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

NXmx Gold Standard at PSI

(Prague), Aug 22th, 2020
## MX endstations at PSI

<table>
<thead>
<tr>
<th>Swiss Light Source</th>
<th>SwissFEL</th>
<th>Versatile academic and high-throughput industrial</th>
<th>Dedicated industrial</th>
<th>Native-SAD</th>
<th>EIGER 16M</th>
<th>EIGER2 16M</th>
<th>PILATUS2 2M</th>
<th>JUNGFRAU 16M</th>
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<th>JUNGFRAU 9M</th>
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**Note:**
- **X06SA (PX)**: Versatile academic and high-throughput industrial with EIGER 16M.
- **X10SA (PXII)**: Dedicated industrial with EIGER2 16M.
- **X06DA (PXIII)**: Native-SAD with PILATUS2 2M → JUNGFRAU 4M (2021) and 10M (2023).
- **Alvra**: Injector with JUNGFRAU 16M.
- **Bernina**: Fixed Target with JUNGFRAU 16M.
- **Cristallina**: In construction (fixed target from Bernina) with JUNGFRAU 9M.
• 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)

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<th><strong>SwissFEL</strong></th>
<th><strong>SLS</strong></th>
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<tr>
<td><strong>X-ray</strong></td>
<td>Femtosecond pulses</td>
<td>Continous beam</td>
</tr>
<tr>
<td><strong>Integration time</strong></td>
<td>10 μs</td>
<td>425 μs</td>
</tr>
<tr>
<td><strong>Framerate</strong></td>
<td>100 Hz (10 ms)</td>
<td>2200 Hz (450 μs)</td>
</tr>
<tr>
<td><strong>Temperature</strong></td>
<td>18°C</td>
<td>-15°C</td>
</tr>
<tr>
<td><strong>Data collection</strong></td>
<td>Mostly continous (injector)</td>
<td>Mostly burst (rotation, raster, fixed target)</td>
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<tr>
<td><strong>User community</strong></td>
<td>Small, experienced, used to HW formats, DIY pipelines</td>
<td>Broad, expects efficient integration with data processing pipelines and high level of automation</td>
</tr>
<tr>
<td><strong>Data backend</strong></td>
<td>Standard servers Linux application (C++ and python)</td>
<td>Task specific architecture Mix of C++ flavors (CPU, CUDA, FPGA HLS)</td>
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SLS MX detector data rates double every 2 years

<table>
<thead>
<tr>
<th>Year</th>
<th>Detector/Model</th>
<th>Resolution</th>
<th>Frame Rate</th>
<th>Frame Rate [GB/s]</th>
</tr>
</thead>
<tbody>
<tr>
<td>2007</td>
<td>PSI PILATUS</td>
<td>6 Mpixel</td>
<td>12.5 Hz</td>
<td>0.2 GB/s</td>
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<tr>
<td>2014</td>
<td>Dectris EIGER</td>
<td>16 Mpixel</td>
<td>133 Hz</td>
<td>3.4 GB/s</td>
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<tr>
<td>2019</td>
<td>Dectris EIGER 2 XE</td>
<td>16 Mpixel</td>
<td>400 Hz</td>
<td>13.5 GB/s</td>
</tr>
<tr>
<td>2020</td>
<td>PSI JUNGFRAU</td>
<td>4 Mpixel</td>
<td>2200 Hz</td>
<td>18.4 GB/s</td>
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<tr>
<td>2022</td>
<td>PSI JUNGFRAU</td>
<td>10 Mpixel</td>
<td>2200 Hz</td>
<td>46.1 GB/s</td>
</tr>
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</table>
• 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

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
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Geometrical HDF5 chunking of images to meet throughput
(either through chunks or separate files à might need VDS)

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Geometrical HDF5 chunking of images to meet throughput (either through chunks or separate files à might need VDS)
JUNGFRAU Pixel Representation

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

• 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)

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

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

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

• Very close to EIGER (but negative counts)
• Well compressed
• Good enough for most MX applications (FEL and synchrotron alike)
• Synchrotron standard
• ADU + gain – directly read out by detector (16-bit)
  – 2-bit: gain level used

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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)

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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
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 JUNGFRAU.
• 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
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• Paul Scherrer Institute
  – MX Group
  – Detector Group
  – Science IT
  – Controls
  – PSD Management

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• HDR MX Community

• Dectris

• IBM, Inno-Boost AG