PAUL SCHERRER INSTITUT

Filip Leonarski :: Beamline Data Scientist :: Paul Scherrer Institut

NXmx Gold Standard at PSI

(Prague), Aug 22th, 2020

MX endstations at PSI

Swiss Light Source	X06SA (PX)	Versatile academic and high-throughput industrial	EIGER 16M
	X10SA (PXII)	Dedicated industrial	EIGER2 16M
	X06DA (PXIII)	Native-SAD	PILATUS2 2M
SwissFEL	Alvra	Injector	JUNGFRAU 16M
	Bernina	Fixed Target	JUNGFRAU 16M
	Cristallina	In construction (fixed target from Bernina)	JUNGFRAU 9M

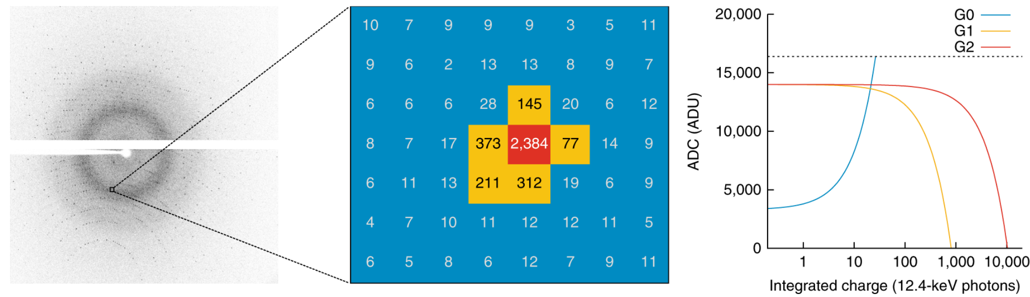
MX endstations at PSI

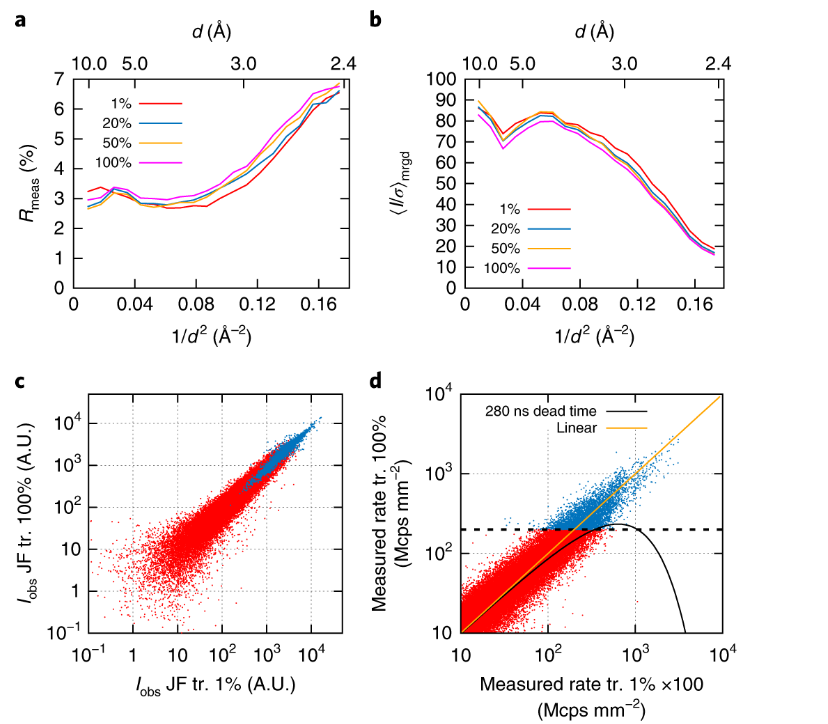
Swiss Light Source	X06SA (PX)	Versatile academic and high-throughput industrial	EIGER 16M
	X10SA (PXII)	Dedicated industrial	EIGER2 16M
	X06DA (PXIII)	Native-SAD	PILATUS2 2M → JUNGFRAU 4M (2021) and 10M (2023)
SwissFEL	Alvra	Injector	JUNGFRAU 16M
	Bernina	Fixed Target	JUNGFRAU 16M
	Cristallina	In construction (fixed target from Bernina)	JUNGFRAU 9M

PAUL SCHERRER INSTITUT

JUNGFRAU

- Adaptive gain charge integrating detector developed at the Paul Scherrer Institute
- Detector necessary for FEL and suitable for synchrotron applications
- High-flux (no count rate correction)
- Low energy (no corner effect)





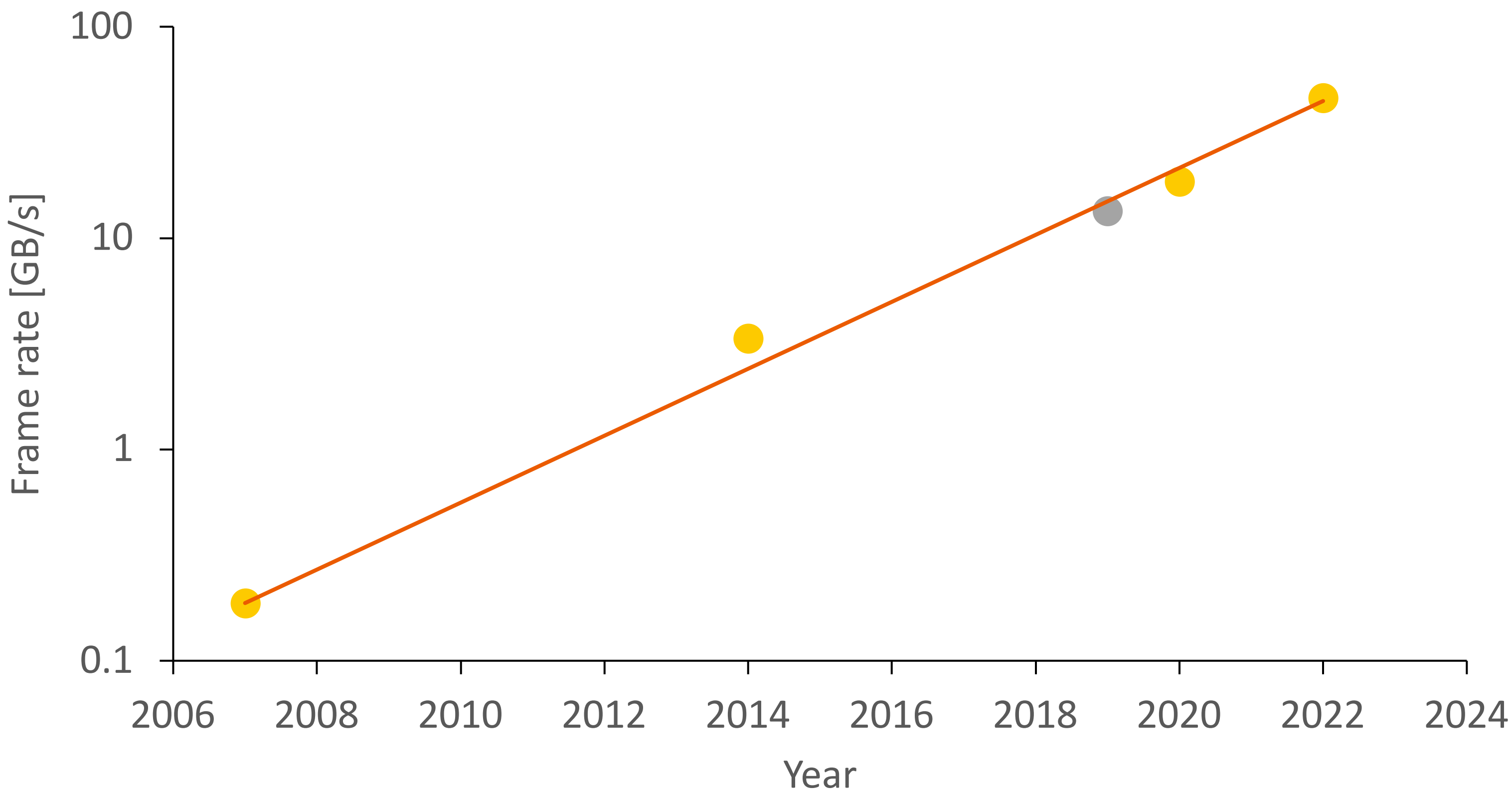
F. Leonarski et al. *Nat. Methods*, **15**, 799-804 (2018)

PAUL SCHERRER INSTITUT

JUNGFRAU at SwissFEL and SLS

	SwissFEL	SLS
X-ray	Femtosecond pulses	Continous beam
Integration time	10 µs	425 µs
Framerate	100 Hz (10 ms)	2200 Hz (450 µs)
Temperature	18^{o}C	-15^{o}C
Data collection	Mostly continous (injector)	Mostly burst (rotation, raster, fixed target)
User community	Small, experienced, used to HW formats, DIY pipelines	Broad, expects efficient integration with data processing pipelines and high level of automation
Data backend	Standard servers Linux application (C++ and python)	Task specific architecture Mix of C++ flavors (CPU, CUDA, FPGA HLS)

SLS MX detector data rates double every 2 years



2007	PSI PILATUS	6 Mpixel	12.5 Hz	**0.2 GB/s**
2014	Dectris EIGER	16 Mpixel	133 Hz	**3.4 GB/s**
2019	Dectris EIGER 2 XE	16 Mpixel	400 Hz	**13.5 GB/s**
2020	PSI JUNGFRAU	4 Mpixel	2200 Hz	**18.4 GB/s**
2022	PSI JUNGFRAU	10 Mpixel	2200 Hz	**46.1 GB/s**

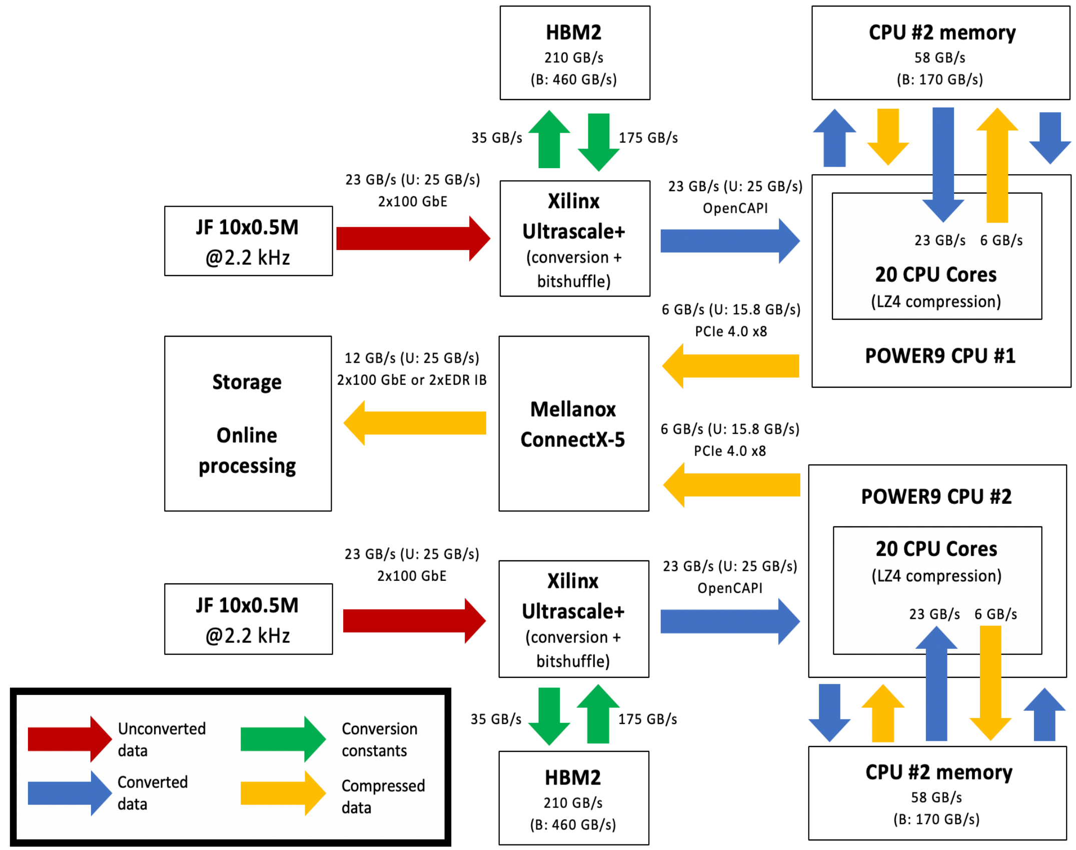
Handling 20 – 50 GB/s is possible in a single server

- Task specific hardware allows to greatly reduce challenge of handling high data rates

- Based on IBM POWER9 architecture

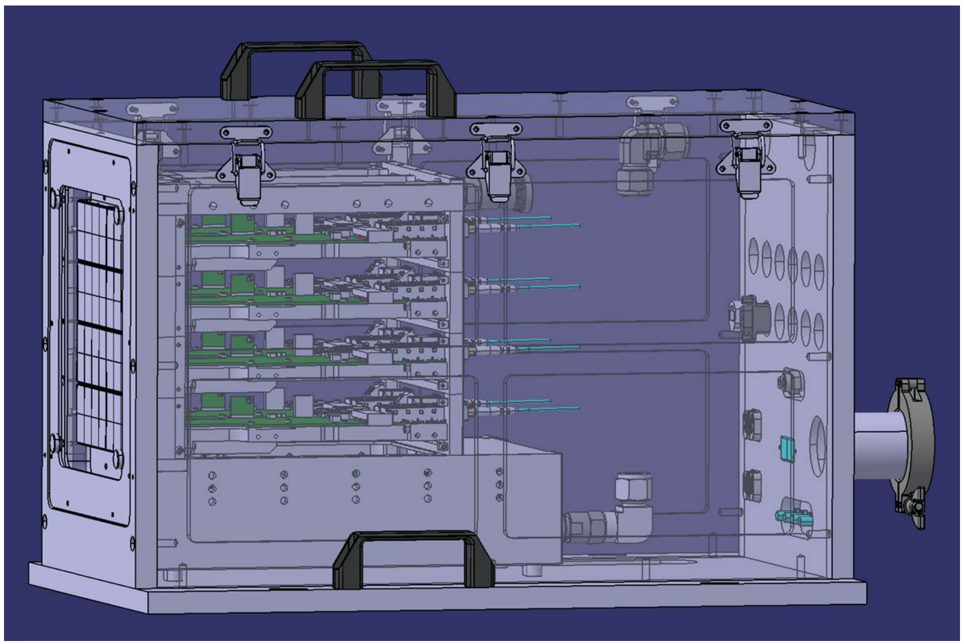
- Successful partnership with IBM to develop FPGA board capable of smoothly handling 2 kHz readout and online conversion

- Among goals are **fully NXmx compliant metadata**

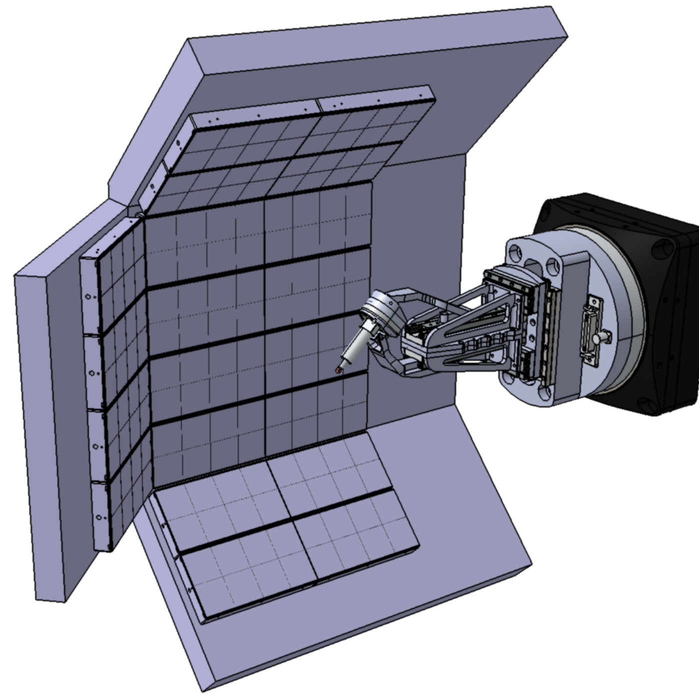


Leonarski et al. *Struct. Dyn.* (2020)

JUNGFRAU for X06DA



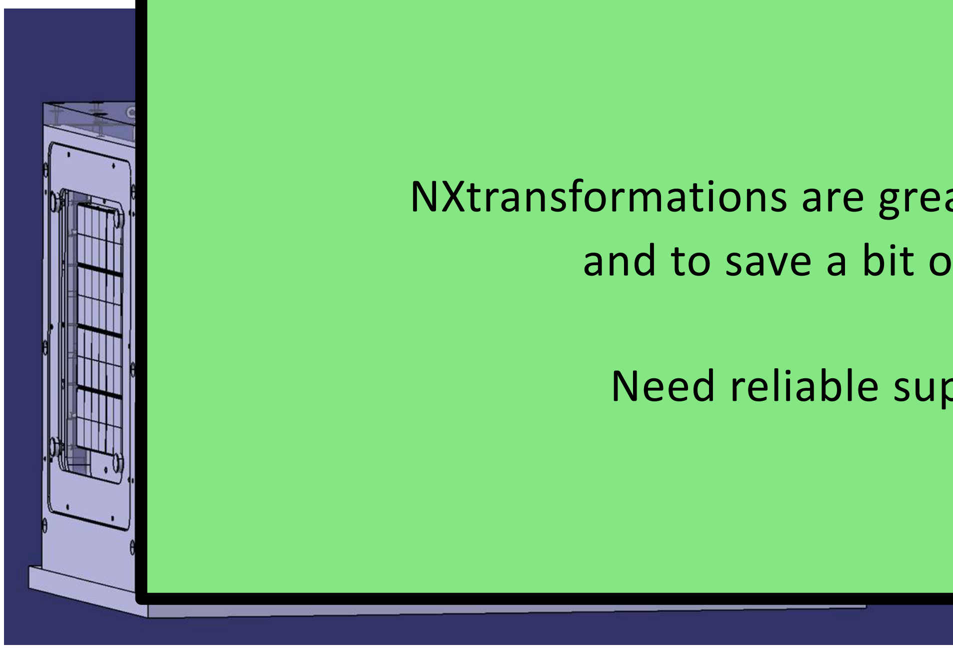
4 Mpixel (2021)

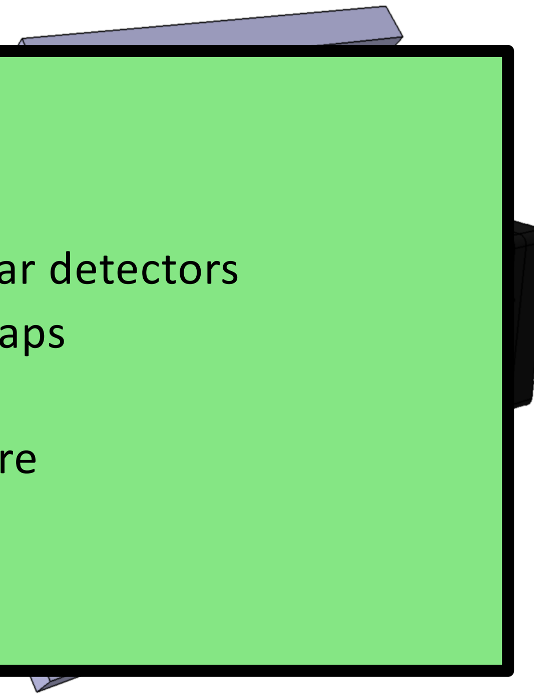


10 Mpixel (2023)

S. Vetter
S. Hasanaj
W. Glettig

JUNGFRAU for X06DA





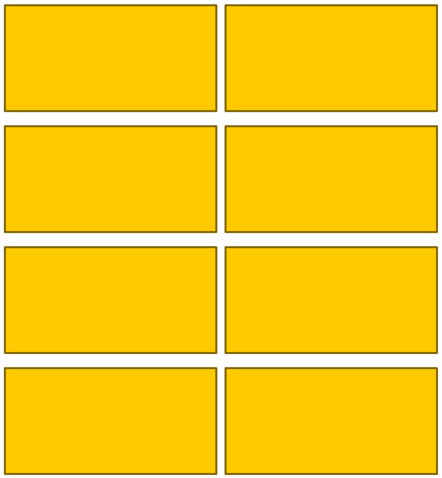
NXtransformations are great for non-planar detectors
and to save a bit of memory on gaps

Need reliable support in software

4 Mpixel (2021)

10 Mpixel (2023)

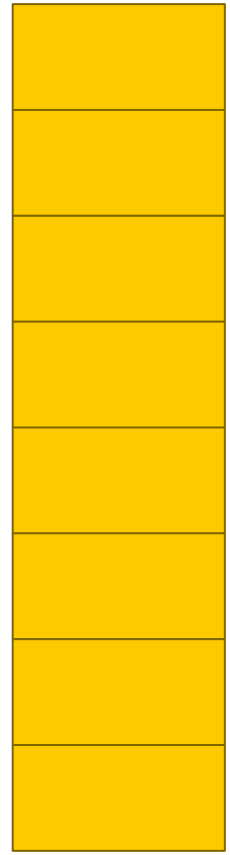
Image representation



"Synchrotron" format

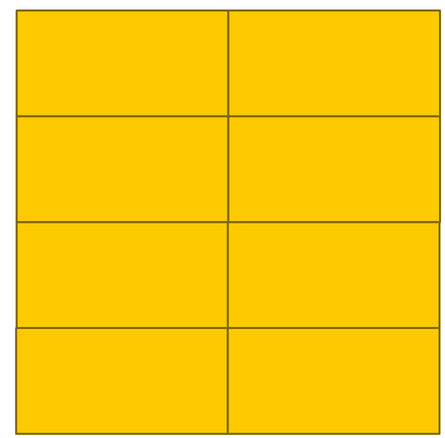
- Modules are placed in the image according to their real position (+/- half pixel)
- Simple for data analysis programs
- One line corresponds to few modules → all of them need to be known for compression
- Virtual datasets possible in HDF5, but performance is a problem

- 235,680 pixels in gaps → 5% more memory space/throughput to store nothing



"XFEL" format

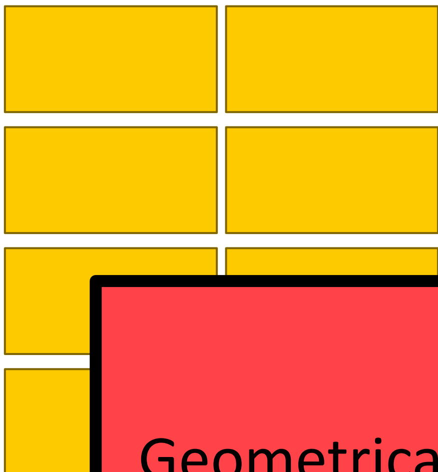
- Modules are placed sequentially
- Needs instructions to rebuild real image for analysis and visualization
- Good for non-planar detectors
- Supported by newer data analysis programs (XDS, DIALS, CrystFEL), but might be less intuitive, esp. for XDS users
- Very nice for data acquisition

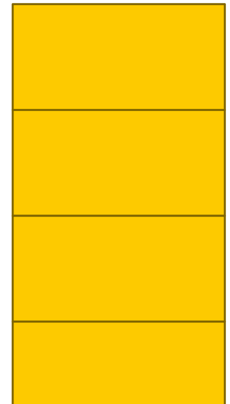


Middle ground

- Close to real geometry
- No gaps

Image representation





“XFEL” format

- Modules are placed sequentially
- Needs instructions to rebuild real image for analysis and visualization
- Good for non-planar detectors
- Supported by newer data analysis programs (XDS, DIALS, CrystFEL), but might be less intuitive, esp. for XDS users
- Very nice for data acquisition

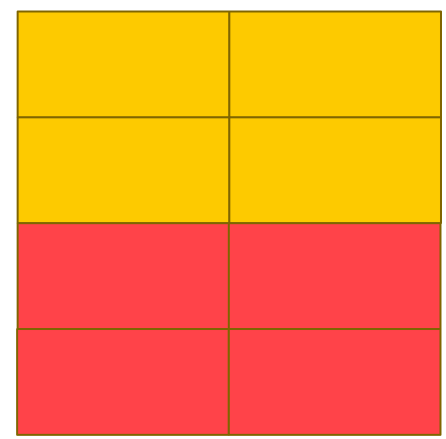
“Synchro

- Modules a
  to their re
- Simple for
- One line c
  of them ne
- Virtual dat
  performan

- 235,680 p
  space/thro

Geometrical HDF5 chunking of images to meet throughput

(either through chunks or separate files → might need VDS)



round

al geometry
- No gaps

JUNGFRAU Pixel Representation

- ADU + gain – directly read out by detector (16-bit)
  - 2-bit: gain level used
  - 14-bit: accumulated charge

- Not compressible
- Not directly useful for data processing
- Easiest to read-out
- Necessary for polychromatic experiments (fluorescence) and for development

- Accumulated energy (eV or keV)
  - Subtract dark current and multiple by conversion factor (both gain and pixel specific)
  - Floating point number (16-, 32- or 64-bit)
  - Can be negative (dark current noise)

- Compression possible, but not optimal
- Commonly used for FEL data processing
- Provides extra precision, but questionable if necessary for MX

- Photon count
  - Divide by X-ray energy
  - Round to integers (half, quarter, etc.)
  - 16- or 32-bit (un)signed integer

- Very close to EIGER (but negative counts)
- Well compressed
- Good enough for most MX applications (FEL and synchrotron alike)
- Synchrotron standard

JUNGFRAU Pixel Representation

- ADU + gain – directly read out by detector (16-bit)
  - 2-bit: gain level used

- Not compressible
- Not directly useful for data processing
- Easiest to read-out
- Necessary for polychromatic experiments

All of these can be provided based on facility practices and user needs.

This should be encoded in NXmx, as critical part of the metadata!

E.g. NXdata could have ”units” attribute (raw ADU, 1 keV, 128 eV, 1/3 photon)

- Photon count
  - Divide by X-ray energy
  - Round to integers (half, quarter, etc.)
  - 16- or 32-bit (un)signed integer

- Very close to EIGER (but negative counts)
- Well compressed
- Good enough for most MX applications (FEL and synchrotron alike)
- Synchrotron standard

PAUL SCHERRER INSTITUT

Considerations for NXmx

1. Different corrections for integrating and photon counting detectors
    1. Replace Boolean fields with corrections with flexible list (fixed dictionary) OR
    2. Provide DOI for paper/technical document/software repository describing corrections
2. Impossible to visualize images at 2 kHz → spot finding and indexing as part of data acquisition pipeline (GPU or FPGA accelerated)
    1. Spot positions or possible indexing solution become integral part of data generated by data acquisition stream – how to store them?
    2. CXIDB has format to store spot information, should these be integrated in NXmx?
3. Compression becomes a hot topic
    1. New lossless and lossy compression algorithm available (e.g. Zstd gives 20% improvement in compression), but how to smoothly integrate them in NXmx?
4. Handling non-standard experiments
    1. Raster scans, small wedges, injector

JUNGFRAU NXmx working group?

I would like to propose an adaptive gain integrating detector working group for NXmx to propose modifications to accommodate calibration data and conversion procedure in the format

More information

- F. Leonarski et al.; JUNGFRAU detector for brighter x-ray sources: Solutions for IT and data science challenges in macromolecular crystallography
  – https://doi.org/10.1063/1.5143480
- S. Redford et al.; Operation and performance of the JUNGFRAU photon detector during first FEL and synchrotron experiments
  – https://doi.org/10.1088/1748-0221/13/11/C11006
- F. Leonarski et al.; Fast and accurate data collection for macromolecular crystallography using the JUNGFRAU detector
  – https://doi.org/10.1038/s41592-018-0143-7
- I. Martiel et al.; X-ray fluorescence detection for serial macromolecular crystallography using a JUNGFRAU pixel detector
  – https://doi.org/10.1107/S1600577519016758

Acknowledgements

- Paul Scherrer Institute
  - MX Group
  - Detector Group
  - Science IT
  - Controls
  - PSD Management

- KEK, CERN, Uni Konstanz, MAX IV, ESRF, DLS, BNL

- HDR MX Community

- Dectris

- IBM, Inno-Boost AG