Update on Science Requirements

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DESY- Hamburg; Germany

Outlook

- Science requirements
  - Single Particle Imaging
  - XPCS
  - XFEL Time Structure

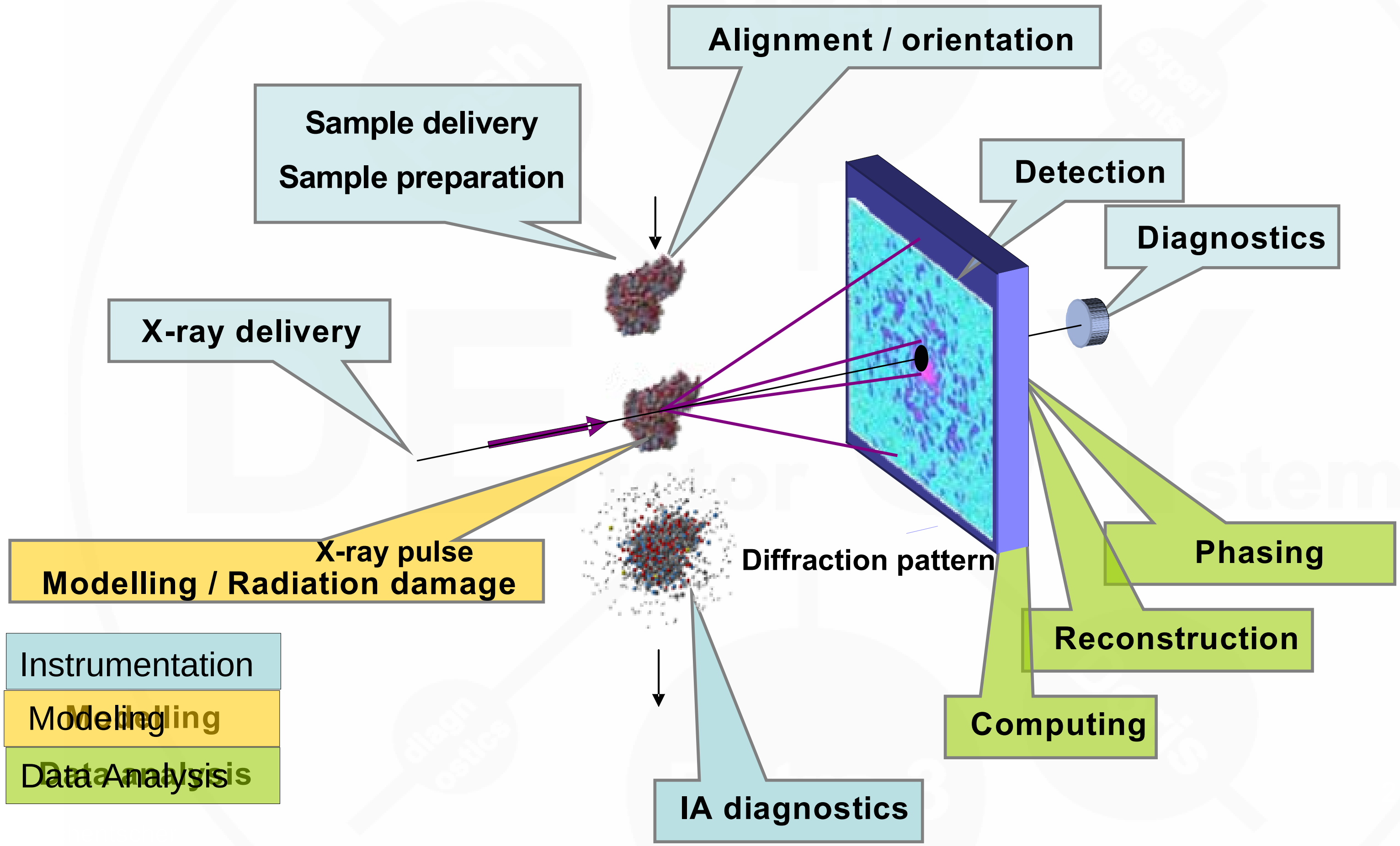
- Status of HORUS, Noise Budget Analysis
  - Analysis of the detector signal as f(Charge Sharing, Amplifier noise, …)
  - Big surprise !

→ SPI requirements

Science Requirements : SPI

Workshop in Uppsala End October 2008

1 instrument – 3 different facets



Science Requirements : SPI

Number of pixels required: limited by the bandwidth

N < 2000 for unmonochromatised

N > 2000 for monochromatised

$$N = \frac{2s\lambda}{\Delta\lambda}$$

- 500 x 500 for 0.3 nm resolution of (75 nm)^2 object s=1 (not safe)
- **2k x 2k** for 0.2 nm resolution of 0.2 micron object s=1
- **2k x 2k** for 0.4 nm resolution of 0.2 micron object s=2 (safer)
- **2k x 2k** for 0.1 nm resolution of 0.05 micron object s=2 (safer)

Single particle imaging is dominated by noise (**counting statistics of quanta**)

- scattered counts per Shannon pixel is *proportional to* λ^2
- number of incident photons per pulse fluence *proportional to* λ

} *Signal α* $\boldsymbol{\lambda^3}$

6 keV (0.2 nm) is 8 times better than 12 keV (0.1 nm)

3 keV (0.4 nm) is 64 times better than 12 keV (0.1 nm)

SASE 1 has a fixed energy of 12,4 keV

→ **SPI impact of the detector**

SPI: The impact of AGIPD on the Technique.

Impact of the detector's dead area on the reconstruction algorithm:

Abbas Ourmazd and co-authors introduced a new reconstruction algorithm.

- There is no need of *a priori information* to classify the data

⇒ Since the molecule's orientation is random, dead area will automatically disappear

- The central Hole remains an issue, and should be kept as small as possible

Single particle imaging is dominated by noise (**counting statistics of quanta + Det/bkg noise**)

- More pixels is better
- Less dead area is better
- Low noise is better *"20 false events on the detector would be an issue"*

But…

→ SPI benchmarking

SPI: Good Benchmarking of the impact of the detector

Noise is an acceptable fact within some limits. ***Calibration is what matters***

"Better a noisy but well calibrated detector than a good poorly calibrated detector"

Ultimate Information is the Joint probability distribution:

- X is the True Mean Count ~ *"Intensity" and its associated "Statistics" (eg. Poisson)*
- Y is the Actual Detector Count

P(X,Y) is the statistical distribution of the detector response for X.

P(X,Y) is explicitly written in the reconstruction algorithm.

XPCS: Where we are

XPCS consortium Meeting — ***End January 2009***

- *The Requirements are a lot less defined*
- *The community is much sm*

Is there any possibility to create a second version of the detector with smaller pixels/less storage capacity?

What does this mean for the Mechanics/Cooling? the Readout Interface?

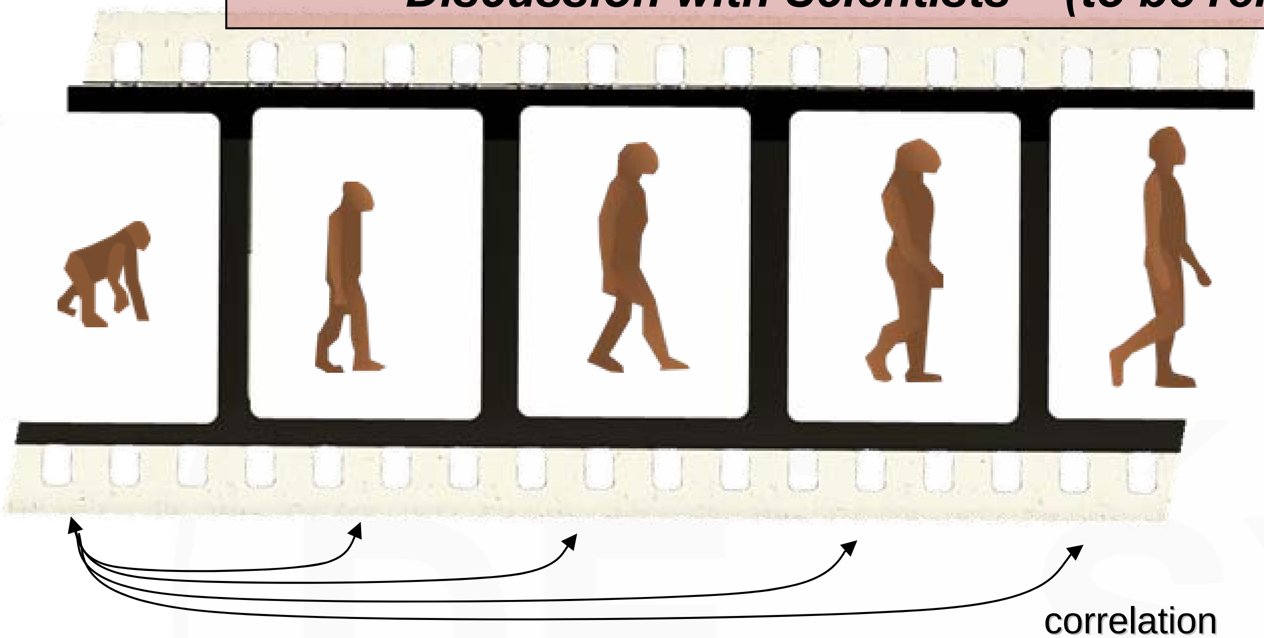
ie. What would be the cost of such a modified version of AGIPD?

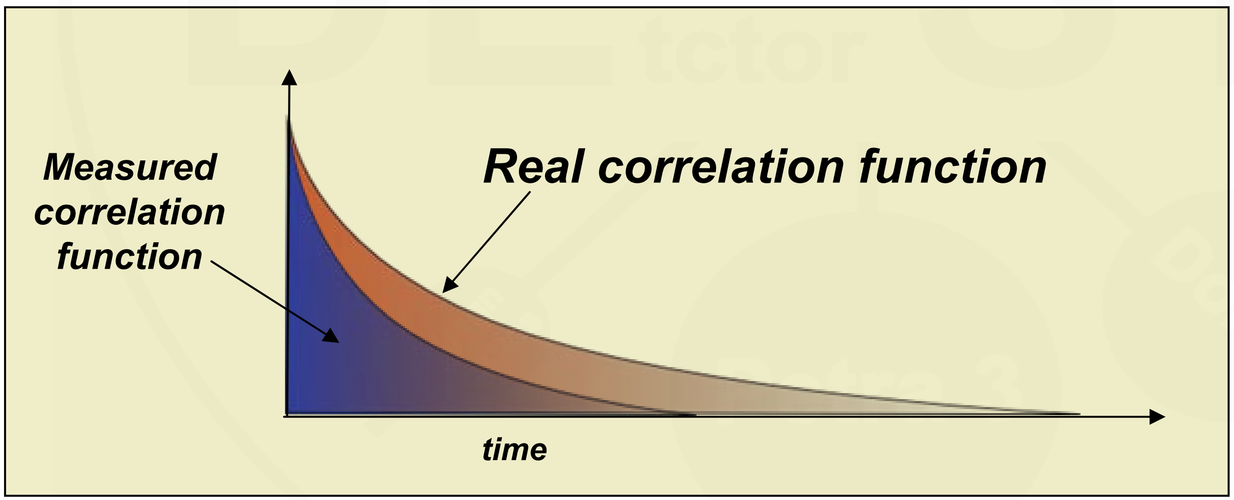
The
Mas *of experiements.*

On the *ue, they do not need many many* ***images: <100***

XPCS: Good benchmarking

XPCS Requirements,
Discussion with Scientists (to be refined a lot)





XPCS Requirements, Discussion with Scientists (to be refined a lot)

Definition of "Single photon Sensitivity"

- *For us it has always meant* *<u>Better than Poisson noise</u>*

- *But for them, a set of data exhibiting Poisson Noise means exactly*
    - *The beam is not coherent*
    - *There is absolutely no correlation in the data set*

This means they are measuring "things" with a precision better than Poisson Statistics

Science Requirements : Summary for us

- 2000x2000 pixels is the **baseline solution** for several experiments
- *Operation of AGIPD at **lower energies** has to envisaged*
- *Poisson Noise may **not be the absolute limit**, we may have to do better…*
- *200x200μm² is a **real problem** for XPCS.* *Need < 100 frames*

  $\Rightarrow$*AGIPD$_{\underline{XPCS}}$ doable (in a second time)?*

Science Requirements : To Does

Studies are ongoing to evaluate the "Luminosity of experiments"

$\Rightarrow$ **Integrated Dose**

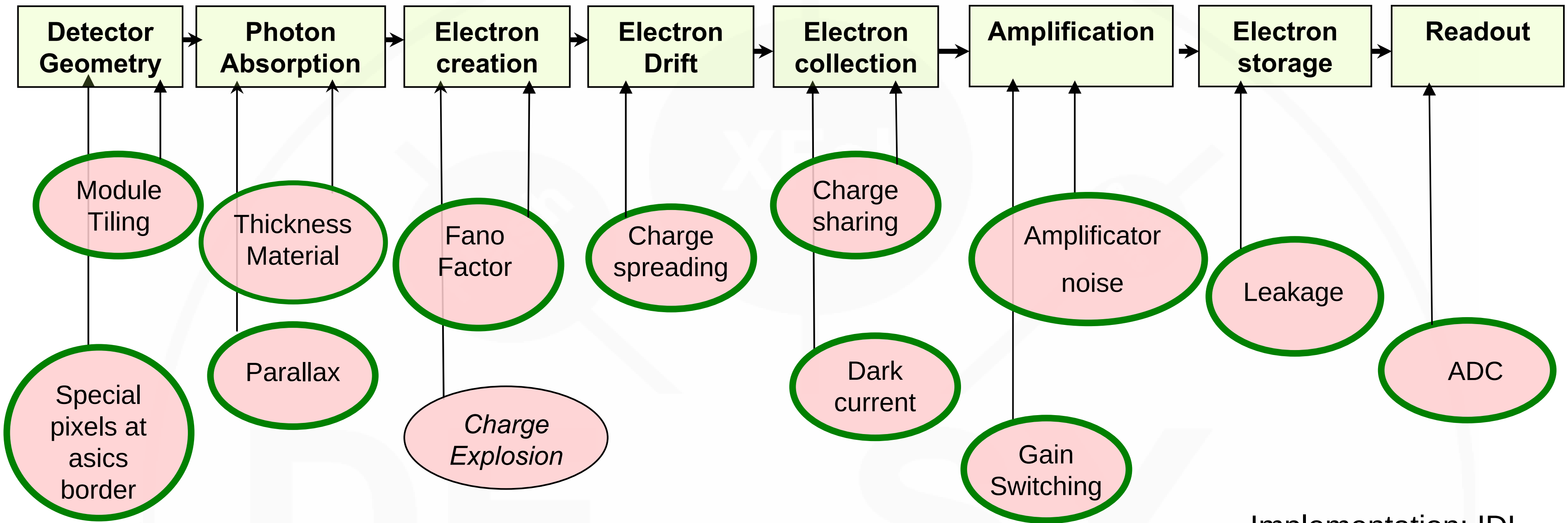
$\Rightarrow$ **Expected data rate**

Depends on many experimental parameters, and improvements in the instrumentation

A related question is that of the Bunch structure of the XFEL. See tomorrow…

Refine and do the different Benchmarking of AGIPD for CDI and XPCS as defined with the scientists

HORUS: a detector simulation program



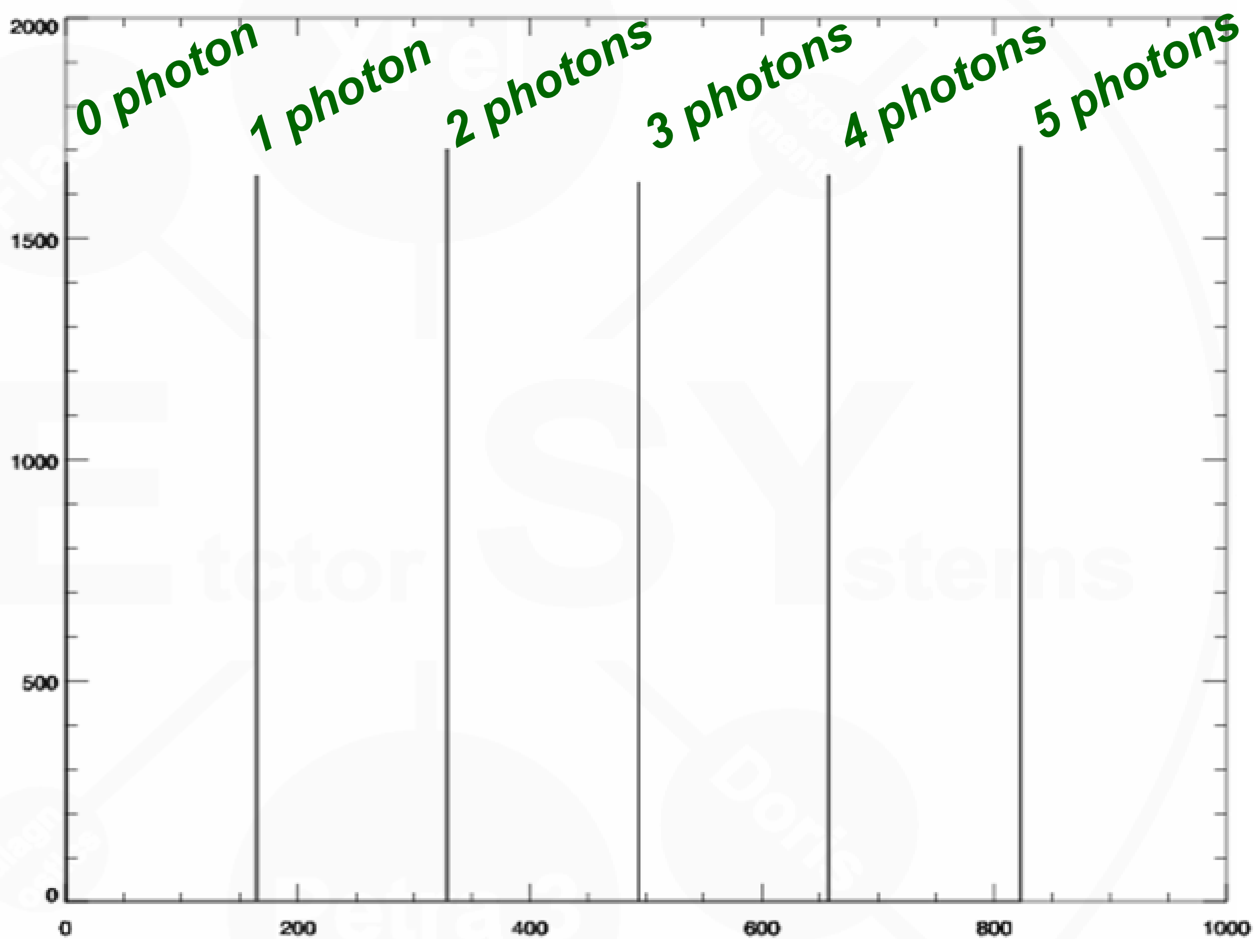
Implementation: IDL

HORUS First Version is finished and tested.
Only minor bugs should still be there

Already some nice results…

Ex. Response to a random image with Intensity 0 ≤ I ≤ 5photons
ie. *# Px (0photons) = # Px (1 photons) = # Px (2 photons) = …*

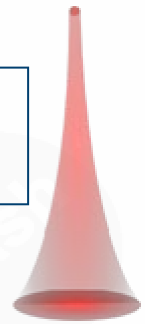
Perfect detector



Standard case:
12keV photons
200µm pixels
500µm thick sensor

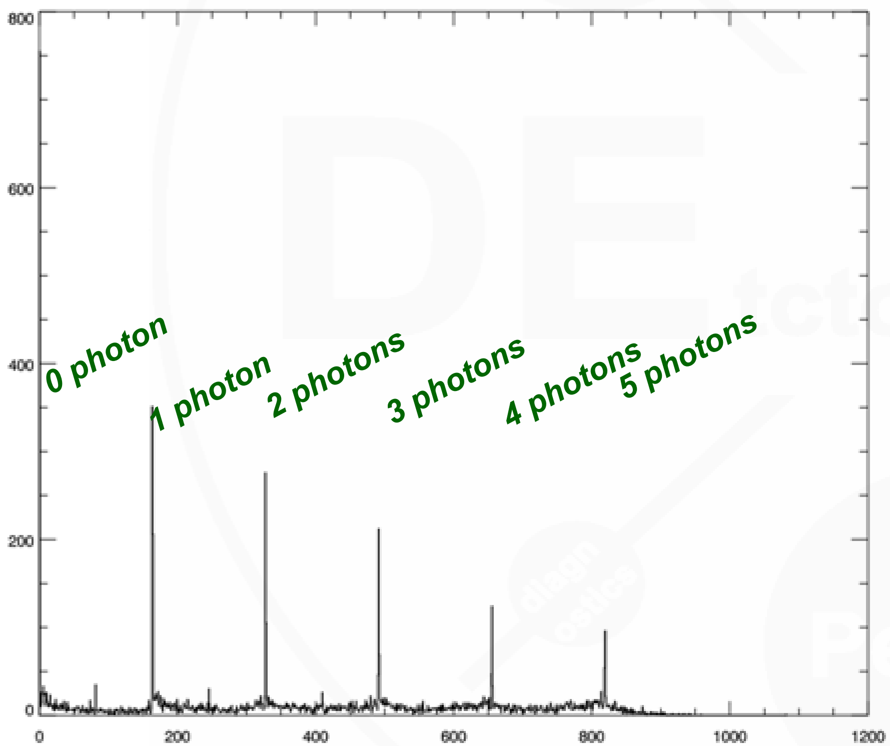
Response to a random image with Intensity 0 ≤ I ≤ 5photons

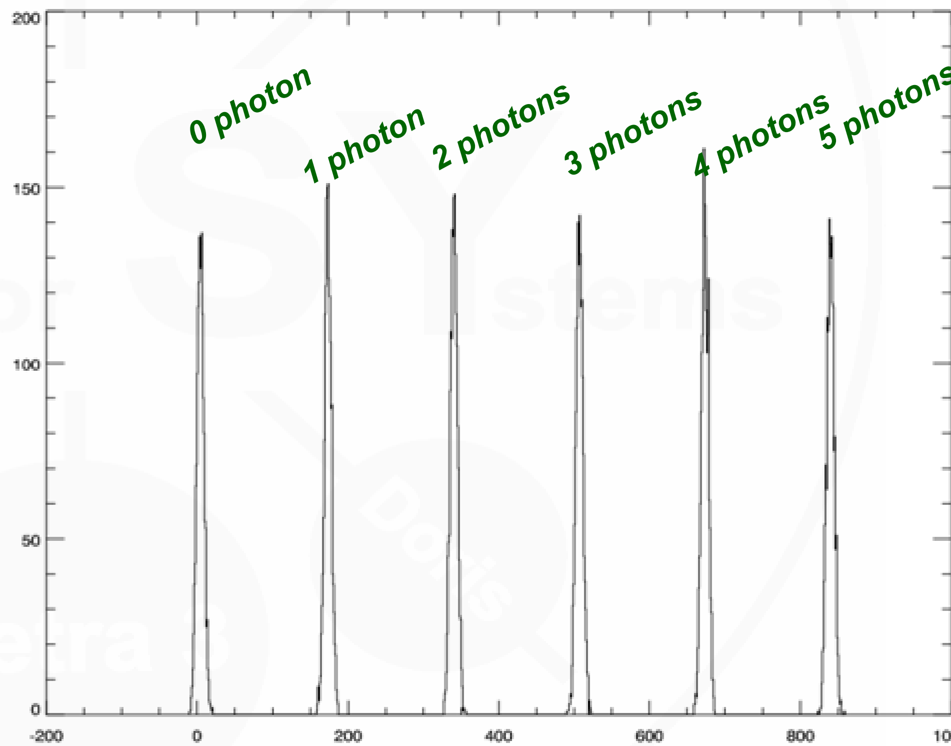
With Charge sharing (only)



With amplifiers noise (only)

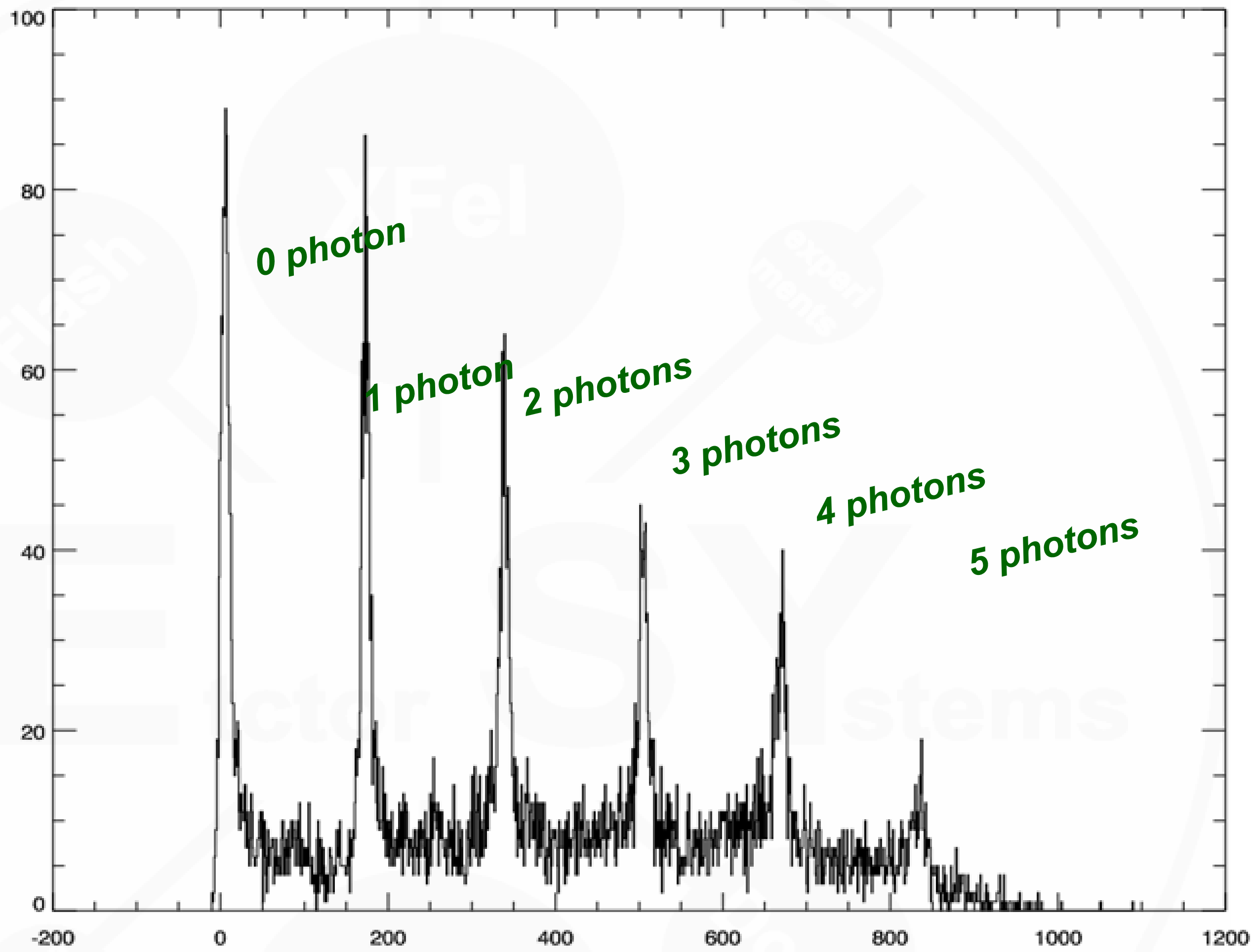
$$Q_n^2 = \frac{\exp(2)}{8}\left[\left(2eI_d + \frac{4kT}{R_p} + i_{na}^2\right)\tau + \left(4kTR_s + e_{na}^2\right)\frac{C^2}{\tau} + 4A_f C^2\right]$$





Response to a random image with Intensity $0 \leq I \leq 5$photons

With everything



Standard case:

12keV photons

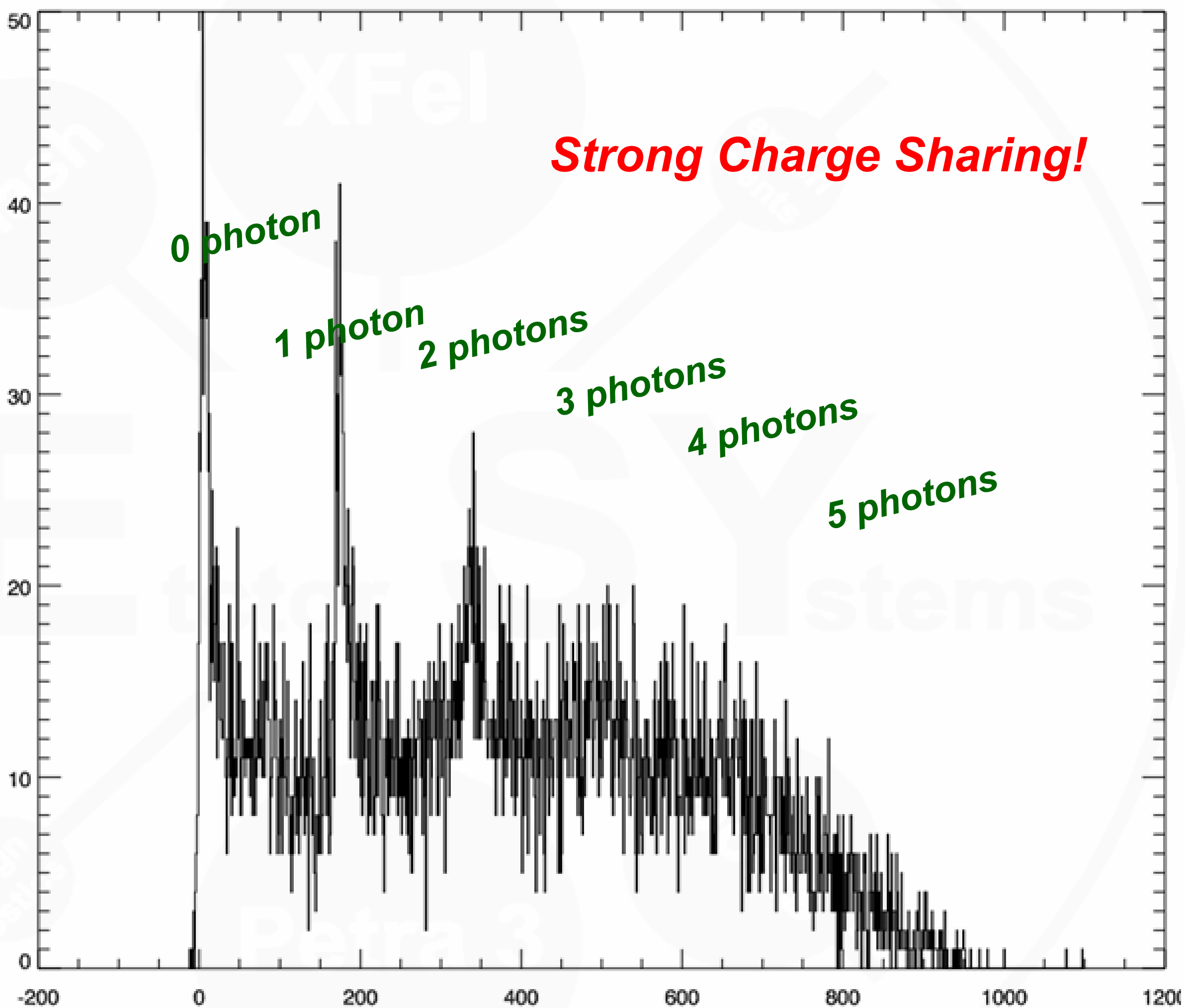
200µm pixels

500µm thick sensor

This looks messy but the resulting image is actually very close to the original one ***(see later for real statistics)***

Response to a random image with Intensity 0 ≤ I ≤ 5photons

With everything



Other case:

12keV photons

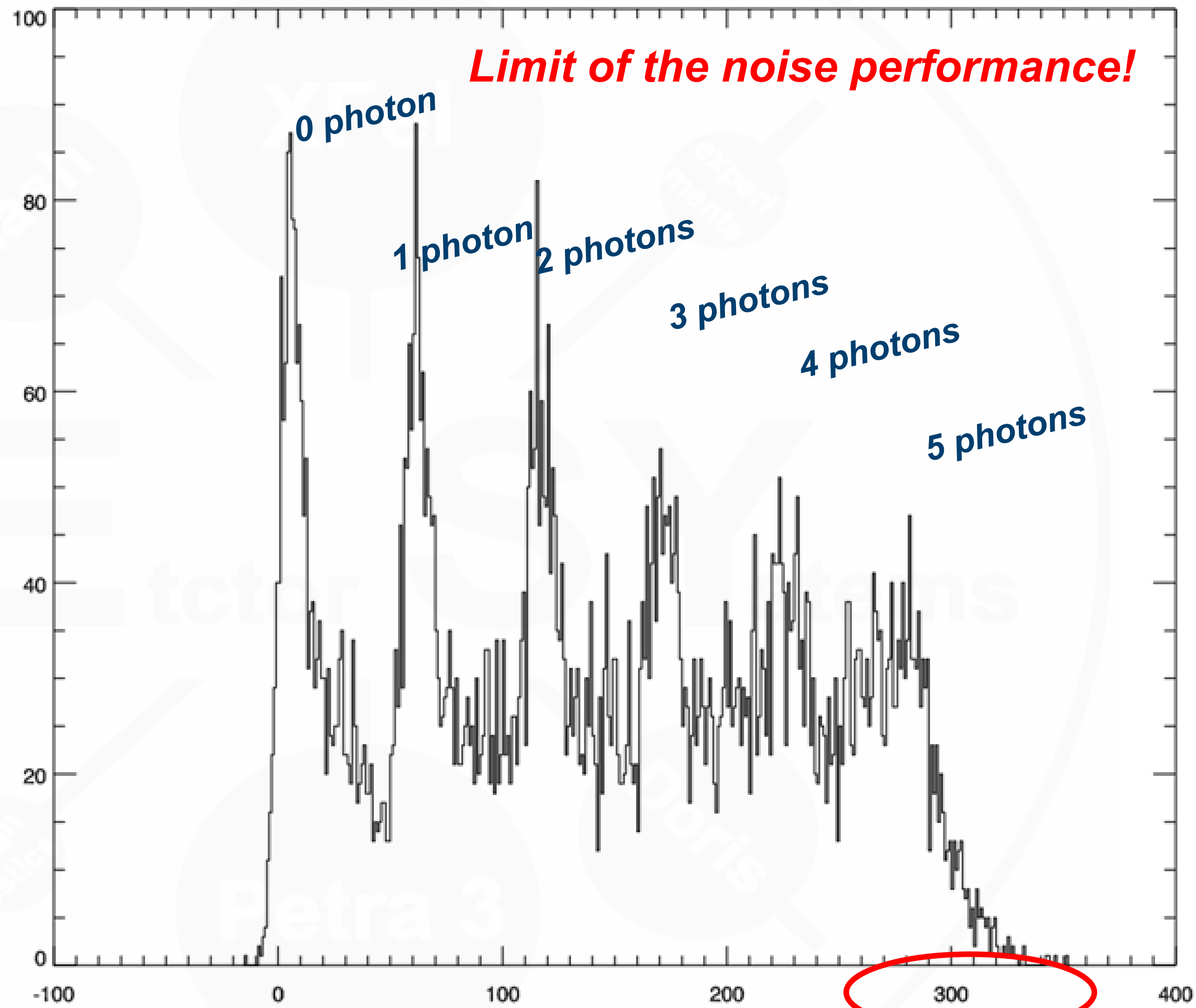
80µm pixels

500µm thick sensor

Response to a random image with Intensity 0 ≤ I ≤ 5photons

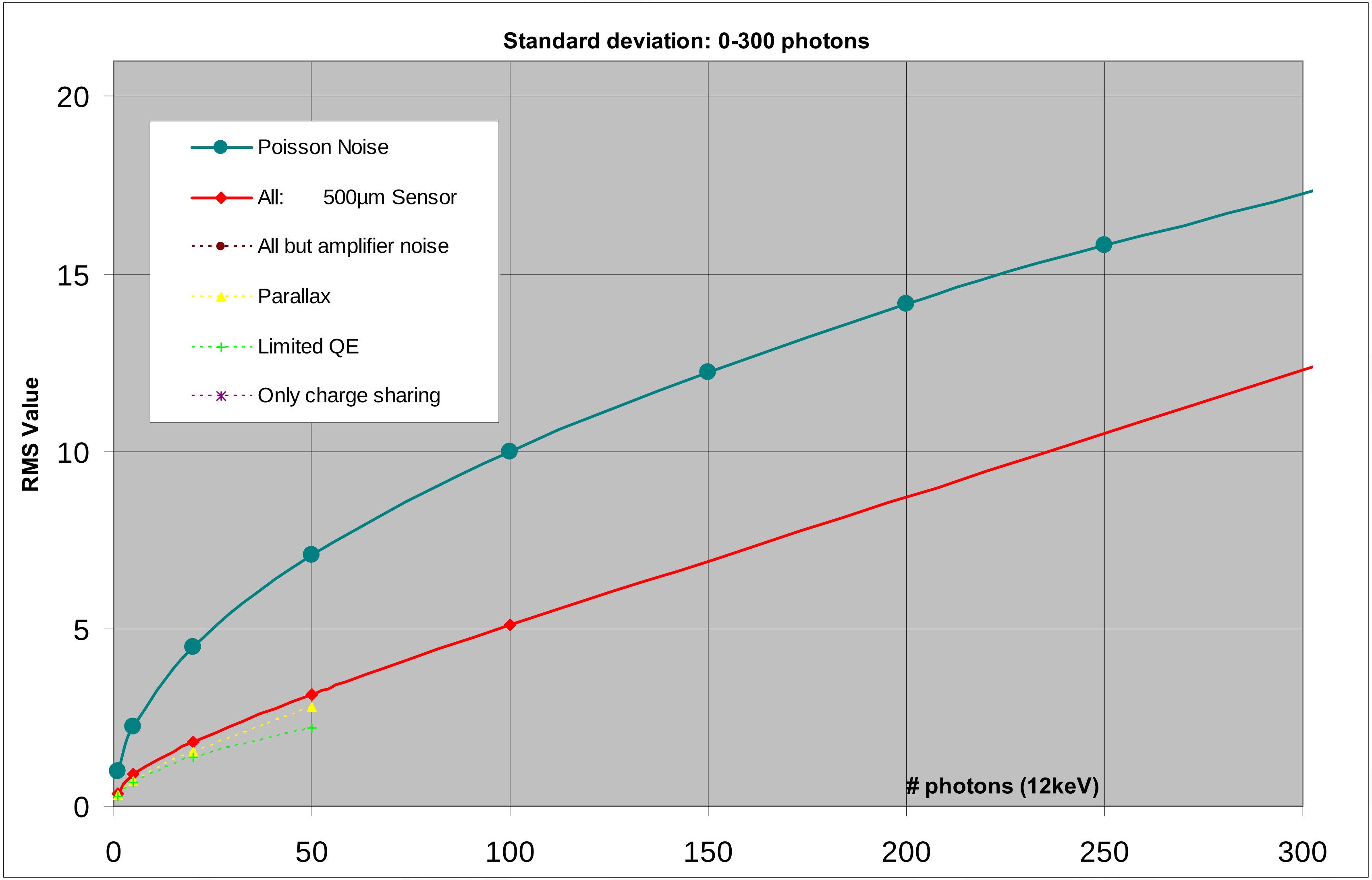
With everything

Standard case:
6keV photons
200µm pixels
500µm thick sensor



→ ***Statistics***

Statistics



$$RMS = \sqrt{\frac{1}{N-1}\sum_{N}\left(I_N - \overline{I_{output}}\right)^2}$$

Conclusion

- ***Lower energies*** *has to envisaged*
- *Poisson Noise may* ***not be the absolute limit***

•*200x200μm² is a* ***real problem*** *for XPCS.* *Need < 100 frames*

⇒*AGIPD$_{XPCS}$ doable (in a second time)?*

- *2000x2000 pixels is certainly to be considered*

- *Complete Noise performance analysis and hard numbers should come soon out of Horus*