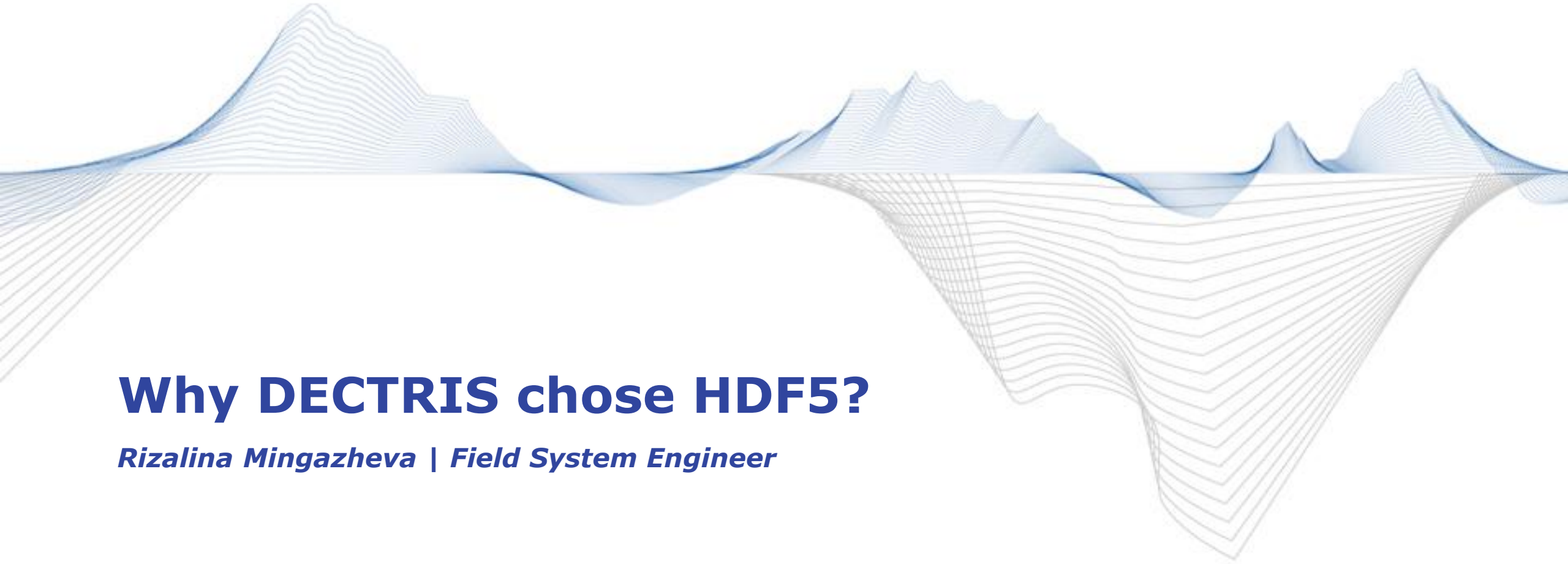
DECTRIS
detecting the future



Why DECTRIS chose HDF5?

Rizalina Mingazheva | Field System Engineer

DECTRIS Ltd.
5405 Baden-Dättwil
Switzerland
www.dectris.com

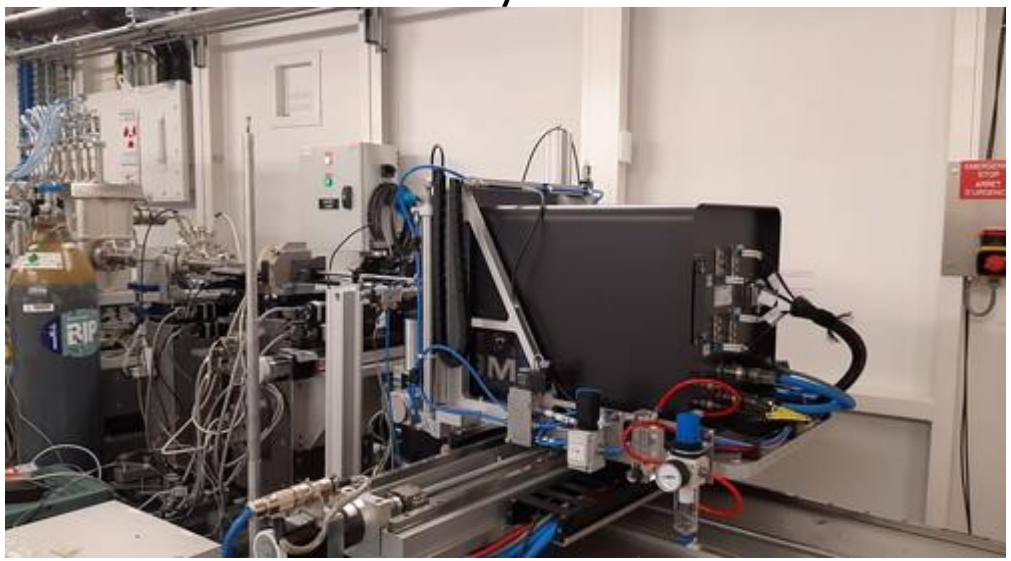
Who is DECTRIS?

DECTRIS: Mission and vision

- Provide the most reliable high-performance X-ray and electron detectors
- Enable scientific discoveries and advance human health by challenging the limits of detection technology

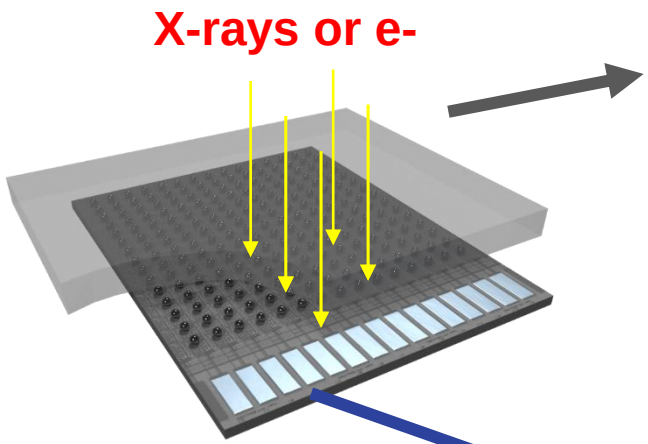
Lab

Syn



DECTRIS detecting the future

Hybrid-pixel X-ray and electron detectors



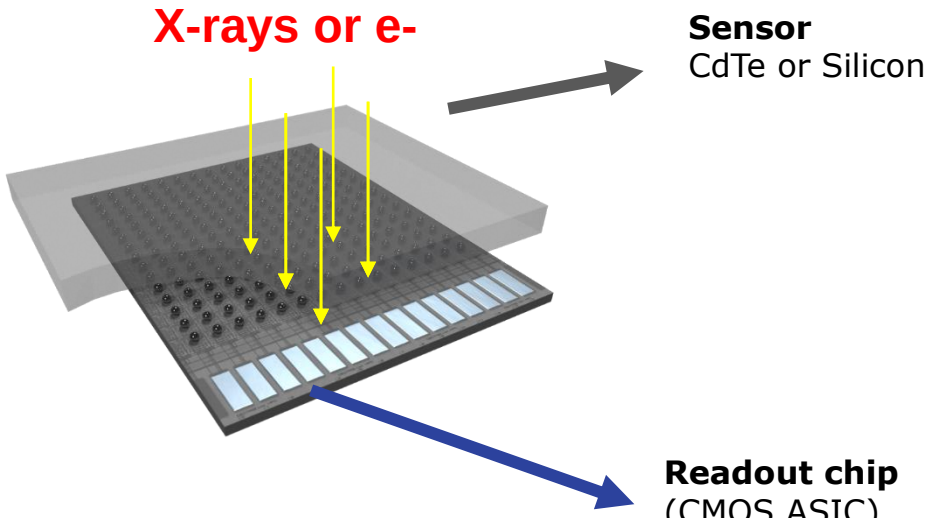
Sensor
CdTe or Silicon

Readout chip
(CMOS ASIC)

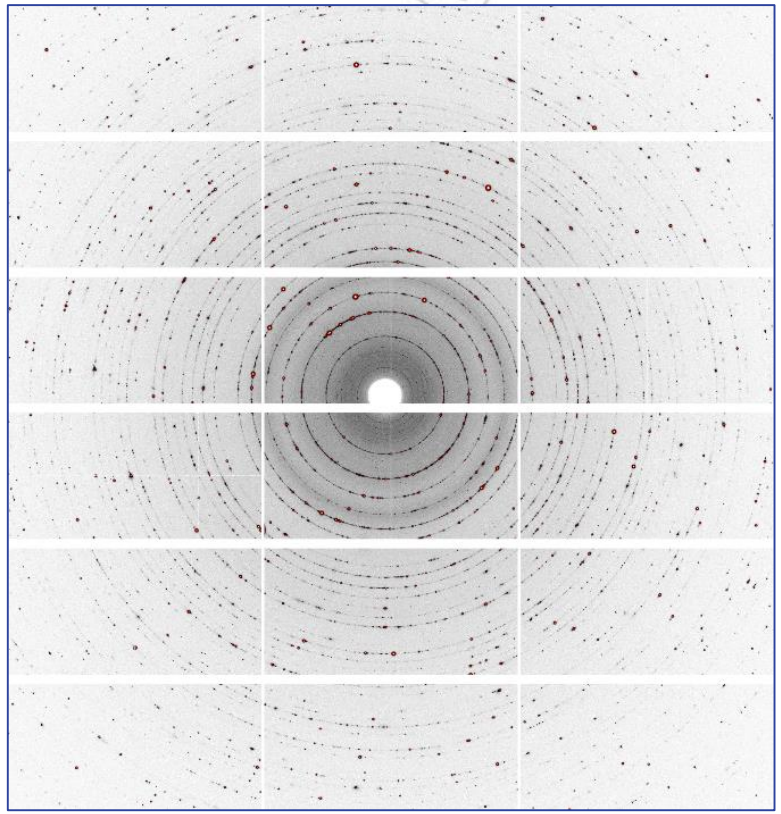
Only interactions with an energy higher than a given threshold are counted

DECTRIS detecting the future

Hybrid-pixel X-ray and electron detectors



9 MPixels!



Courtesy of Michael Hanfland, ESRF ID15B

Only interactions with an energy higher than a given threshold are counted

DECTRIS detecting the future

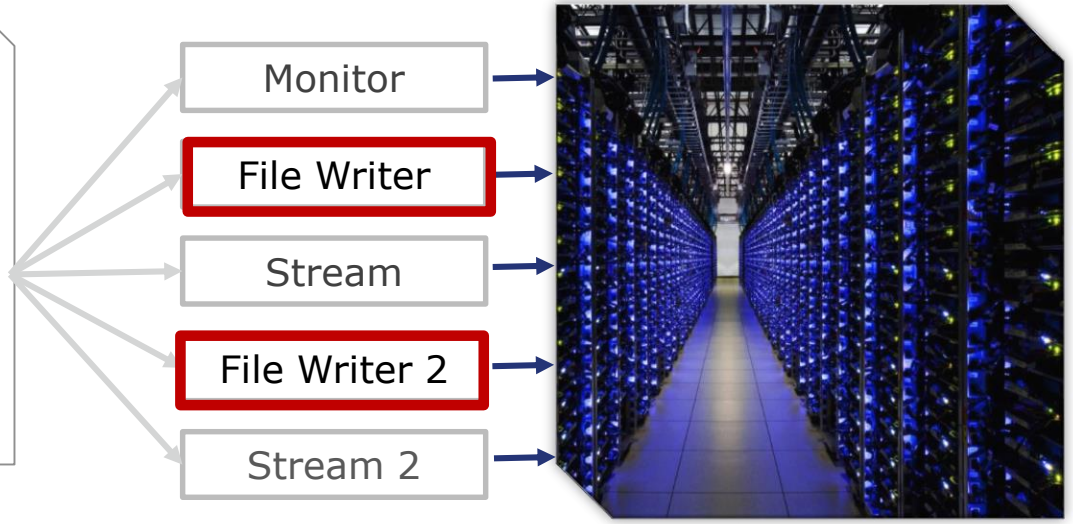
The flagship of our portfolio – EIGER2

Up to 16 Mpixels counting at 550Hz => Output 20GB/s before compression

* EIGER2 – two energy discriminating thresholds

EIGER/EIGER2 Data Interfaces

– Data interfaces enable access to image series



Filewriter/Filewriter2

Why HDF?

Driving force behind - frame rate

- 2011: start of the EIGER1 development
- Next generation detectors/requirement for a container file-format with fast and efficient compression

A new data format should be:

- Easy readable
- Universal
- Fast

HDF /NeXus

https://www.nexusformat.org/

HDF5 & NeXus

HDF5 – data format for recorded data

However:

- What to include in the data file?
- Which data type?
- How to name it?
- Where to put it?

NeXus:
an international
data standard

```
/
|
+-- entry
     |
     +-- data
     +-- instrument
     |    |
     |    +-- beam
     |    +-- detector
     |         |
     |         +-- detectorSpecific
     |         +-- geometry
     |         |    |
     |         |    +-- orientation
     |         |    +-- translation
     |         |
     |         +-- goniometer
     |         +-- module
     |         +-- transformations
     |
     +-- sample
          |
          +-- goniometer
          +-- transformations
          +-- beam
```

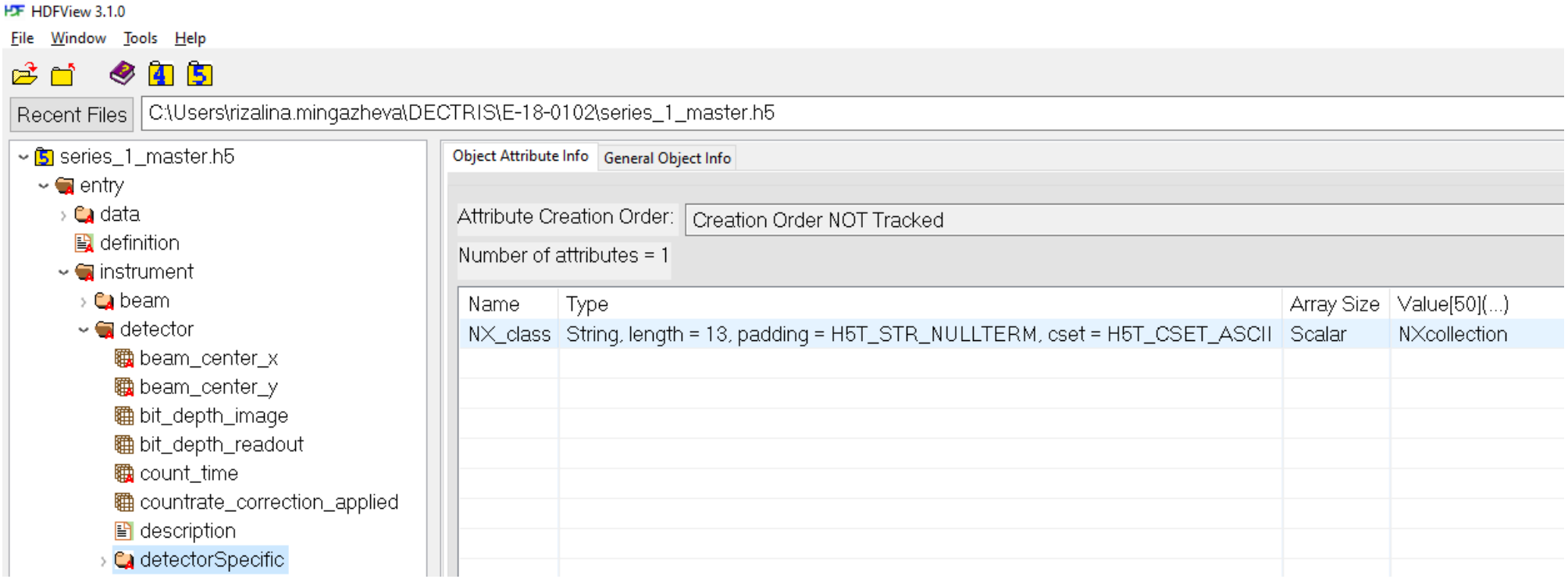
@NX_class = NXentry

@NX_class = NXdata

Inside of DECTRIS's HDF5 file

Human readable format:
Group names

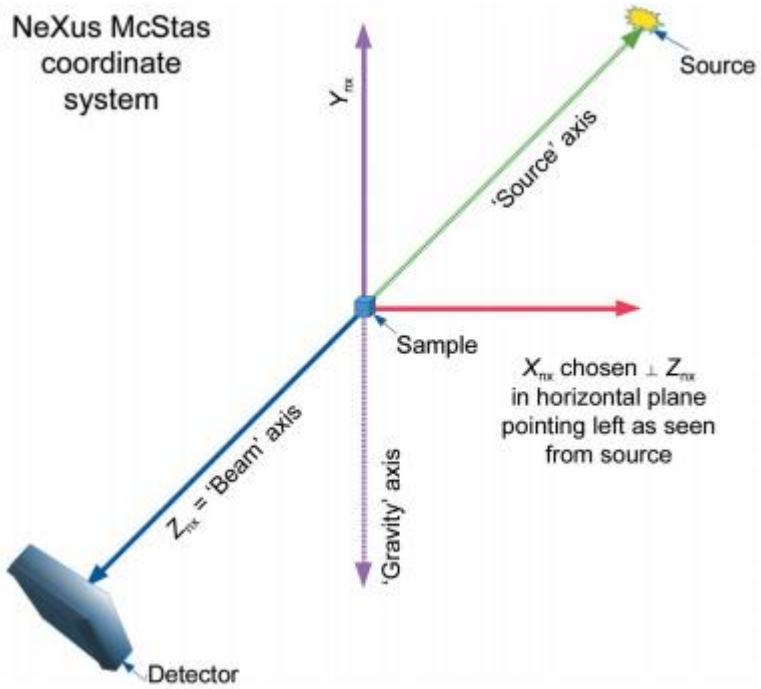
NX class names:
Type of object



DECTRIS detecting the future

NXmx Gold standard

- Facilitates the independent processing of data
- Focus on interoperability and reusability.



- entry
  - data
    - data_000001
  - definition
  - instrument
    - beam
    - detector
  - sample
    - beam
    - goniometer
    - transformations

Gold Standard for macromolecular crystallography diffraction data

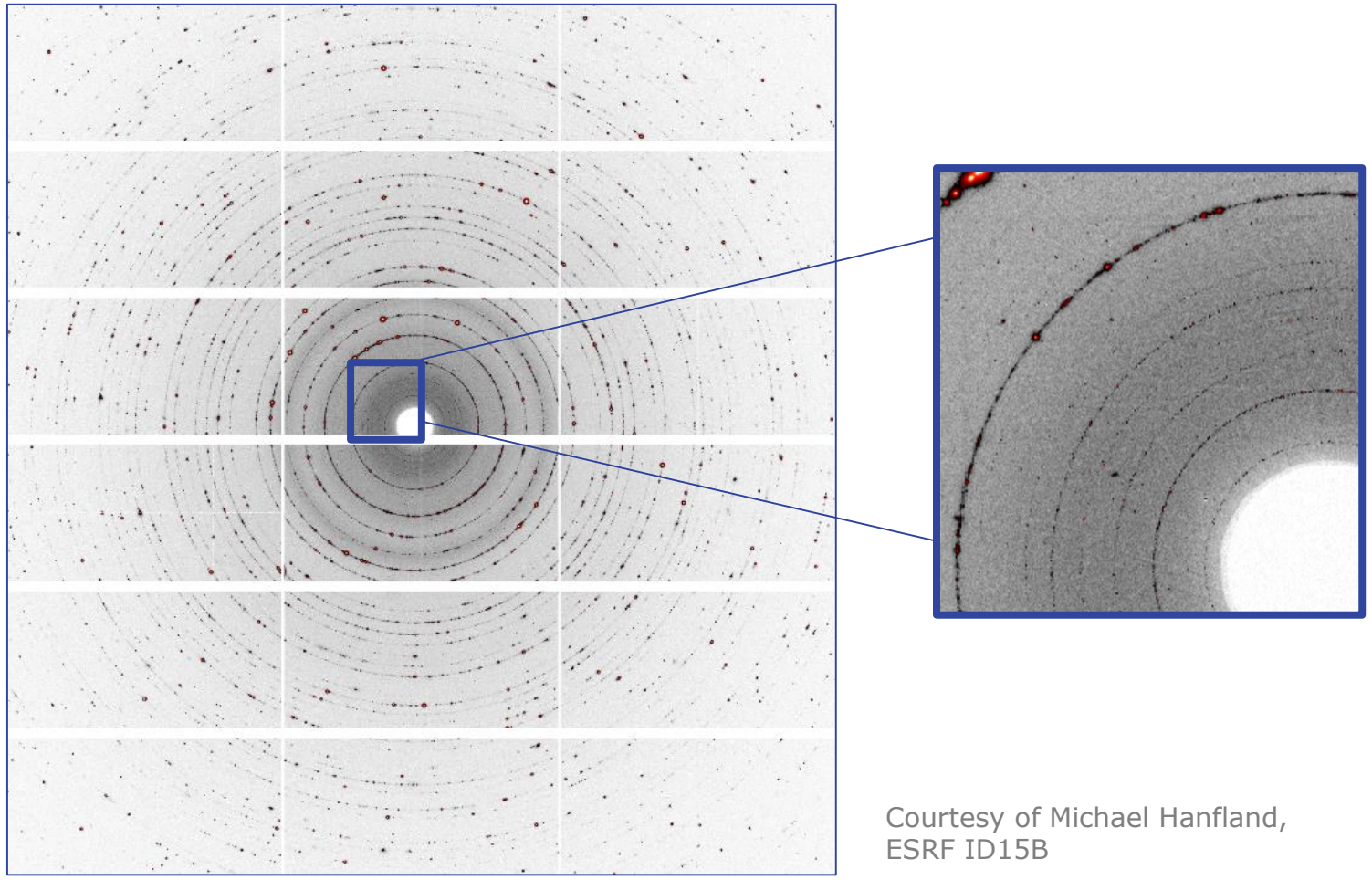
Herbert J. Bernstein
Ronin Institute for Independent Scholarship

EUROPEAN HDF USERS GROUP SUMMER 2021
7 - 8 JULY 2021

Bernstein et al., IUCrJ (2020). 7, 784–792

DECTRIS detecting the future

Why two energy discriminating thresholds?



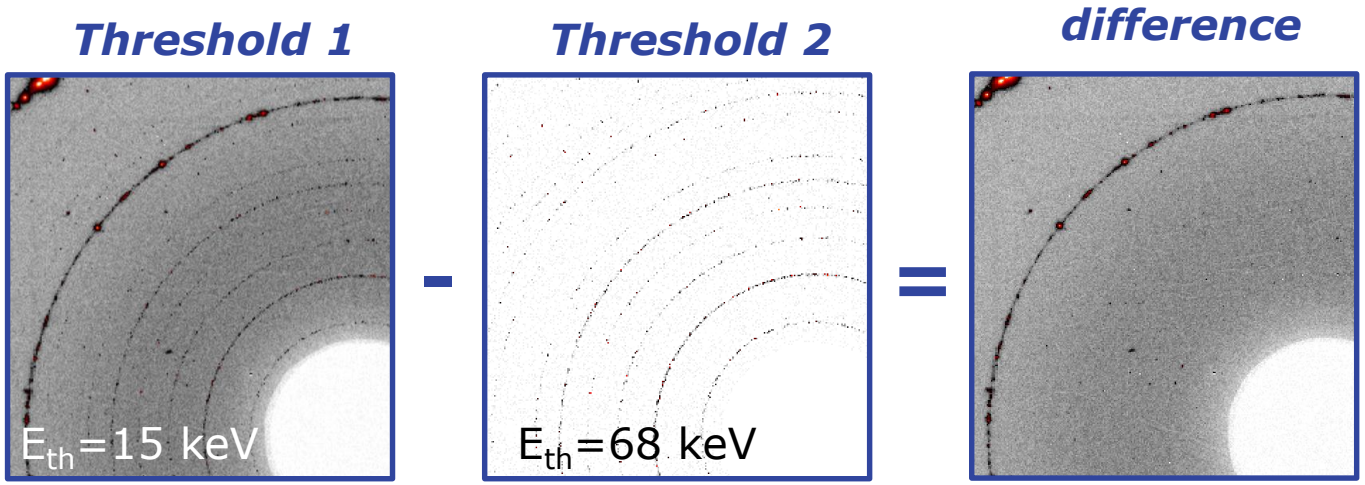
Courtesy of Michael Hanfland, ESRF ID15B

Experimental Condition

- *Detector:* ***EIGER2 X CdTe 9M***
- *Sample:* LaB_6
- *Energy: 30 keV*
- *Higher-Harmonic energy: 90 keV*

- *Unwanted diffraction rings from Higher-Harmonic contribution at low angles*

Two thresholds



Courtesy of Michael Hanfland,
ESRF ID15B

EIGER2 Advantage

- *Separation of different scattering contributions by energy*
- *Subtraction of unwanted signals*

Cleaner Diffraction Patterns

Filewriter2: Current involvement

- Reserve field prefix `DECTRIS_` documentation
  #993 opened on Mar 1 by soph-dec NXDL 2022.03
- NXdetector: Type of `GEOMETRY` group is deprecated
  #967 opened on Jan 18 by soph-dec
- NXmx: Change `entry/end_time_estimated` from "required" to "recommended"
  #966 opened on Jan 18 by soph-dec
- NXmx: Definitions for multi-channel (thresholds) data NIAC should review
  #940 opened on Aug 17, 2021 by soph-dec NXDL 2022.03
- NXdetector/NXmx: Add countrate_correction_lookup_table
  #975 opened on Feb 3 by soph-dec • Review required NXDL 2022.03
- NXdetector: Add virtual_pixel_correction_applied NIAC vote needed
  #942 opened on Aug 19, 2021 by soph-dec • Approved NXDL 2022.03
- NXdata: Fix type of AXISNAME_indices bug
  #941 opened on Aug 18, 2021 by soph-dec • Approved NXDL 2022.03

Filewriter 2

Challenge: how to store three images in one data file?

Alpha version will be available with next release 2022.1 (Aug ‘22)

Features

- Full nxmx (v1.0) support
- Multi threshold images
- Virtual data sets

Stay tuned!

Plans

- Gather feedback from pilot groups (data pipelines, image analysis)
- Release Filewriter2 Q4/22 or Q1/23

DECTRIS at HDF5 USER GROUP (HUG) 2021

1. *Herbert J. Bernstein*
   Gold Standard for MX diffraction data

2. *Jon Wright, ESRF*
   Experiences with GPU decompression for bitshuffle + LZ4 data

3. *Graeme Winter, DLS*
   Live Eiger Analysis with HDF5 & SWMR

Contact for further discussion

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Field System Engineer
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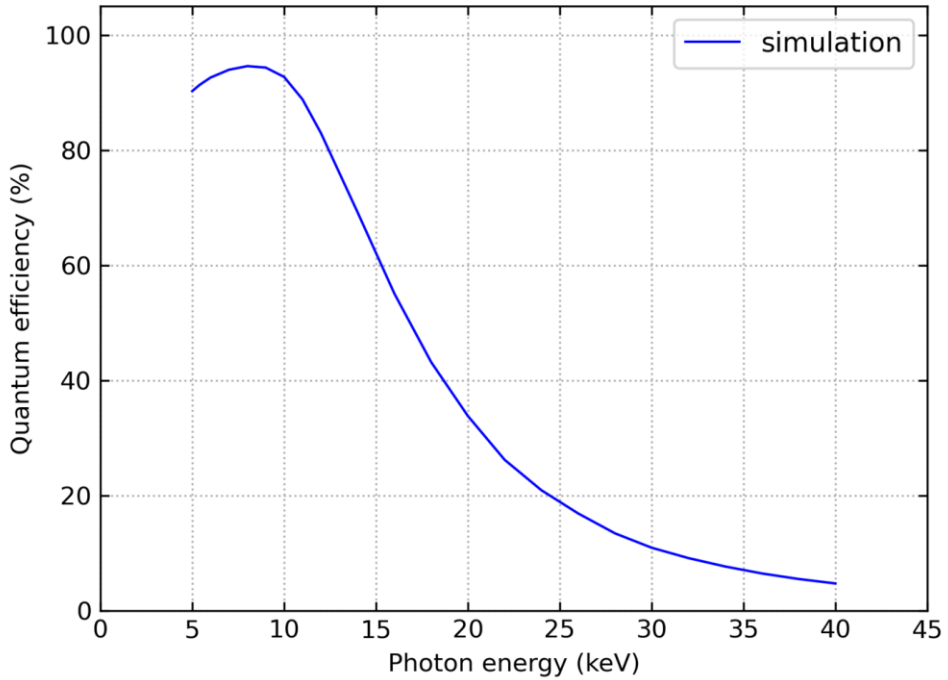
Diego Gämperle:
Product Owner – customer software
Email: diego.gaemperle@dectris.com

Backup slides

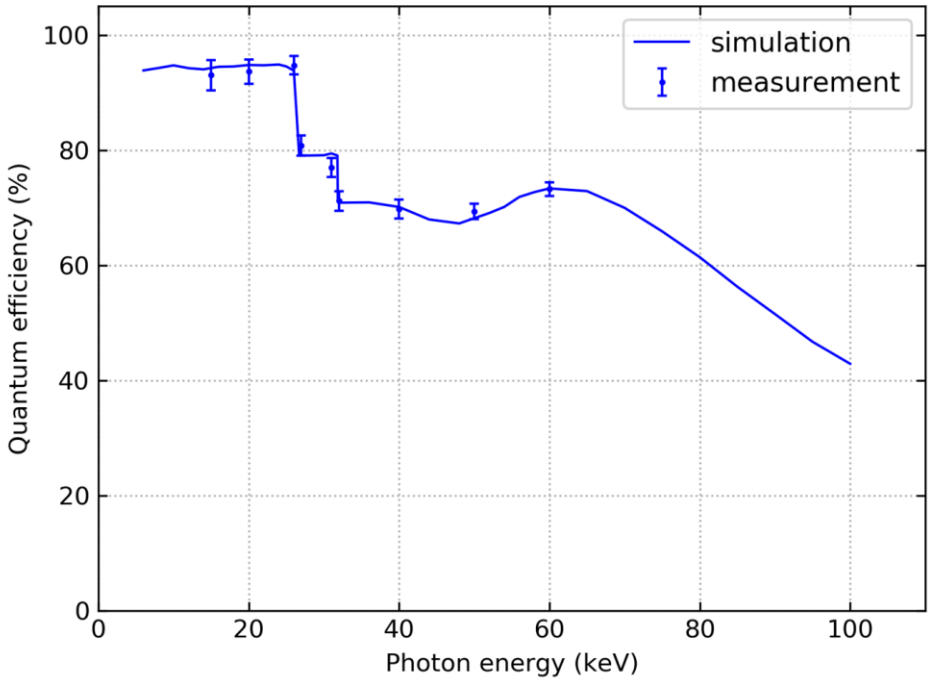
EIGER2 Sensor Materials

Silicon



Ideal for for 6 - 20 keV

CdTe



High Efficiency for 8 - 100 keV

P. Zambon, Nuclear Inst. and Methods in Physics Research, A 892 (2018) 106–113

DECTRIS detecting the future

Current portfolio – Electron Detection

DECTRIS ELA

Unleashing the full potential of Electron Energy Loss Spectroscopy

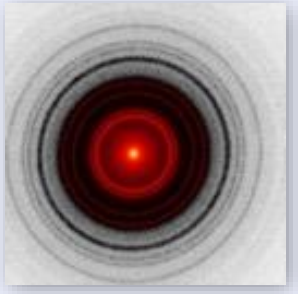
APPLICATIONS

EELS, 4D-STEM

SPECIFICATIONS

1024 x 512 pixels
4.5 kHz
>1 pA/pixel

DECTRIS QUADRO



The entry-level Hybrid-Pixel Detector

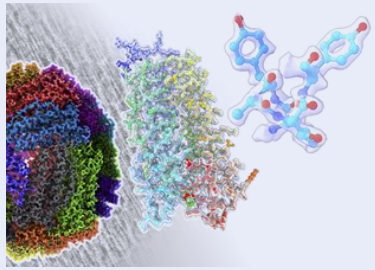
APPLICATIONS

Electron Diffraction
Small-molecule µED

SPECIFICATIONS

512 x 512 pixels
4.5 kHz (18 kHz with ROI)
>1 pA/pixel

DECTRIS SINGLA



Optimized for CryoEM at 100 keV

APPLICATIONS

CryoEM, µED

SPECIFICATIONS

1024 x 1062 pixels
4.5 kHz
5-200 keV

DECTRIS
detecting the future

X-Ray Products

MYTHEN2 X

Photon counting strip detectors

50 µm strips, 1 kHz

MYTHEN

PILATUS3 S/X

Photon counting area detectors

172 µm pixels, Si & CdTe

PILATUS

EIGER2 S/X/XE

Photon counting area detectors

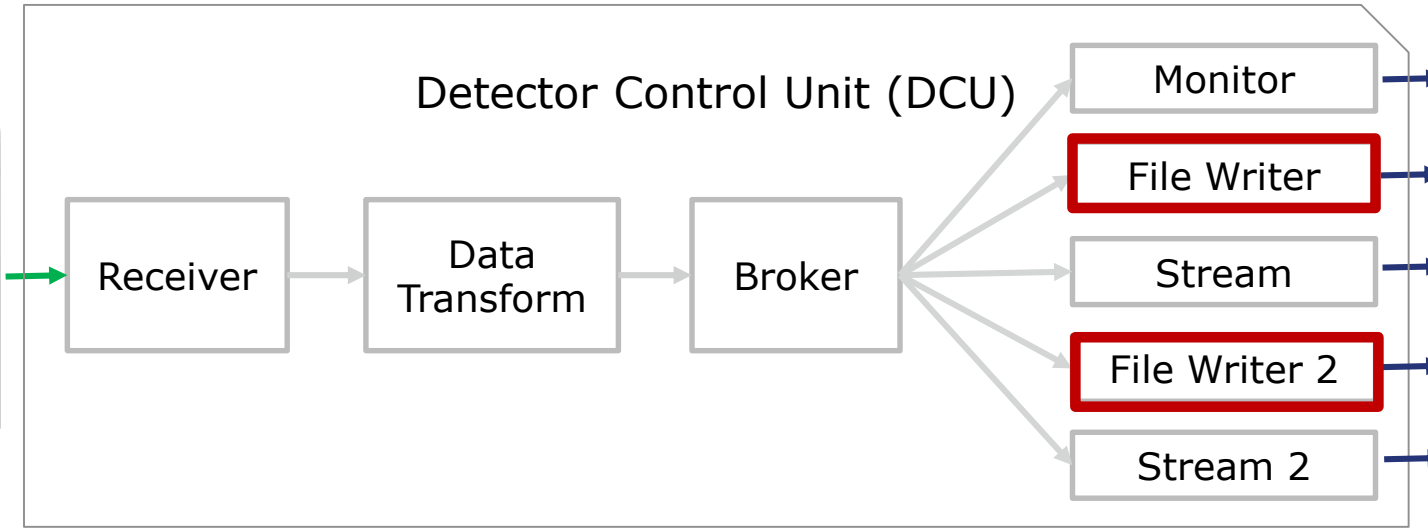
75 µm pixels, Si & CdTe

EIGER

DECTRIS detecting the future

EIGER/EIGER2 Data Interfaces

- Data interfaces enable access to image series
- Multiple data interfaces are available
  - different beamlines/laboratories have different requirements
- Multiple data interfaces can be active simultaneously
  - no more than 2 high performance interfaces active at any given time



DECTRIS
detecting the future

New features in HDF5: direct_write

Functionality:

The new function is easy to use. We can write uncompressed and precompressed data, and we are able to read them back (given the applied compression algorithm is implemented as a HDF5 – Filter)

Performance:

The performance of the new function is high and achieves nearly the native performance of writing directly to a Unix file. It is nearly independent of chunk size, but for very small chunks, the performance breaks down.

Credits:

The implementation of the new direct_write function is financed by PSI and Dectris Ltd.

New features in HDF5: filter plugin

Problem:

Users want to read our (compressed) data with proprietary programs like matlab, IDL, or with different languages like C/C++, python, java, …
Writing a filter wrapper for each language and program is tedious or even impossible. Filters used: snappy, lz4

Solution:

The HDF5 group implements a filter plugin mechanism, which allows us to write one library (.so, .dll) containing the filter. This library can then be preloaded by the program, and the filter is automatically applied when H5Dread/H5Dwrite is called.

Credits:

The implementation of filter plugin function is financed by DESY.

ious involvement and learnings

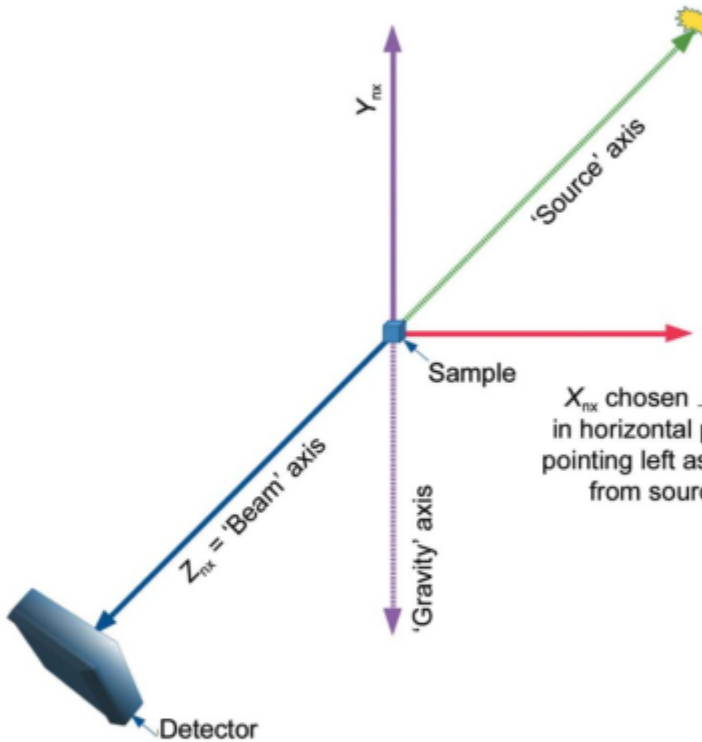
ed a lot

rt of the community is essential.

ndreas Förster was everytime a strong contributor.

olution does not necessary fit all, but we work on it.

standardized data format involves effort, but it's worth it!



Bernstein et al., IUCrJ (2020).

Gold Standard for macromol
crystallography diffraction d