallax Correction

X-rays impacting at oblique angles have different path lengths in the silicon sensor

→ Increasing shift of the spot centroids towards larger 2θ!

→ Asymmetric broadening of the peak profiles towards larger 2θ!



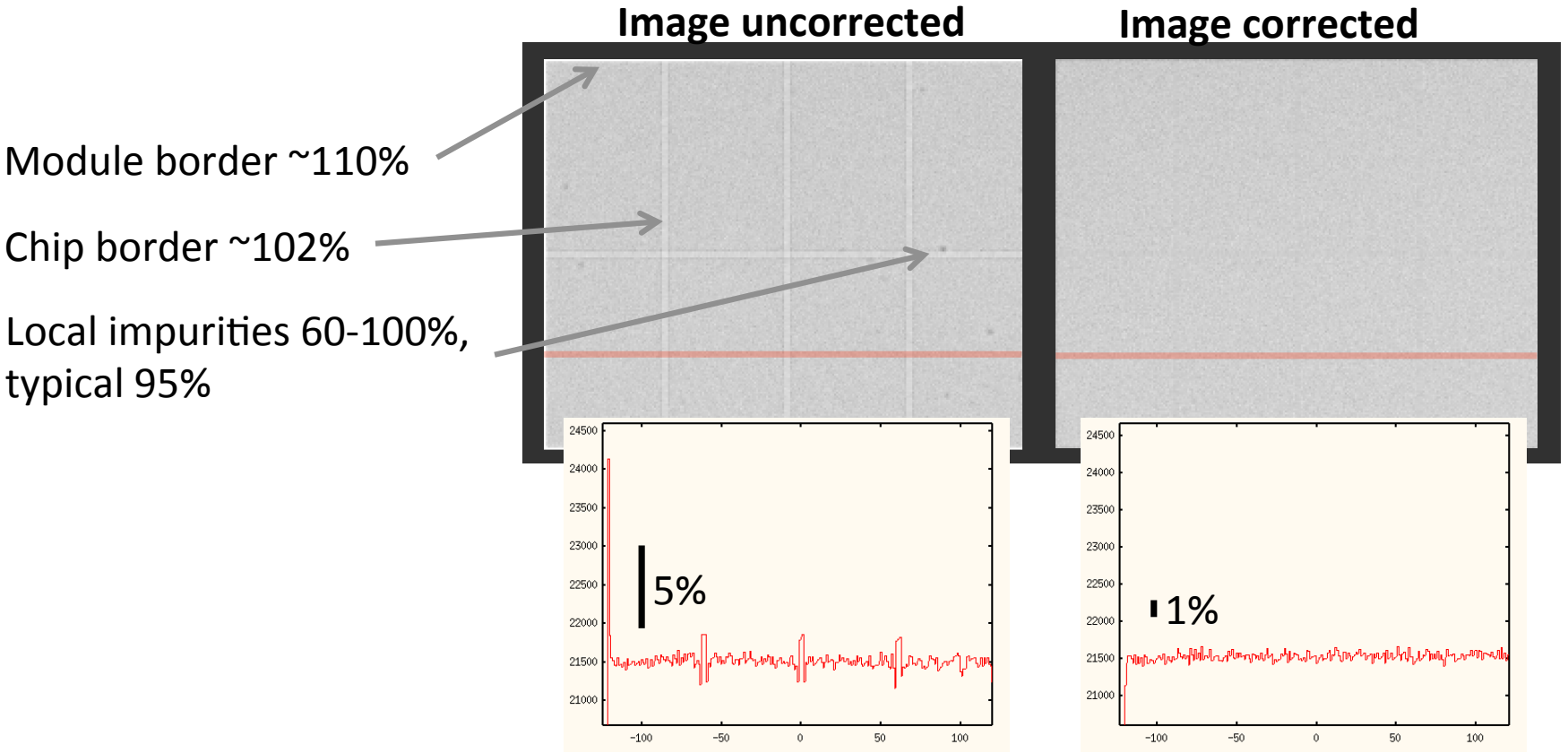
Geometrical Distortions

- Module Positional Error: σ: 0.25 pixel
  max: 0.8 pixel
- Module Angular Error: < 1 mrad
- Lithography errors: < 1 micron

- Module units geometrically perfect
  - No correlations across module
- Refine module positions from diffraction data but fix positional error within module
- Program should make use of processing history

Flat field correction

Intensity variations can be compensated with a flat field



Flatfield

XSCALE.LP - /sls/X06SA/Data10-staff/e11206/BLstartup/20111201/2/GO_insulin_ff_off_mask_on/xscale/ <@x06da-cn-1>

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SUBSET OF INTENSITY DATA WITH SIGNAL/NOISE >= -3.0 AS FUNCTION OF RESOLUTION

RESOLUTION LIMIT	NUMBER OF REFLECTIONS OBSERVED	UNIQUE	POSSIBLE	COMPLETENESS OF DATA	R-FACTOR observed	R-FACTOR COMPARED expected	I/SIGMA	R-meas	Rmrgd-F	Anomal Corr	SigAno
10.00	161	48	54	88.9%	1.3%	1.4%	153	79.59	1.6%	0.8%	41%	0.967
6.00	649	169	171	98.8%	1.2%	1.5%	634	80.12	1.4%	0.9%	8%	0.946
5.00	613	150	151	99.3%	1.3%	1.5%	605	87.12	1.4%	0.9%	54%	1.082
4.00	1241	342	345	99.1%	1.2%	1.5%	1218	81.60	1.4%	0.9%	29%	0.978
3.00	3328	917	935	98.1%	1.3%	1.5%	3270	77.14	1.6%	1.0%	17%	0.924
2.50	4507	1157	1166	99.2%	1.7%	1.7%	4442	68.90	1.9%	1.2%	14%	0.988
2.20	4972	1253	1277	98.1%	1.8%	1.9%	4890	59.00	2.1%	1.5%	13%	0.963
2.00	4657	1306	1331	98.1%	2.2%	2.2%	4551	45.83	2.6%	1.9%	5%	0.863
1.80	7719	1953	1980	98.6%	3.2%	3.3%	7585	33.91	3.7%	3.0%	4%	0.856
1.50	20086	5240	5272	99.4%	6.9%	7.0%	19826	16.43	7.9%	8.0%	4%	0.818
1.40	10627	2860	2871	99.6%	17.8%	18.7%	10478	6.64	20.7%	22.1%	0%	0.762
1.30	12903	3784	3843	98.5%	33.9%	36.1%	12575	3.26	39.9%	44.9%	0%	0.736
1.20	8463	3929	5177	75.9%	56.9%	60.6%	7047	1.40	71.4%	92.6%	2%	0.721
total	79926	23108	24573	94.0%	2.0%	2.2%	77274	23.01	2.4%	6.8%	4%	0.832

========== STATISTICS OF INPUT DATA SET ==========

FF off, Mask on

XSCALE.LP - /sls/X06SA/Data10-staff/e11206/BLstartup/20111201/2/GO_insulin_ff_on_mask_on/xscale/ <@x06da-cn-1>

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SUBSET OF INTENSITY DATA WITH SIGNAL/NOISE >= -3.0 AS FUNCTION OF RESOLUTION

RESOLUTION LIMIT	NUMBER OF REFLECTIONS OBSERVED	UNIQUE	POSSIBLE	COMPLETENESS OF DATA	R-FACTOR observed	R-FACTOR COMPARED expected	I/SIGMA	R-meas	Rmrgd-F	Anomal Corr	SigAno
10.00	162	46	54	85.2%	1.6%	1.5%	154	80.68	1.8%	0.7%	52%	1.062
6.00	642	169	171	98.8%	1.3%	1.5%	627	78.53	1.5%	0.9%	47%	0.960
5.00	608	150	151	99.3%	1.2%	1.5%	600	85.72	1.4%	0.8%	54%	1.052
4.00	1234	342	345	99.1%	1.3%	1.5%	1210	80.26	1.5%	0.9%	36%	1.017
3.00	3269	917	935	98.1%	1.3%	1.5%	3209	75.64	1.6%	1.0%	14%	0.916
2.50	4508	1158	1166	99.3%	1.7%	1.7%	4442	68.38	1.9%	1.2%	16%	0.985
2.20	4960	1254	1277	98.2%	1.8%	1.9%	4878	58.55	2.1%	1.4%	25%	0.950
2.00	4615	1303	1331	97.9%	2.2%	2.2%	4504	45.61	2.6%	2.0%	7%	0.851
1.80	7691	1951	1980	98.5%	3.3%	3.3%	7559	33.87	3.8%	3.1%	12%	0.901
1.50	20014	5235	5272	99.3%	6.9%	7.0%	19744	16.47	7.9%	7.9%	3%	0.828
1.40	10650	2866	2877	99.6%	18.1%	18.6%	10500	6.72	21.1%	21.7%	-1%	0.782
1.30	12858	3773	3837	98.3%	34.2%	36.1%	12523	3.28	40.2%	45.0%	0%	0.752
1.20	8471	3933	5177	76.0%	59.1%	61.0%	7050	1.40	73.9%	96.5%	1%	0.734
total	79682	23097	24573	94.0%	2.1%	2.2%	77000	22.86	2.4%	6.8%	5%	0.844

========== STATISTICS OF INPUT DATA SET ==========

FF on, Mask on

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SUBSET OF INTENSITY DATA WITH SIGNAL/NOISE >= -3.0 AS FUNCTION OF RESOLUTION

RESOLUTION LIMIT	NUMBER OF REFLECTIONS OBSERVED	UNIQUE	POSSIBLE	COMPLETENESS OF DATA	R-FACTOR observed	R-FACTOR COMPARED expected	I/SIGMA	R-meas	Rmrgd-F	Anomal Corr	SigAno
10.00	157	47	54	87.0%	1.4%	1.4%	149	82.29	1.6%	0.7%	40%	0.842
6.00	654	169	171	98.8%	1.2%	1.5%	641	82.59	1.4%	0.9%	24%	1.036
5.00	612	150	151	99.3%	1.3%	1.5%	605	89.38	1.5%	0.8%	47%	1.109
4.00	1280	344	345	99.7%	1.2%	1.5%	1257	84.73	1.4%	0.9%	28%	0.967
3.00	3394	917	935	98.1%	1.3%	1.5%	3333	79.49	1.6%	0.9%	21%	0.947
2.50	4599	1156	1166	99.1%	1.7%	1.7%	4542	70.15	1.9%	1.2%	14%	0.986
2.20	5068	1253	1277	98.1%	1.8%	1.9%	4995	59.33	2.1%	1.5%	12%	0.965
2.00	4818	1313	1331	98.6%	2.3%	2.3%	4716	45.82	2.7%	2.1%	2%	0.891
1.80	7848	1956	1980	98.8%	3.3%	3.4%	7723	33.21	3.8%	3.1%	3%	0.852
1.50	20490	5243	5272	99.4%	7.3%	7.5%	20250	15.84	8.4%	8.6%	2%	0.813
1.40	10811	2863	2871	99.7%	19.2%	20.1%	10660	6.30	22.3%	23.9%	0%	0.762
1.30	13028	3786	3843	98.5%	36.4%	39.2%	12711	3.05	42.8%	49.0%	2%	0.712
1.20	8512	3943	5177	76.2%	60.5%	65.7%	7086	1.31	75.6%	99.8%	4%	0.698
total	81271	23140	24573	94.2%	2.1%	2.3%	78668	22.97	2.4%	7.1%	3%	0.829

========== STATISTICS OF INPUT DATA SET ==========

FF off, Mask off

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SUBSET OF INTENSITY DATA WITH SIGNAL/NOISE >= -3.0 AS FUNCTION OF RESOLUTION

RESOLUTION LIMIT	NUMBER OF REFLECTIONS OBSERVED	UNIQUE	POSSIBLE	COMPLETENESS OF DATA	R-FACTOR observed	R-FACTOR COMPARED expected	I/SIGMA	R-meas	Rmrgd-F	Anomal Corr	SigAno
10.00	162	46	54	85.2%	1.6%	1.5%	154	79.21	1.8%	0.7%	55%	1.058
6.00	639	169	171	98.8%	1.3%	1.6%	624	76.97	1.5%	0.9%	50%	0.968
5.00	610	150	151	99.3%	1.2%	1.6%	602	84.29	1.4%	0.8%	54%	1.008
4.00	1234	342	345	99.1%	1.3%	1.6%	1210	78.83	1.5%	1.0%	30%	0.965
3.00	3277	914	935	97.8%	1.4%	1.6%	3209	74.49	1.6%	1.0%	5%	0.915
2.50	4529	1154	1166	99.0%	1.7%	1.7%	4469	67.64	2.0%	1.2%	16%	0.967
2.20	4975	1254	1277	98.2%	1.8%	2.0%	4896	57.75	2.1%	1.5%	23%	0.946
2.00	4670	1306	1331	98.1%	2.3%	2.3%	4570	45.12	2.7%	2.1%	6%	0.857
1.80	7764	1949	1980	98.4%	3.3%	3.3%	7642	33.60	3.8%	3.2%	13%	0.902
1.50	20416	5241	5272	99.4%	7.0%	7.2%	20171	16.36	8.1%	8.1%	2%	0.827
1.40	10862	2869	2877	99.7%	17.9%	18.8%	10719	6.70	20.8%	20.8%	-3%	0.779
1.30	13015	3775	3837	98.4%	34.4%	36.6%	12690	3.25	40.4%	45.2%	-1%	0.759
1.20	8537	3940	5177	76.1%	59.3%	61.9%	7127	1.38	74.1%	97.9%	-2%	0.710
total	80690	23109	24573	94.0%	2.1%	2.3%	78083	22.58	2.4%	6.8%	3%	0.839

========== STATISTICS OF INPUT DATA SET ==========

FF on, Mask off

PILATUS3

New Features

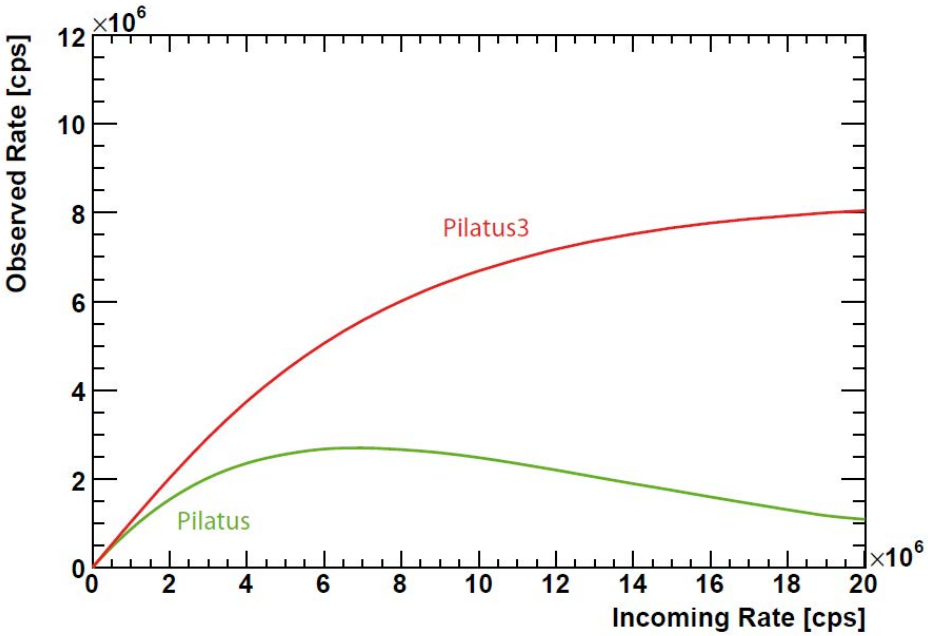
- instant retrigger technology for non-paralyzable counting
- counter overflow handling
- reduced readout time
- compatibility with CdTe sensors

Benefit

- improved data quality at high count rates
- increased frame rates

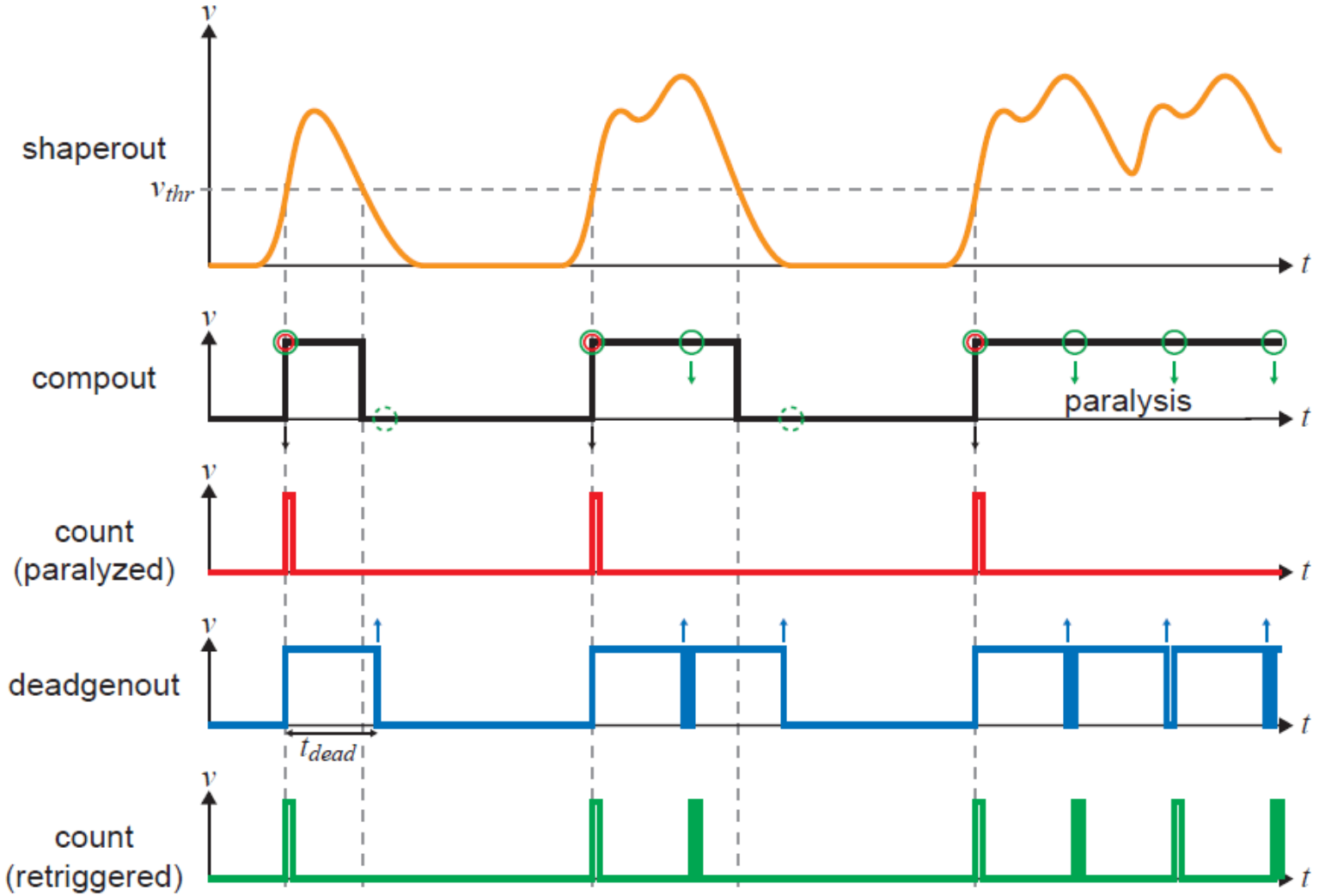
Performance

Simulated counting performance of PILATUS and PILATUS3 detectors:



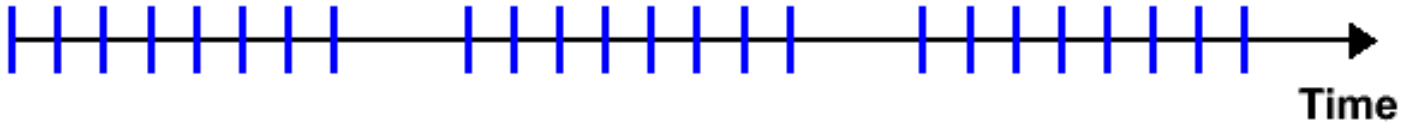
(Monte-Carlo system simulations, continuous source, photon energy 12 keV, low gain, pulse width 95 ns, threshold energy 6 keV, dead time overlap 1.25)

Instant Retrigger TechnoMode

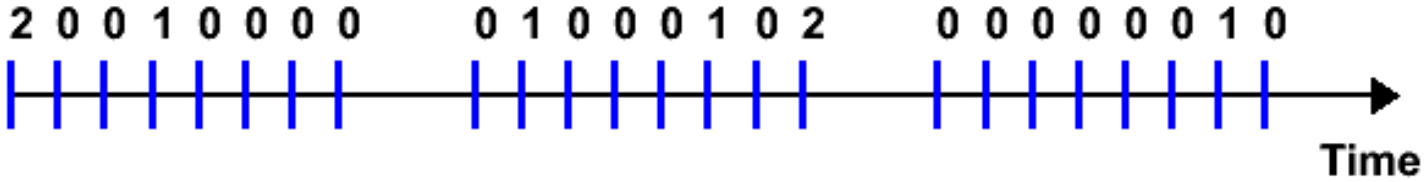


Monte-Carlo (MC) Simulation

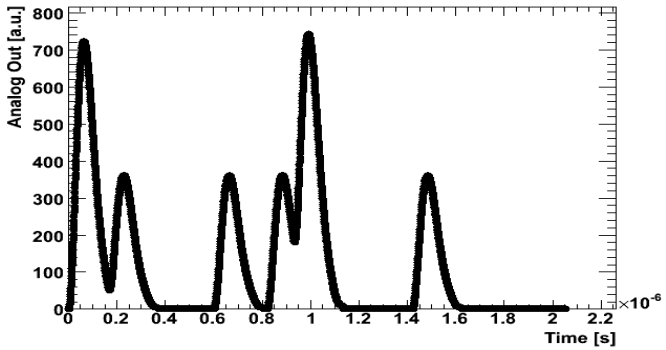
1. Build bunch structure



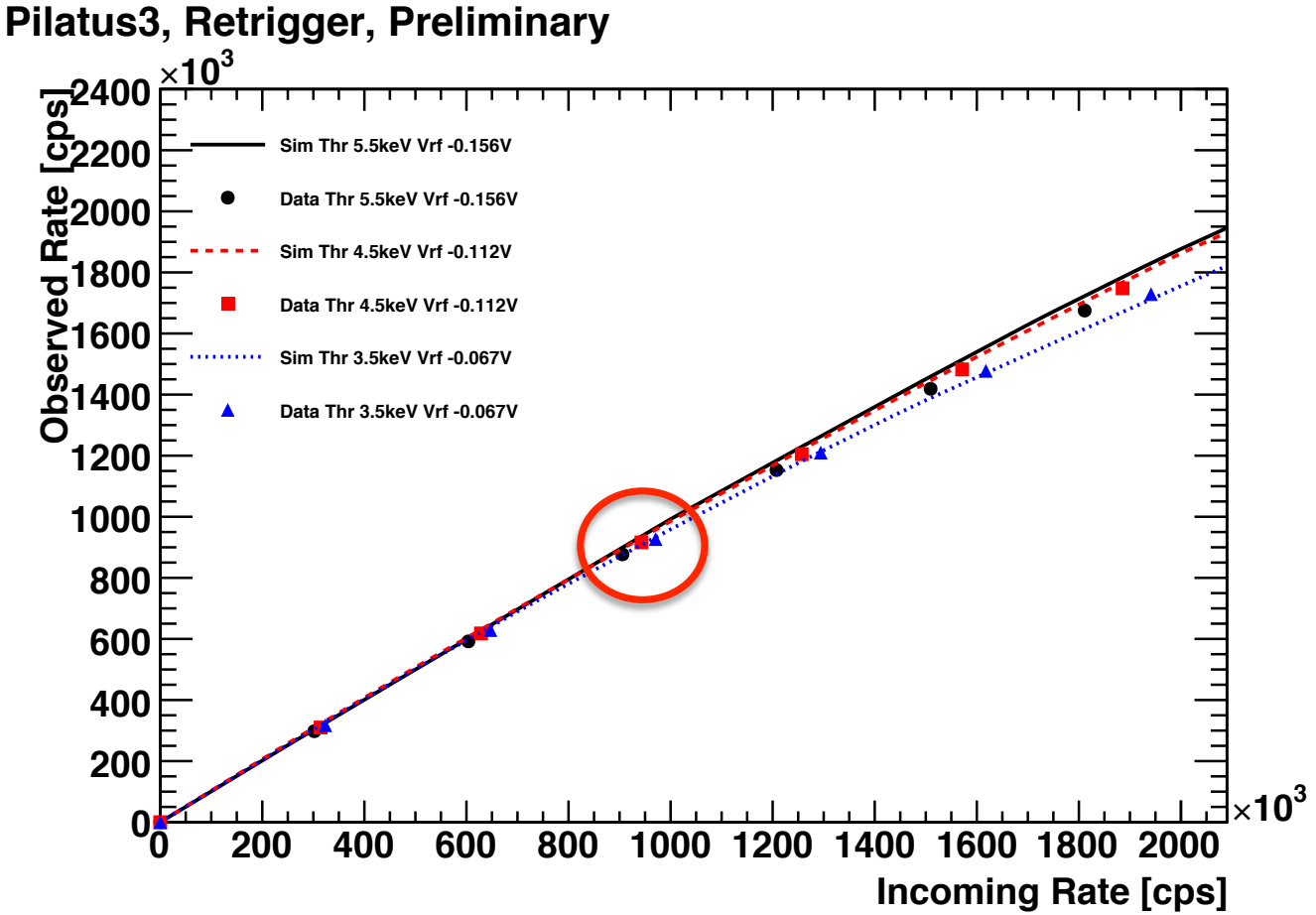
2. Determine number of photons in each bunch according to Poisson statistics



3. Input as stimulus file for Cadence Simulator: Spice simulation of amplifier, comparator and counter

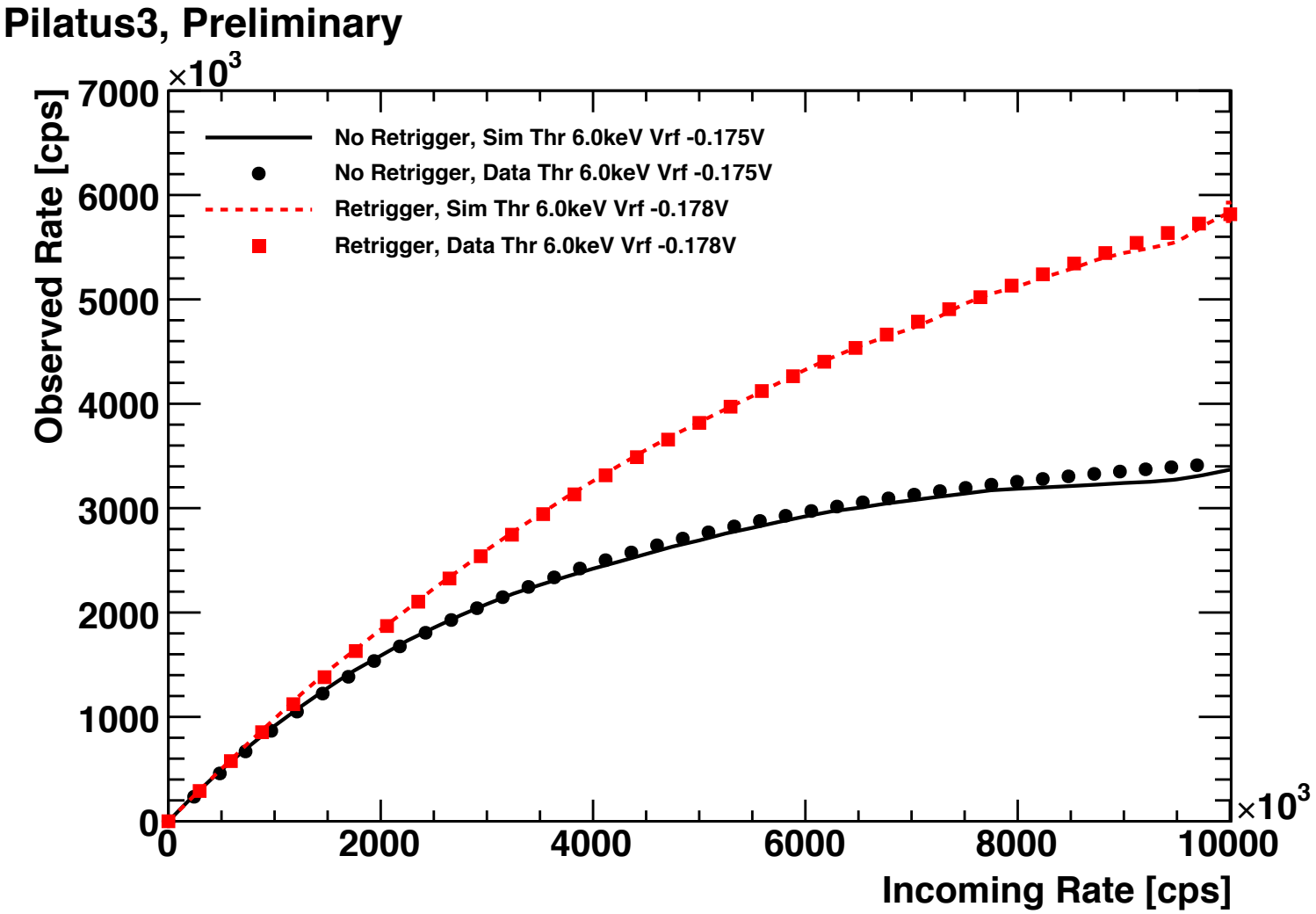


Retrigger mode: High rates



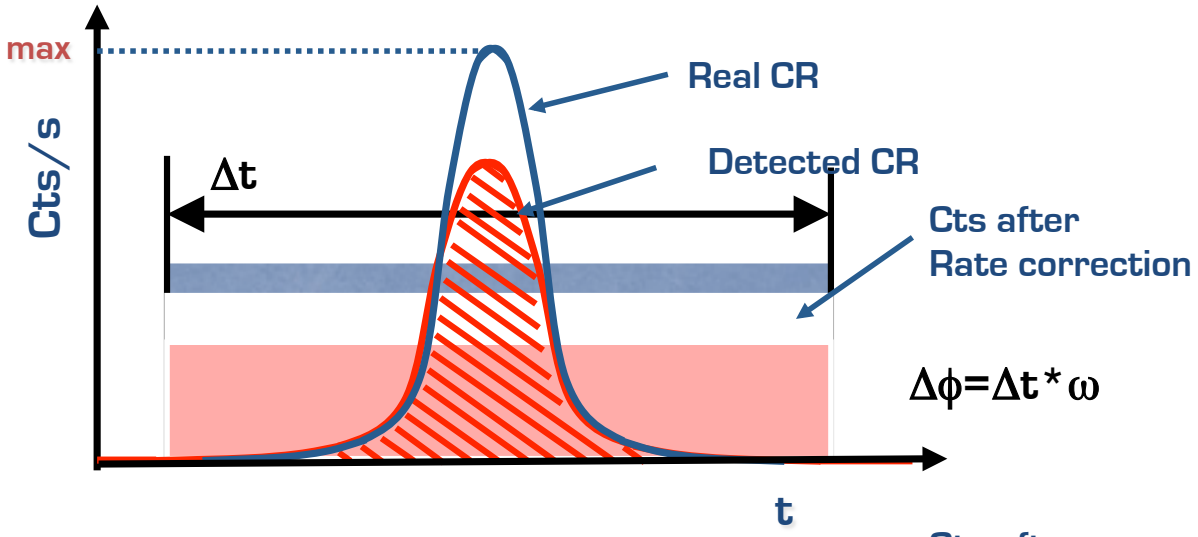
Deviation (fast settings)	10^6 cps	10^7 cps
Before correction	4%	44%
After correction	1 %	few percent

Comparison standard – retrigger mode Pilatus 3

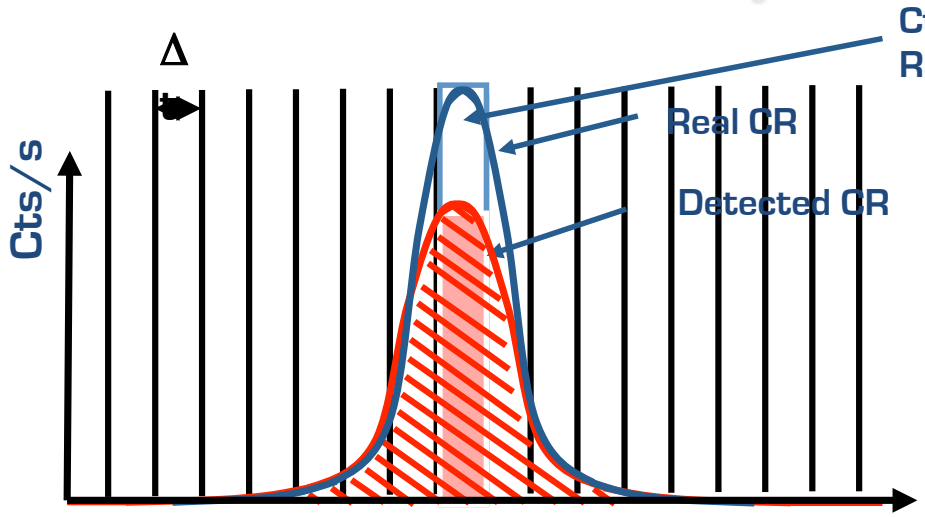


Excellent Agreement for retrigger mode up to 10^7 cps

Count rate correction in the non-constant case



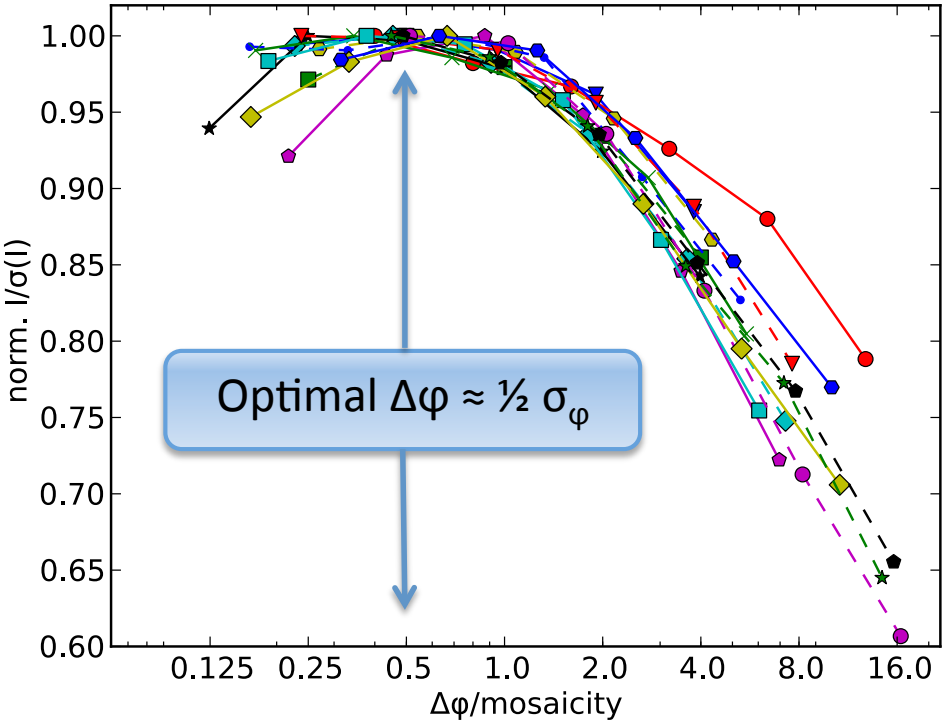
Conventional Integration leads to an underestimation of very strong reflections

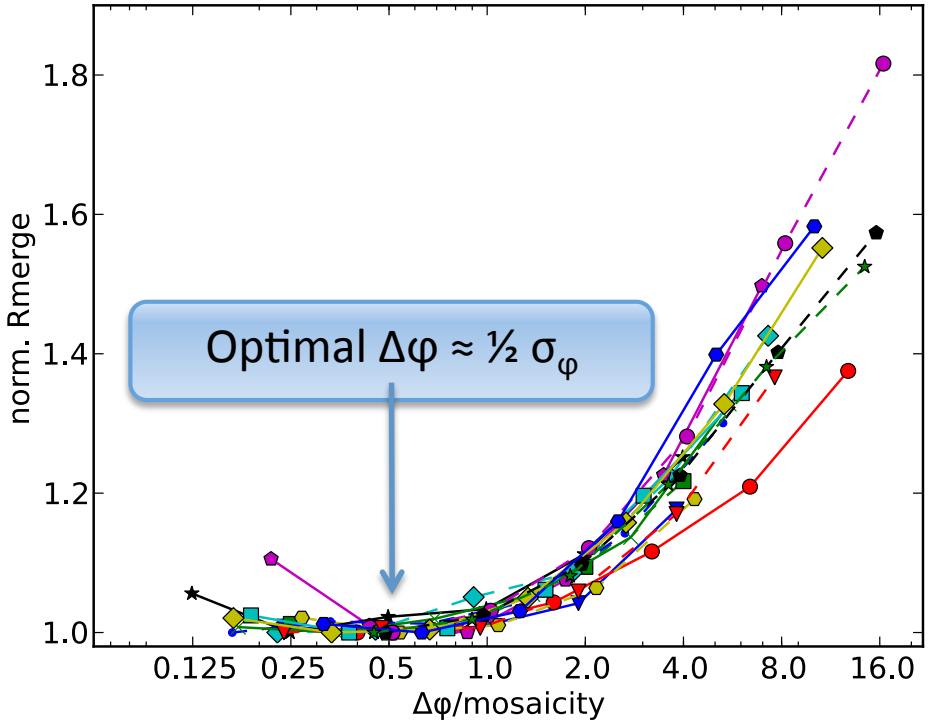


If Δϕ<= mosaicity then the reflection intensity is reconstructed with a precision < 1%

➔ Apply Rate Correction based on Reflection Profile (derivative)

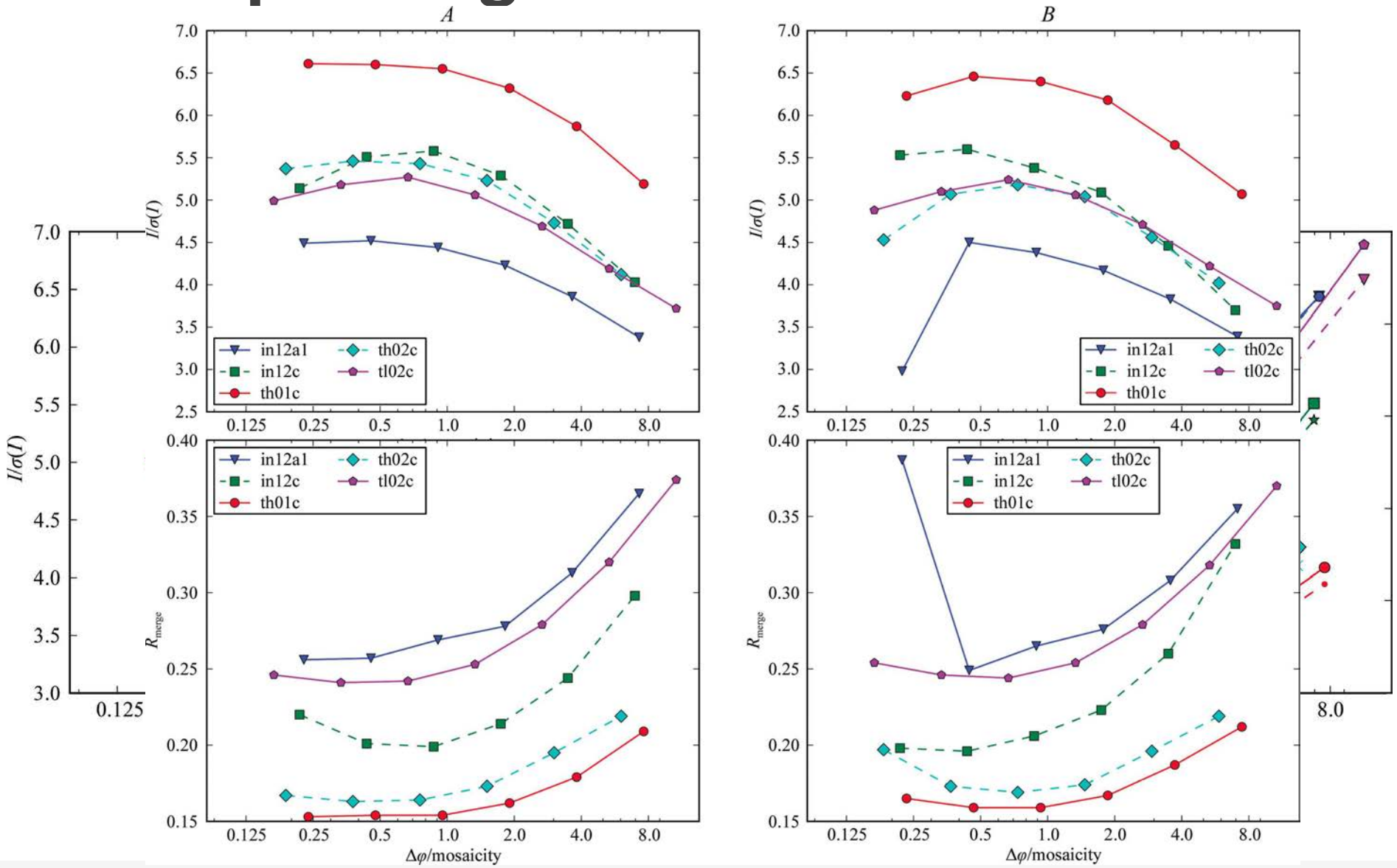
Fine φ-slicing: Highest shell statistics





- Best data at Δφ = ½ mosaicity (σ_φ)
- Highest shell statistics improve substantially
  => integration software should process fine phi-sliced data very stably

Fine φ-slicing: Artifacts

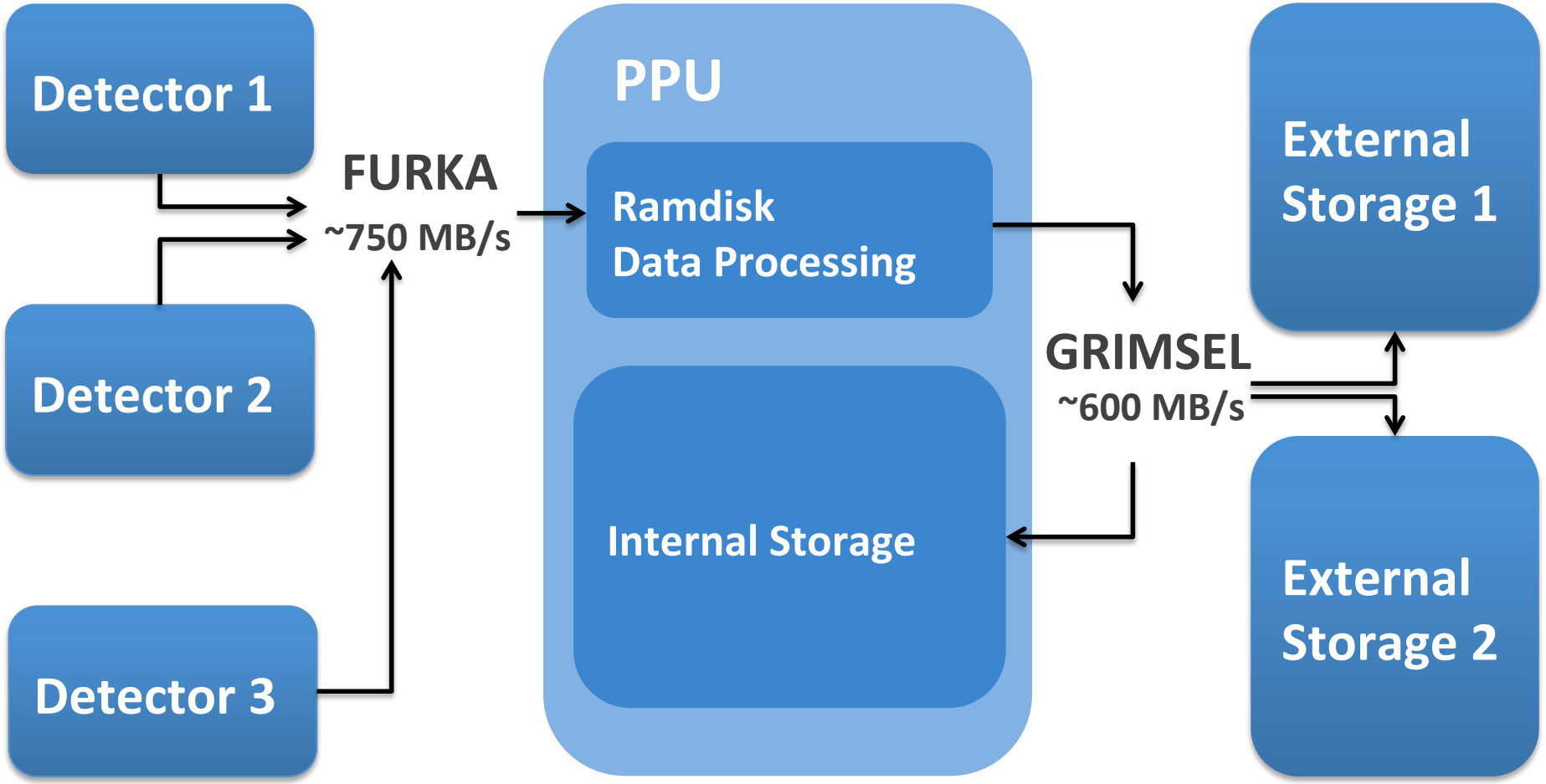


Large Area Fast Detector Systems

System Name	Frame Rate (Hz)	Image size compressed (MB)*	Data rate (MB/s)
Pilatus 6M	12	6	72
Pilatus 6M FAST	25	6	150
Pilatus3 6M	100	6	600
Eiger 16M	180	16	2880

*Assuming current CBF Format and byte forward compression

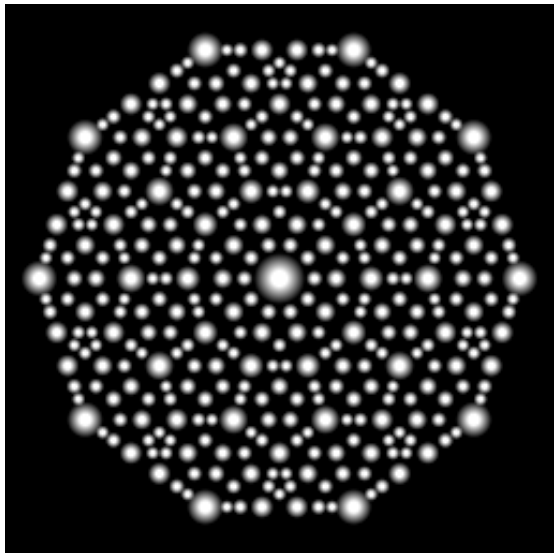
Products Extensions:
PILATUS Processing Unit - PPU



ALBULA

Main Features

- Life view modes
  - Watch directory
  - Movie mode
  - Slave mode



- Real-time image statistics and arithmetic tools (peak-finder, region of interest)
- Synchronization of multiple images

File format for EIGER

- EIGER will pose new challenges in data handling: frame rates up to 3 kHz, data rates up to 5 GB/s
- HDF5 is a promising candidate:
  - already widely used: NASA, LCLS
  - BSD-style open-source license for C, C++, Fortran, Python libraries
- Currently being evaluated by DECTRIS and PSI
- After positive current evaluation, test data sets will be made available in October on www.dectris.com
- HDF5toCBF converter for backward compatibility is planned

Conclusions

- Energy and flat-field calibrations provided by DECTRIS
- Dead time correction based on parameterised MC simulation (time structure, threshold, gain) taking reflection profile into account by DECTRIS
- Positional error difficult to access and calibrations not optimal
  - ➢ Refine positions of modules from diffraction
- QE fully determined by Si – absorption
  - ➢ Error estimates based on photon counting statistics

Conclusions

- Dials is a unique chance to further improve data from single photon counting detectors
- “True photon statistics” should be applied
- As simple as can be, should be extended later
- As little corrections as possible
- Clear division btw detector manufacturer corrections and corrections in the processing
- Cope with ever brighter beamlines
- Cover features of new Pilatus3 and Eiger

Suggestions

- Improve processing stability for very fine ϕ-sliced data
- Improve processing statistics of ‘crystal limited’ diffraction data
- Look into high frame rate capabilities (> 100 Hz) of next generation pixel detectors