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Filip Leonarski :: MX Group :: Paul Scherrer Institut

Using the Jungfrau Charge Integrating Detector for MX at Synchrotron Facilities

HDR MX Meeting Auckland

Presentation Plan

- Jungfrau Detector Characteristics
- Jungfrau Pixel Output
- Data Conversion
- HDF5 Practicalities

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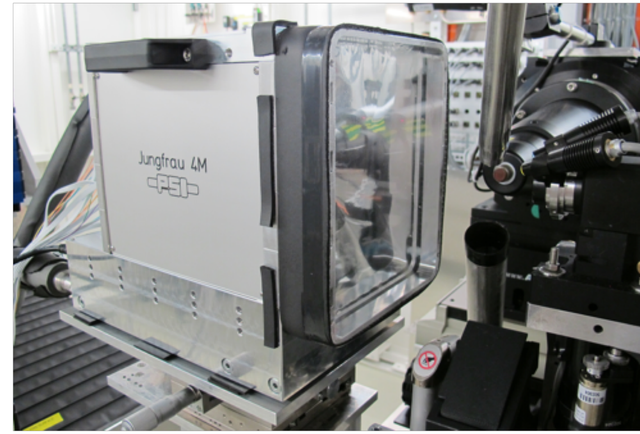
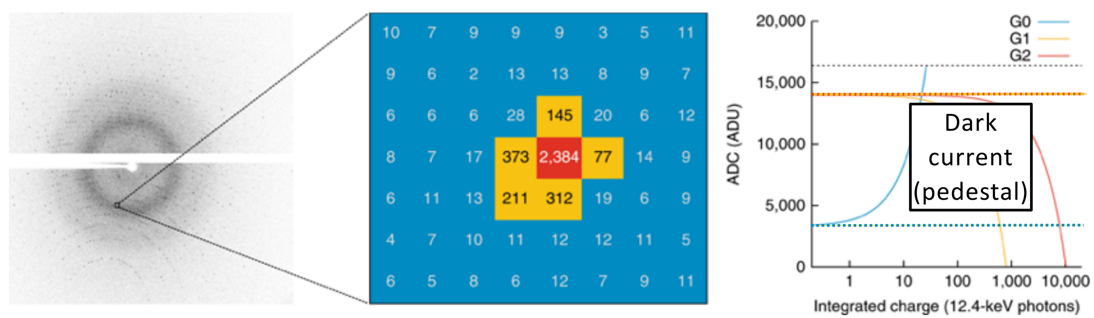
Jungfrau Detector Characteristics

Jungfrau Detector

- Designed for SwissFEL, but with synchrotron applications in mind
- Charge integrating
- Shares EIGER design
  - Pixel size 75x75 µm
  - One ASIC = 256x256 pixels
  - One module = 4x2 ASICs = 1024x512 pixels
- Adaptive gain
  - High dynamic range
  - Single photon sensitivity



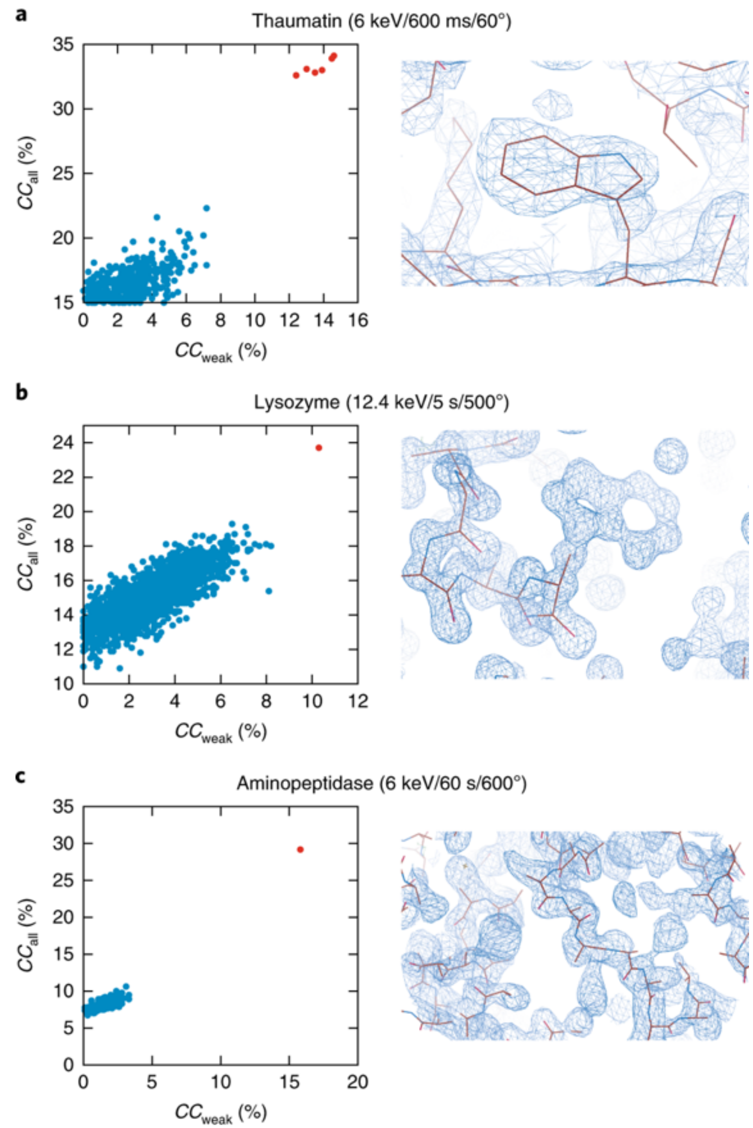
JF4M at X06SA / SLS



Leonarski *et al.*, Nat Methods, 15, 799-804 (2018)

Jungfrau for Macromolecular Crystallography

- Photon counting detectors are **state-of-the-art** for conventional MX
- Jungfrau can improve results for certain particular areas:
  - Low energy MX (≤ 6 keV)
    - Threshold limitations in HPC
  - High dose-rate experiments
    - Count-rate limitation in HPC
- Jungfrau is necessary for sources with short, intense pulses:
  - XFEL
  - Pink beam and chopper



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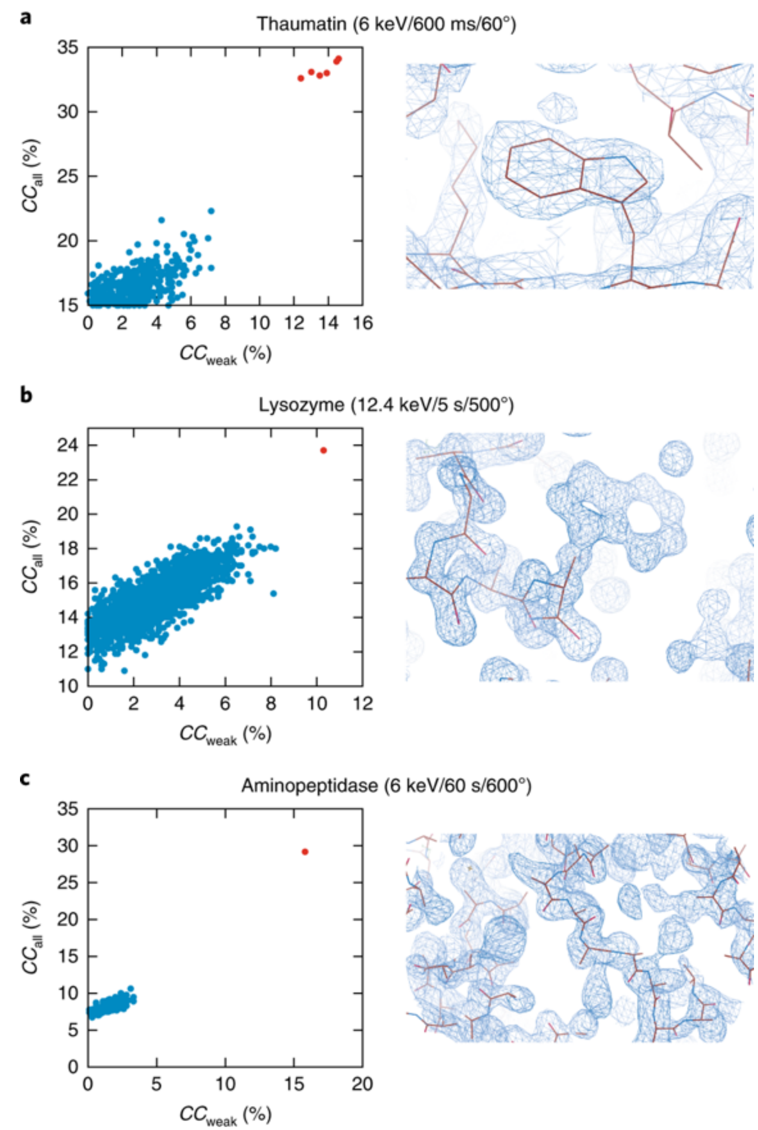
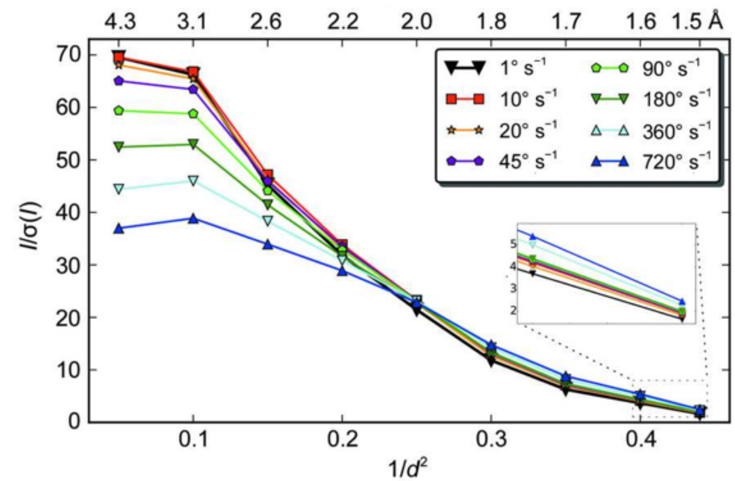


Leonarski *et al.*, Nat Methods, 15, 799-804 (2018)

High Dose-rate Strategy

- Photon counting detectors introduce imprecisions for pixels with high photon rate due to pile-up effect

- In practice with a photon counting detector, for a well diffracting crystal one needs to attenuate beam and slow down measurement to get the best performance (see Casanas *et al.*, Acta Cryst, D72, 2016)



Casanas *et al.*, Acta Cryst, D72, 1036-1048 (2016)

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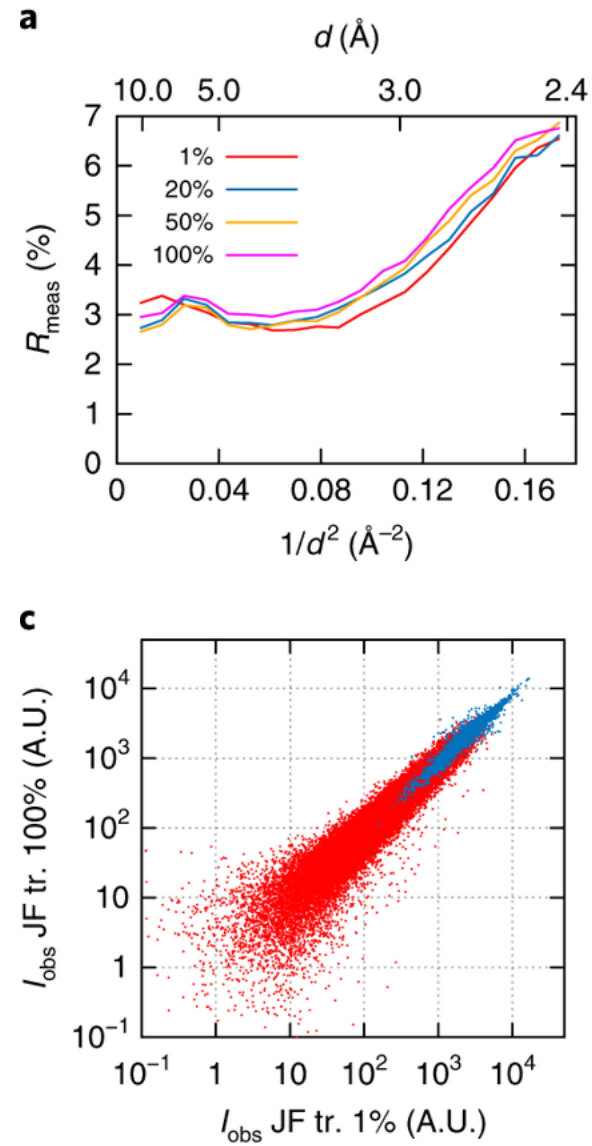
- **Jungfrau has no such limitation**



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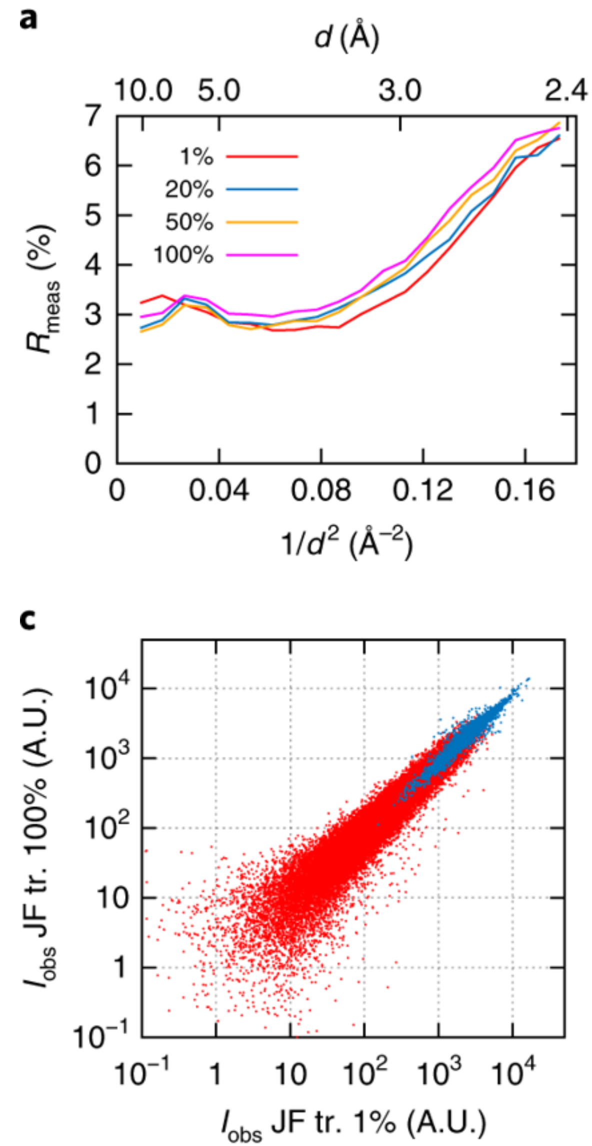
- **Jungfrau has no such limitation**

- Jungfrau + DLSR, better magnets and novel sample delivery methods:
  – Higher beamline throughput
  – Fragment screening methods (<10s/xtal)
  – Routinely 100% flux and 50-100°/s with good data



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Jungfrau Pixel Output

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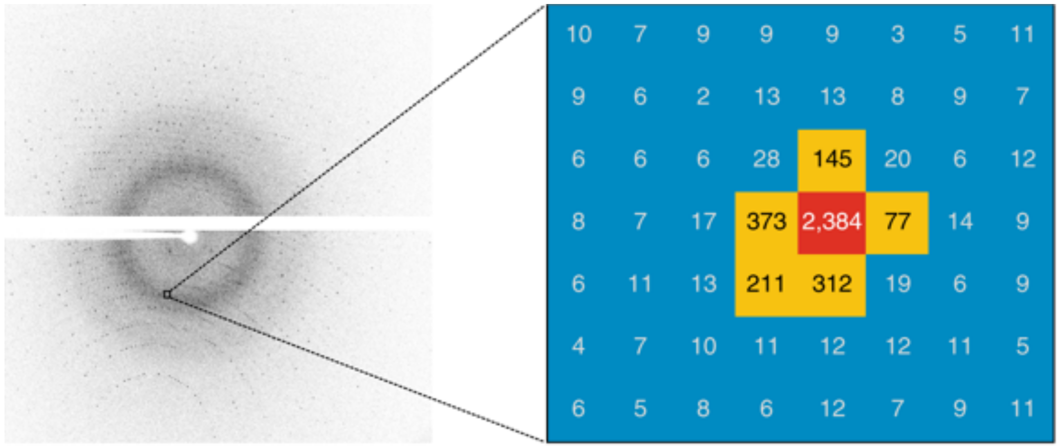
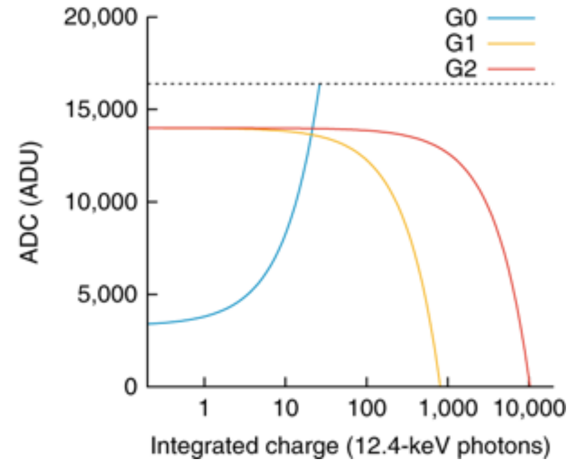


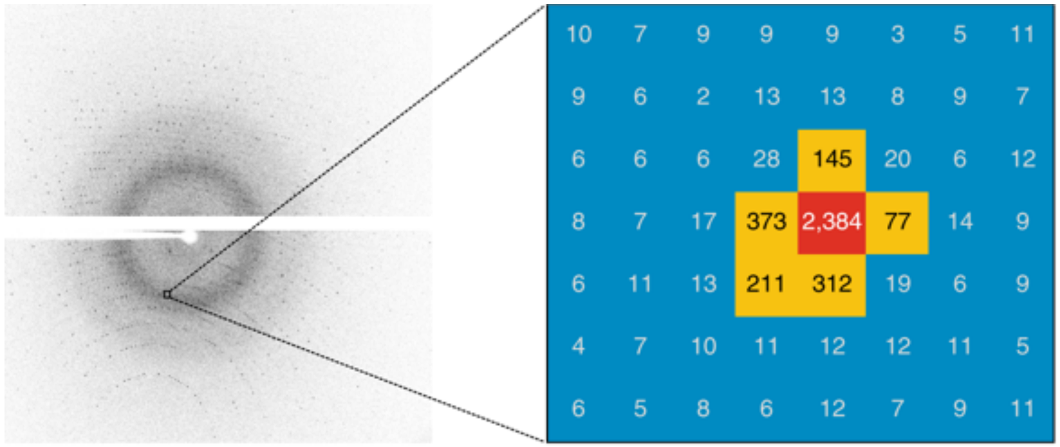


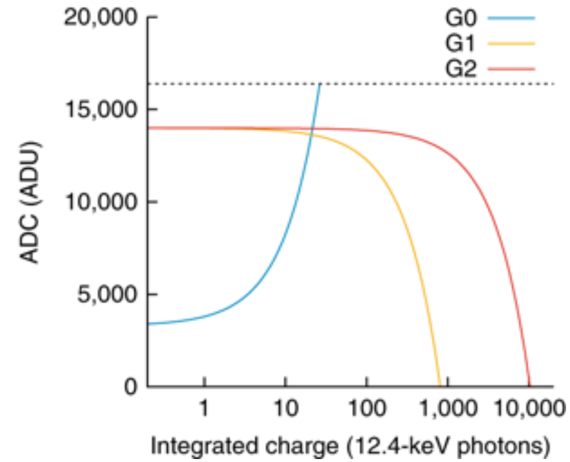
Pixel output in JF: 0101010111110011

Gain: 0001010111110011 00:G0 01:G1 11:G2

ADC value: 0001010111110011

Jungfrau Pixel Output





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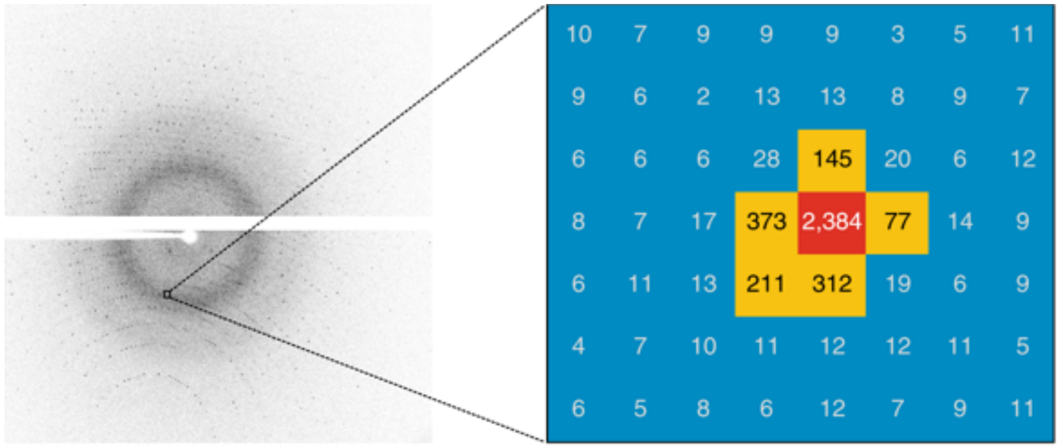
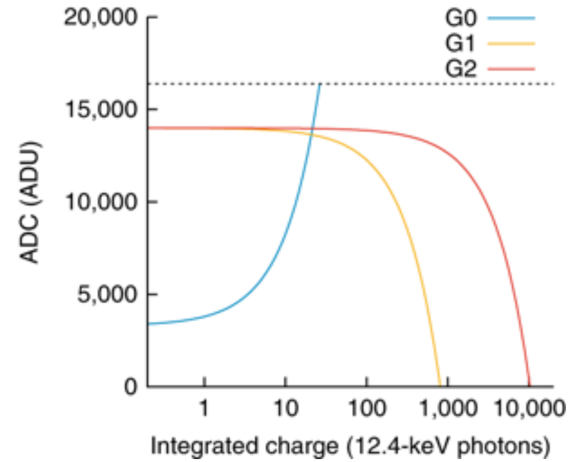
ADC value: 0001010111110011

Photon number: $= \frac{ADC - pedestal}{gain * photon\ energy}$

Jungfrau Pixel Output





Pixel output in JF: 0101010111110011

Gain: 0001010111110011 00:G0 01:G1 11:G2

ADC value: 0001010111110011

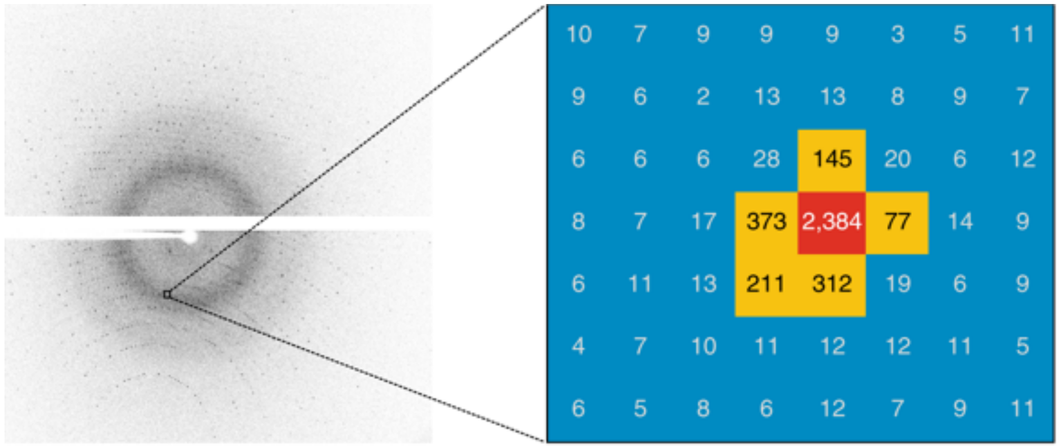
Dedicated dark run

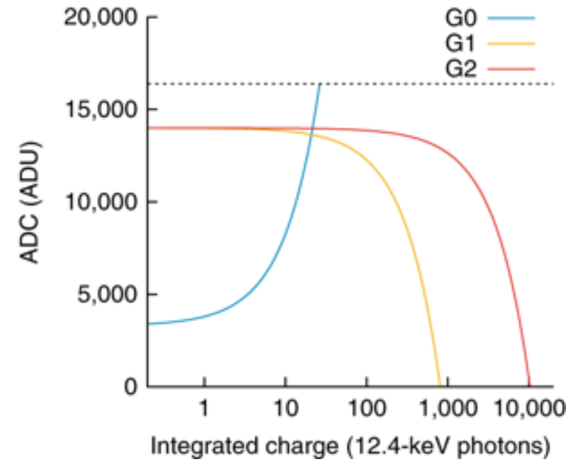
Photon number: $= \frac{ADC - pedestal}{gain * photon\ energy}$

Prior calibration

Gain and pedestal factors are specific for pixel and gain setting

Jungfrau Pixel Output





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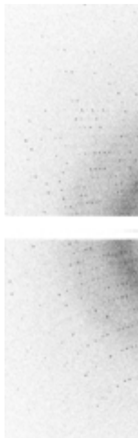
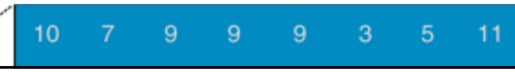
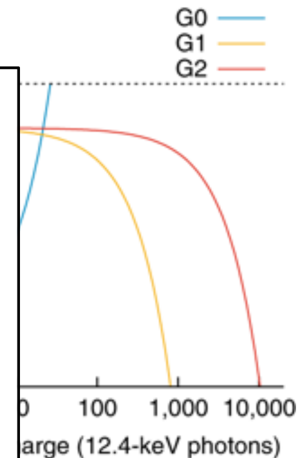
G0 pedestal varies with time and needs to be tracked

Jungfrau Pixel Output



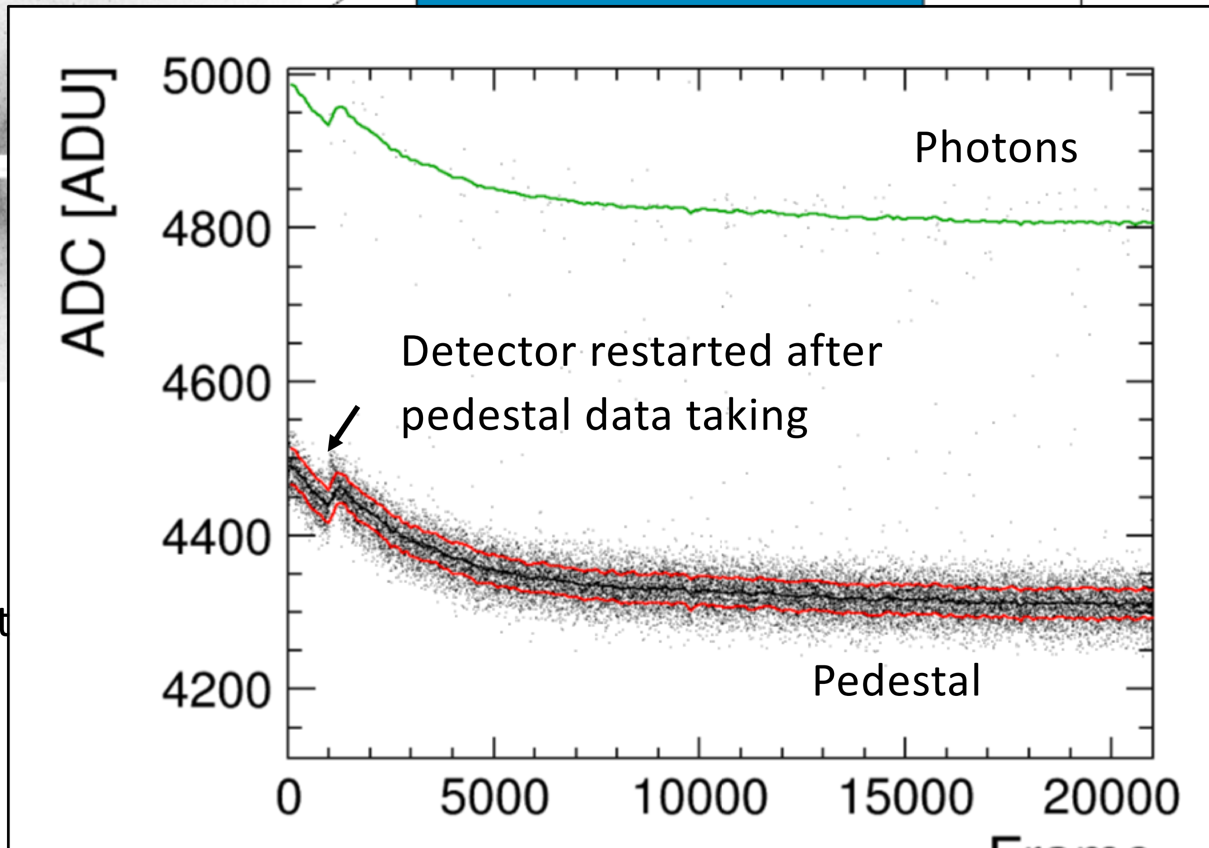




Pixel output

Gain: G2

ADC value:



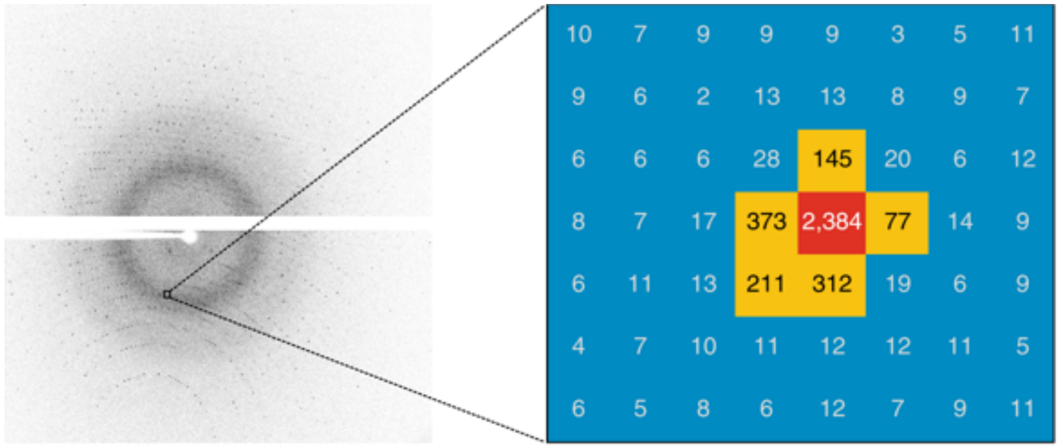
Redford *et al.*, JINST, 13, C11006

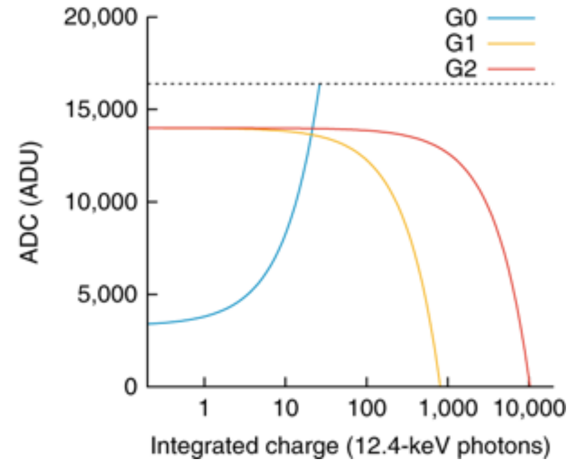
Photon number: $= \frac{ADC - pedestal}{gain * photon\ energy}$

es with longer integration time and higher temperature

(higher framerate is always better)

Jungfrau Pixel Output





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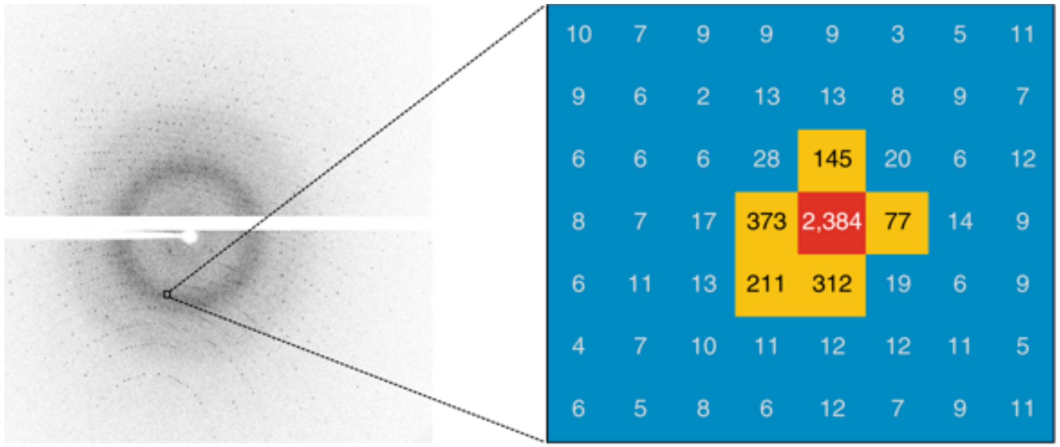
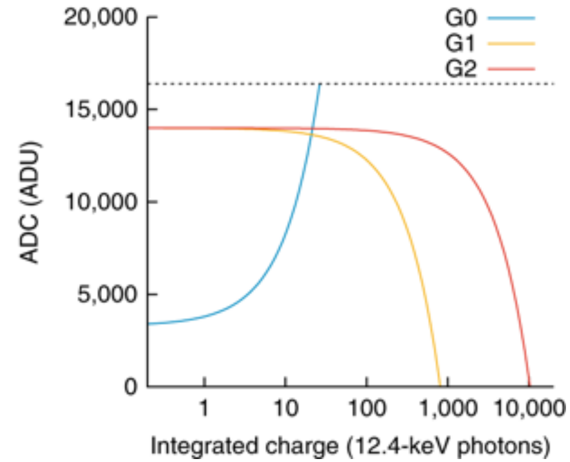
Pedestal increases with longer integration time and higher temperature
(higher framerate is always better)

Jungfrau Pixel Output





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Floating point number

- Negative counts possible (not handled by data processing software at the moment)
- Fractional counts relevant (charge sharing)

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Data Conversion

Jungfrau Data Conversion

- Currently, both raw data and converted data are stored
- Raw data do not compress very well
- Raw data are necessary for detector development
- Raw data will most likely not benefit end user
- Converted data are already of very good quality
- For user operation only converted data should be kept and these will be very similar to data produced by EIGER
  – Currently we imitate EIGER very well (REST interface and HDF5)

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Jungfrau Data Conversion Challenge

- Fast operation is necessary for good detector performance
  – 1.1 kHz at the moment, 2.4 kHz next year

- Pedestal values depend on temperature of the sensor and should be collected within a short delay from the experiment

- One needs to convert ADUs to photons to add frames together:
  – 5916 ADU in G0 + 300 ADU in G1 = ?

- Since conversion factors are specific for pixel, gain setting and detector conditions, hardware lookup tables cannot be used for that purpose

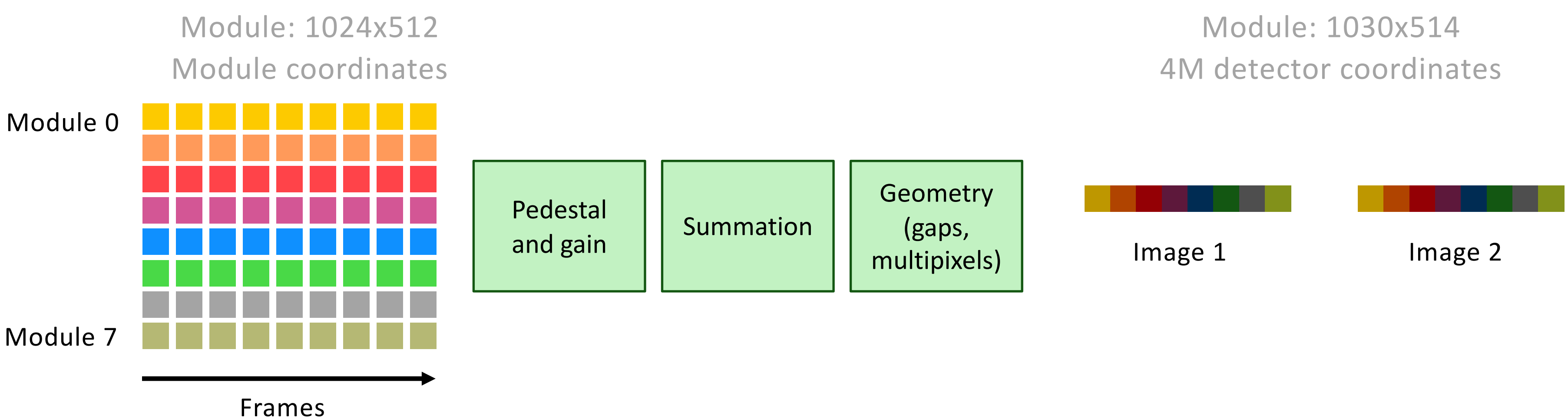
- One needs a floating point unit: CPU, GPU or Field Programmable Gate Array (FPGA)

Jungfrau Data Conversion Challenge

- Data flow for 4M detector:
  - 4,194,304 pixels x 16-bit = 8 MB
  - 8 MB * 1.136 kHz = 9 GB/s (72 Gbit/s or 8x10 GbE links)
  - 8 MB * 2.400 kHz = 19 GB/s (153 Gbit/s or 16x10 GbE links)
- Raw data need to be received by a computer, before calculations can be performed on CPU/GPU
- There is no space for transmission control protocol (TCP) overhead, so if frames are not received, they are lost
- x86-64/Linux machines are not designed for real time applications
- With HPE DL580 Gen10 (4x12C Intel Xeon 6148 + 1.5 TB of RAM) we can handle both data receiving and data conversion for 4M @ 1.1 kHz, but not simultaneously

Converter Architecture

- Input data
  - Placed in 4 RAM disks (2 modules per RAM disk)
  - Separate files per module
  - Modules (even pixels) are independent for conversion purpose
- Output data
  - Compressed HDF5 file with NeXuS (Dectris flavor) metadata for Albula/Neggia
  - Compression operates on full images, so needs to combine all modules in one place
  - It is currently impossible to have separate HDF5 files for each region



Jungfrau Data Conversion Challenge

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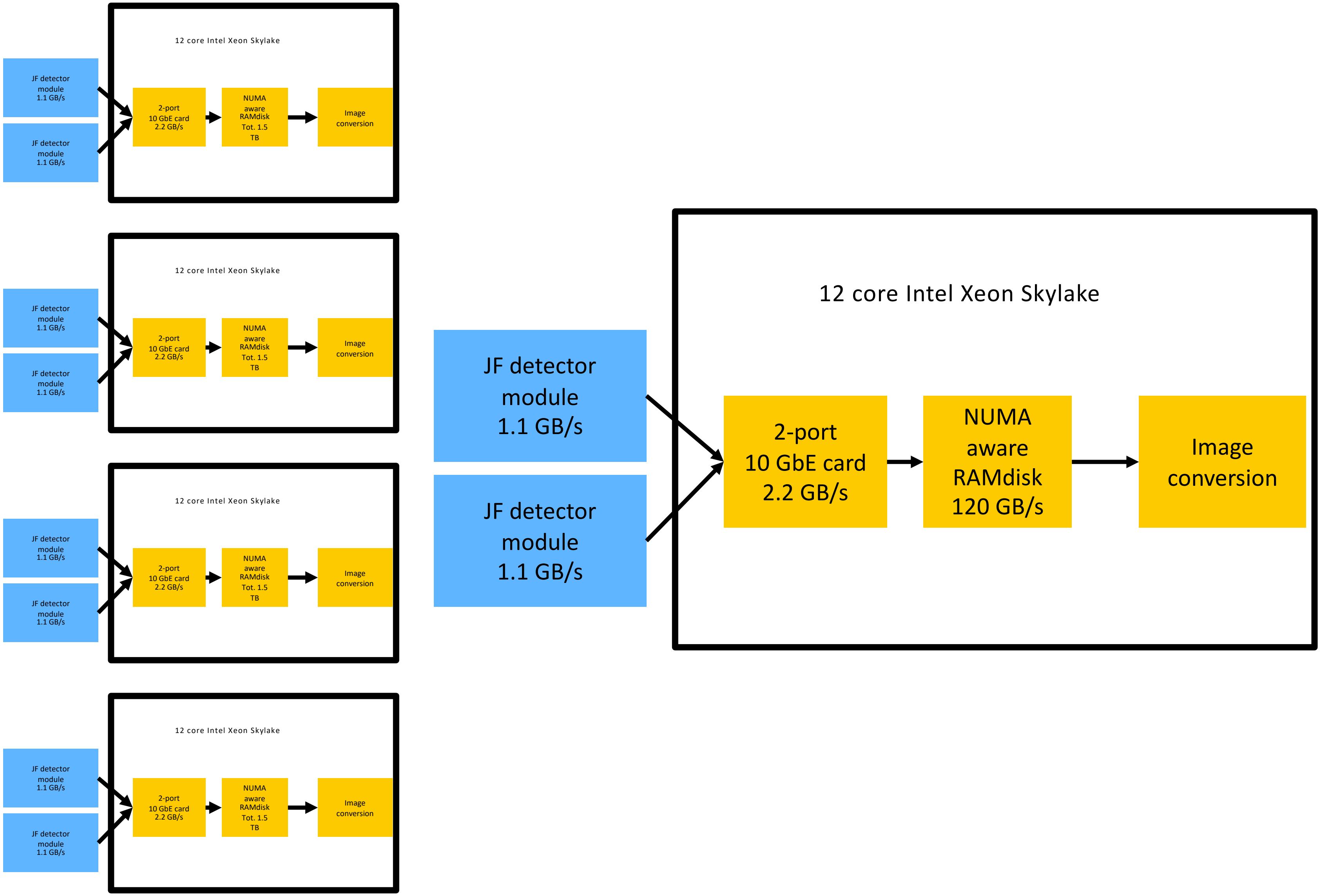

Total Performance

- 32 converter threads (4 per module)
- 16 writer threads
- Single instruction multiple data optimizations (AVX-512 for Intel Xeon)

- Protein crystal
  - 87290 frames (+3000 pedestal)
  - 3 s pedestal
  - ~76 s of data collection

Summation	Execution [s]	Per frame [us]	Throughput* [GB/s]
1	41.7	478	17.5
5	19.2	220	38.1
10	15.3	175	47.9
20	17.3	198	42.4

* - throughput based on input frame size only, i.e. 8 MB/frame time

- Execution time includes all steps, from reading raw data to writing final HDF5
- Compression time is non-deterministic (depends on data entropy)

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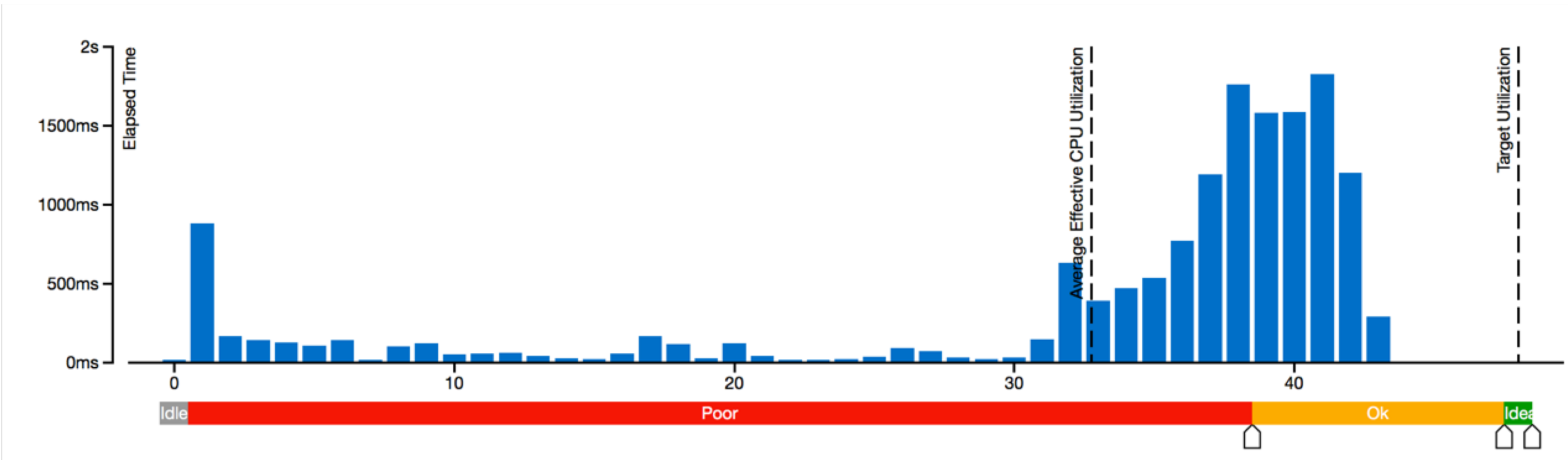
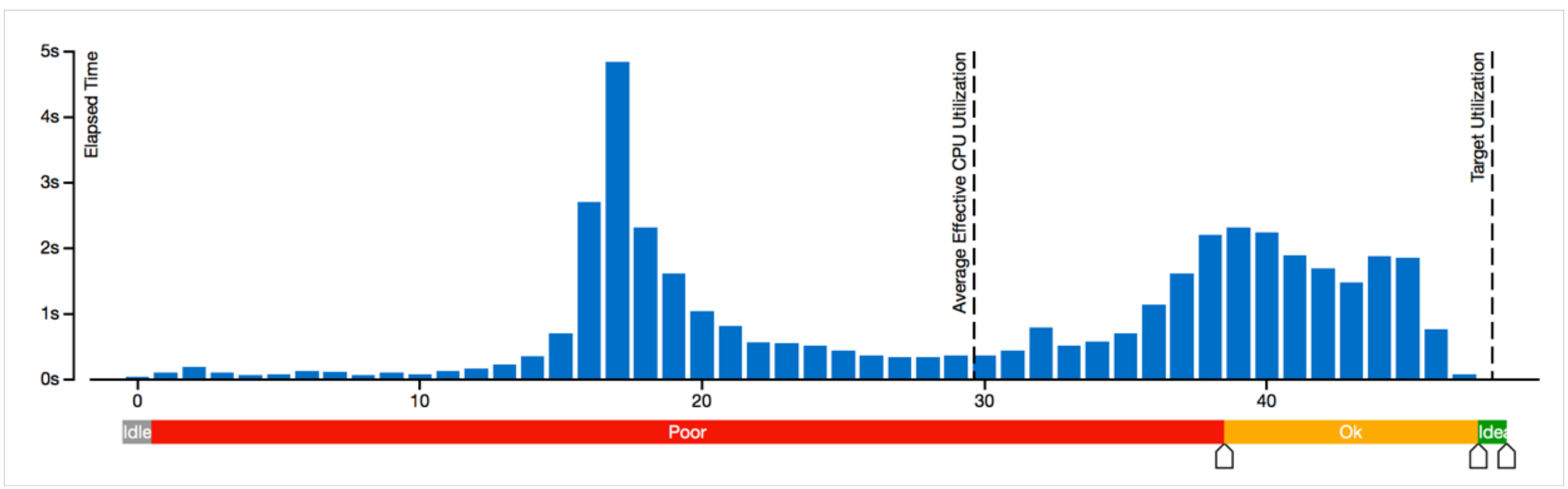
Core Utilization – Intel VTune



Summation of 10



Summation of 1

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Floating-Point Unit Load – Intel VTune

Elapsed Time: 15.265s

SP GFLOPS: 200.012

Effective CPU Utilization: 68.2%

Average Effective CPU Utilization: 32.749 out of 48

Effective CPU Utilization Histogram

Memory Bound: 52.3% of Pipeline Slots

Cache Bound:	19.4%	of Clockticks
DRAM Bound:	23.6%	of Clockticks
NUMA: % of Remote Accesses:	0.0%	

FPU Utilization: 3.3%

SP FLOPs per Cycle:	2.137 Out of 64
Vector Capacity Usage:	100.0%
FP Instruction Mix:	
% of Packed FP Instr.:	100.0%
% of 128-bit:	0.0%
% of 256-bit:	0.0%
% of 512-bit:	100.0%
% of Scalar FP Instr.:	0.0%
FP Arith/Mem Wr Instr. Ratio:	1.169

Summation of 10

Elapsed Time: 41.725s

SP GFLOPS: 73.079

Effective CPU Utilization: 61.7%

Average Effective CPU Utilization: 29.628 out of 48

Effective CPU Utilization Histogram

Memory Bound: 48.0% of Pipeline Slots

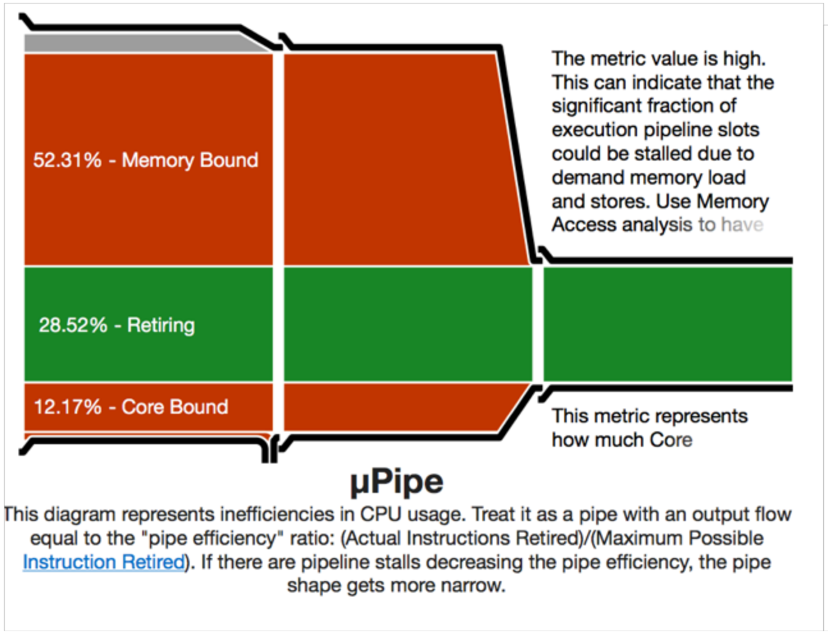
Cache Bound:	21.0%	of Clockticks
DRAM Bound:	20.8%	of Clockticks
NUMA: % of Remote Accesses:	0.0%	

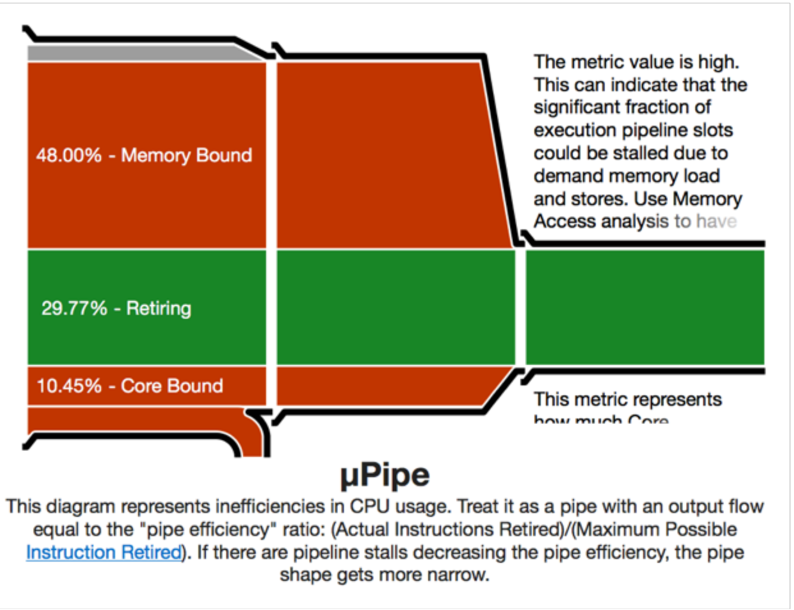
FPU Utilization: 1.3%

SP FLOPs per Cycle:	0.803 Out of 64
Vector Capacity Usage:	97.8%
FP Instruction Mix:	
% of Packed FP Instr.:	97.7%
% of 128-bit:	0.1%
% of 256-bit:	0.0%
% of 512-bit:	97.6%
% of Scalar FP Instr.:	2.3%
FP Arith/Mem Wr Instr. Ratio:	0.417

Summation of 1

Microarchitecture Utilization – Intel VTune





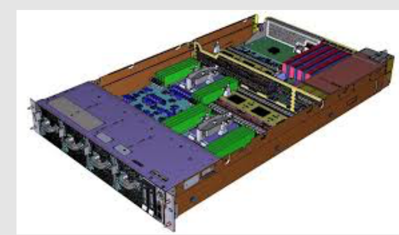
Summation of 10

Summation of 1

Data Challenge Conclusions

- Data receiving needs to be offloaded by network boards with FPGA chips, writing raw frames directly to memory without CPU/kernel involvement

- Jungfrau 4M @ 1.1 kHz possible in real time
- Jungfrau 10M @ 2.4 kHz – most likely impossible with a single PC
- Computational complexity is very limited (3% of FPU utilization)



- Memory transfers are the limiting factor
  - GPU is not easy answer, as PCI Express is a bottleneck
  - More severe problem for multi-PC system
  - Splitting data files for 2D regions could help a lot

- Architectures optimized for higher data throughput are needed (IBM POWER) or hybrid architectures FPGA+Xeon / FPGA+ARM

Data Challenge Conclusions

High data rate challenge of Jungfrau is driven by operational reasons, mainly related to dark current, however solving the challenge will benefit MX scientific goals

High dose-rate strategy requires fast framerate detectors to achieve reasonable phi-slicing – to get 0.10^{o}/image one needs:

1.0 kHz for full area of the detector at 100^{o}/s rotation speed
2.0 kHz for full area of the detector at 200^{o}/s rotation speed

2.4 kHz for full area of the detector at 360^{o}/s rotation speed → 0.15^{o}/image

Data processing will need to follow and we already need to think on GPU/FPGA/TPU/? implementations, due to Moore's Law limitations

HDF5 Practicalities

HDF5 Format Practicalities

- **Virtual datasets** would allow data from separate modules could be compressed and written independently, without a need to gather all data before

- **Parallelization** is highly limited by lack of fully thread-safe libhdf5

- **Signed integer** for photon counts: pedestal distribution can result in negative counts

- **Amplification factor (gain) in metadata**: Jungfrau can report partial (half, quarter) photons in case of charge sharing, fixed-point format (2, 4, 8 or 16 counts per photon) would be better and easier than floating point storage

- **No count rate correction** and **per pixel** saturation level

- **Compression**
  - Bitshuffle: AVX-512 instructions library, FPGA implementation should be trivial
  - Hardware accelerated compression (IBM POWER9, NVIDIA GPUs)

- **Sparse data format**: assuming 0 or 1 photons per pixel/frame Jungfrau allows to calculate energy and position with precision higher than one pixel for each photon

- **Metadata**: For XFEL applications each frame is associated with metadata – saving these results in a very poor performance

My thanks go to

- PSI Detector Group
  - Sophie Redford
  - Aldo Mozzanica
  - Bernd Schmitt
- PSI MX Group
  - Zac Panepucci
  - Meitian Wang
- PSI IT Group
  - Leonardo Sala
  - Dmitry Ozerov
  - Heiner Billich
  - Derek Feichtinger
- Photon Factory KEK
  - Naohiro Matsugaki
  - Yusuke Yamada
- Dectris
  - Stefan Brandstetter
  - Andreas Förster