CENTRE FOR
X-RAY TOMOGRAPHY

DEPARTMENT OF PHYSICS AND ASTRONOMY
RADIATION PHYSICS GROUP

PTYCHOGRAPHY USING HYPERSPECTRAL X-RAY SENSORS: IMPLEMENTATION AND APPLICATION

Frederic Van Assche

GHENT
UNIVERSITY

OUTLINE

1. Introduction

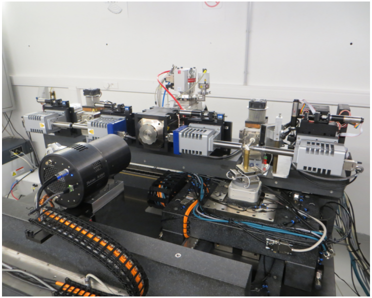
2. Software

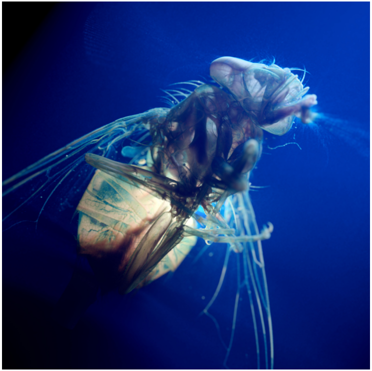
3. Ptychography

4. Conclusions

UGCT SPECTRAL

UGENT CENTRE FOR X-RAY TOMOGRAPHY





Ptychography
using
Hyperspectral X-ray imaging

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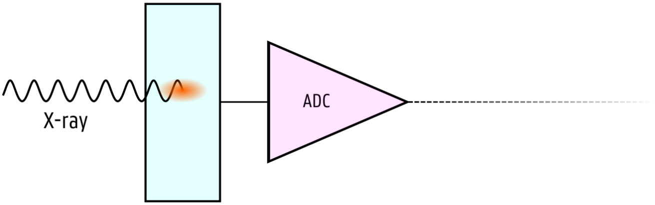
HYPERSPECTRAL X-RAY DETECTORS



Photon counting hyperspectral

HYPERSPECTRAL X-RAY DETECTORS

- pnCCD
- HEXITEC
- Mönch
- ePix

- Timepix

FLUX LIMITATIONS

Measuring a photon's energy

$\Downarrow$

Detecting photons individually

Maximum flux rates are limited

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CORE PRINCIPLES

1. Stable and reliable
2. Every pixel of every frame processed and used in real time
3. Retain flexibility inherent in hyperspectral datastreams

Initial version

- Developed to replace pnCCD-based SLcam software
- Proven reliability track record over multiple beamtimes
- Network transparent collection of small single-purpose processes

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ØMQ

NEW DEVELOPMENTS

Redesigned architecture

- Fully detector-agnostic: actual frame grabbing done in plugin requiring only small API
- Plugin based frame conditioning, processing and integration
- Central configuration and calibration store
- DAQ components autodiscover eachother

New detectors

- HEXITEC
- HEXITEC Quad

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BASIC PROCESSING STEPS

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2. Apply overall calibration (gains, ADC offsets, ...)
3. Select pixels above noise thresholds
4. Cluster finding and reconstruction (= charge sharing correction)
5. Event filtering and processing
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PERFORMANCE

- HEXITEC-sized 80x80 pixel frames, 16 bit per pixel
- 100k real frames replayed in loop from RAM
- Around 38 kHz frame rate processed in real time

Nearing 4 Gbps on single thread of i7-7700K
240 megapixel/s

- Still room for optimisations, focus was on functionally correct code for now
- Can be scaled up by spawning more worker processes
- ...or distributing over multiple machines

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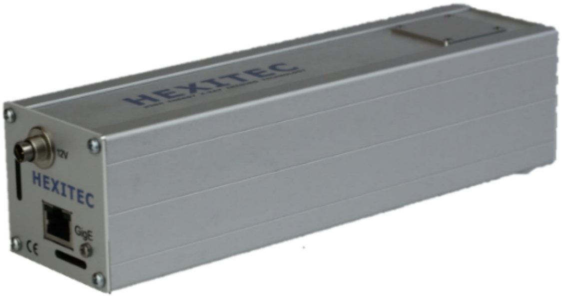
HEXITEC

- Full design-spec 9 kHz framerate available
- 800 eV FWHM @ 60 keV



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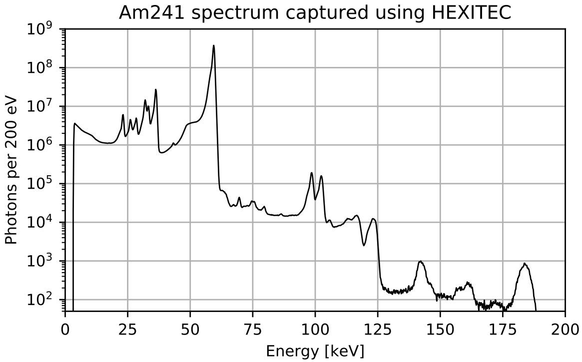

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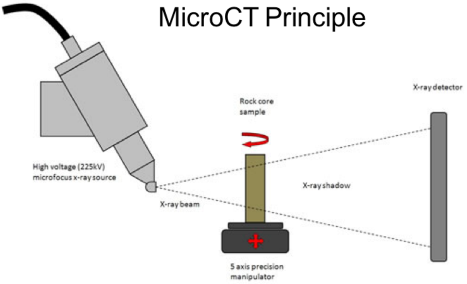
CONVENTIONAL IMAGING

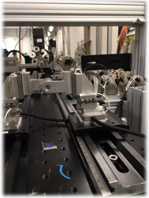
CENTRE FOR X-RAY TOMOGRAPHY



FAR-FIELD PTYCHOGRAPHY

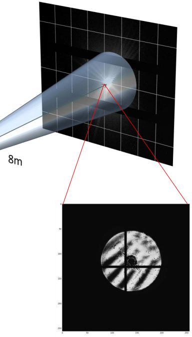
diamond

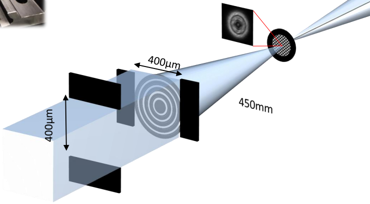
Condensing Optics



- Capture all of the available coherent flux
- Have control over the beam size on the specimen
- The dynamic range requirements of the detector are reduced

- FZP: High resolution / ptychography
  - Collaboration with PSI (C.David, F.Doring)
- KB: Lower resolution / XRF
- CRL: Increasing flux





Courtesy of Darren Batey – Diamond Light Source

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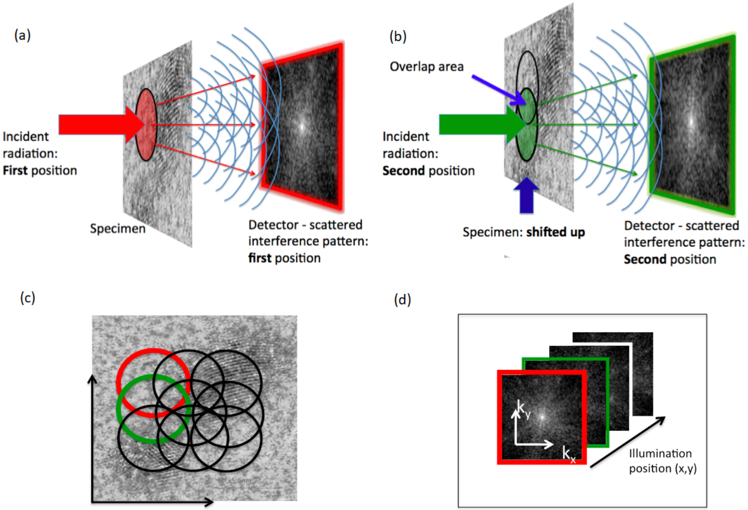

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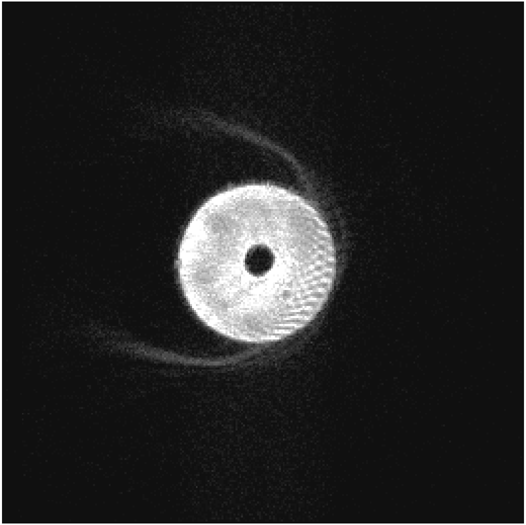
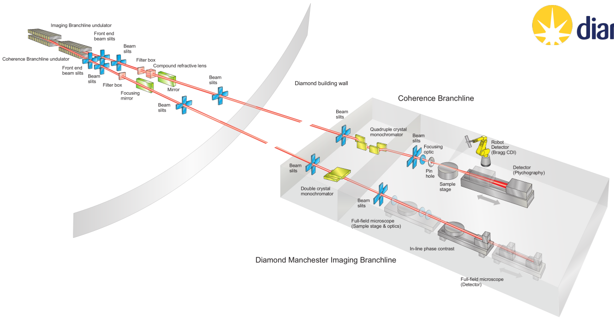


DIAMOND LIGHT SOURCE I13-1

CENTRE FOR X-RAY TOMOGRAPHY



diamond

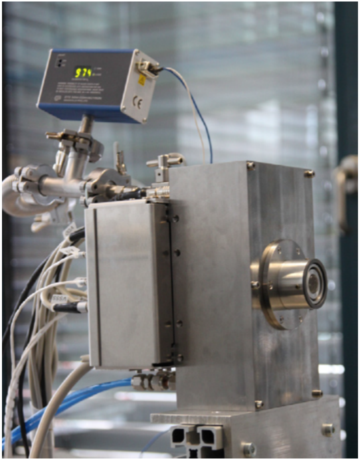
- Fresnel Zone Plate (FZP) focusing optics
- pnCCD detector placed 4.05 m downstream of sample
- Main beam energy around 8339 eV Ni K-edge

SLCAM

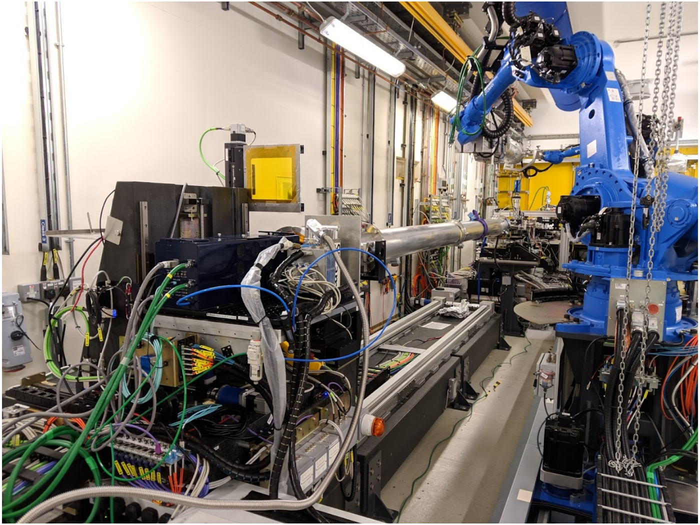
SLcam specs

Device type	Photon counting CCD
Readout	Wire-bonded ASIC
Sensor material	450 μm Si
Pixel count	264 × 264
Pixel size	48 μm
Framerate	400 Hz
Energy FWHM	147 eV @ Mn Kα

X-ray Microspectroscopy and Imaging
XMI
Universiteit Gent - Ghent University



HYPERSPECTRAL PTYCHOGRAPHY



SETUP AND RESOLUTION CHECK

Parameters

- Beam: centered on 8339 keV, $\sim$ 1 eV bandwidth
- 6 µm beam size on sample
- Sample: Siemens star
- 16 x 16 sampling grid, 1.5 µm step size
- 80 s acquisition time per step

SETUP AND RESOLUTION CHECK

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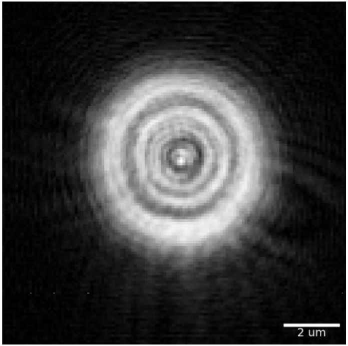
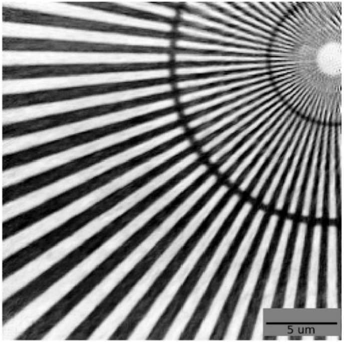




In final stage of review with Scientific Reports

Results

- Detector FWHM 172 eV at Ni K-edge
- Reconstructed resolution better than 200 nm

POLYCHROMATIC PTYCHOGRAPHY

Parameters

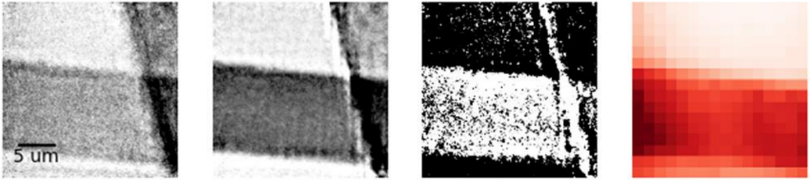
- Beam: 180 eV bandwidth
- Sample: Cu-Ni grid pair, 12.5 μm bar widths

Goal

Discriminating the Ni grid from the Cu grid from a single ptychographic acquisition using a pink beam spectrum

POLYCHROMATIC PTYCHOGRAPHY

CENTRE FOR X-RAY TOMOGRAPHY



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Below Ni-K Above Ni-K Difference XRF

POLYCHROMATIC PTYCHOGRAPHY

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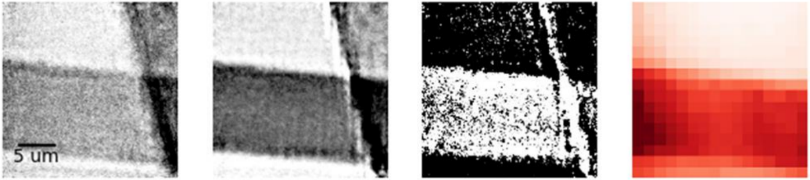

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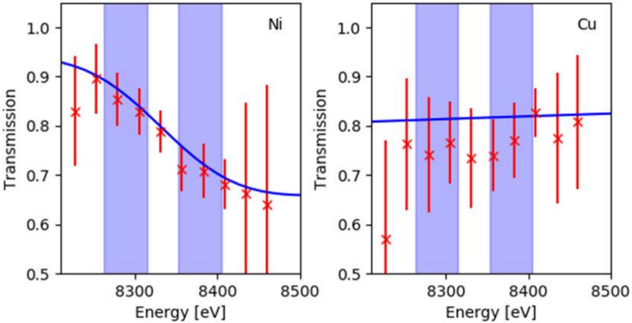

CHALLENGE 1: ENERGY CORRECTION

Problem

Ptychography reconstruction requires precisely defined setup parameters

- Optics behaviour is energy dependent
- In observed energy range: beam size from 11 µm to 2 µm

- Detector FWHM is great, but still finite
- Energy bins can actually contain majority of wrong energy events

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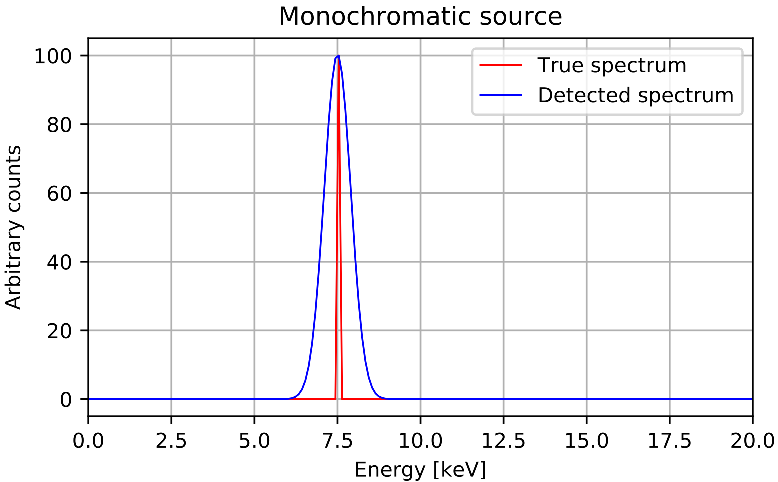

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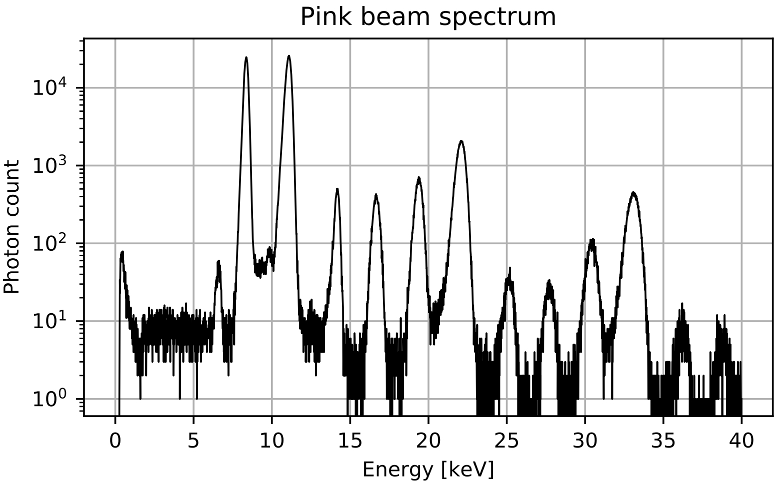

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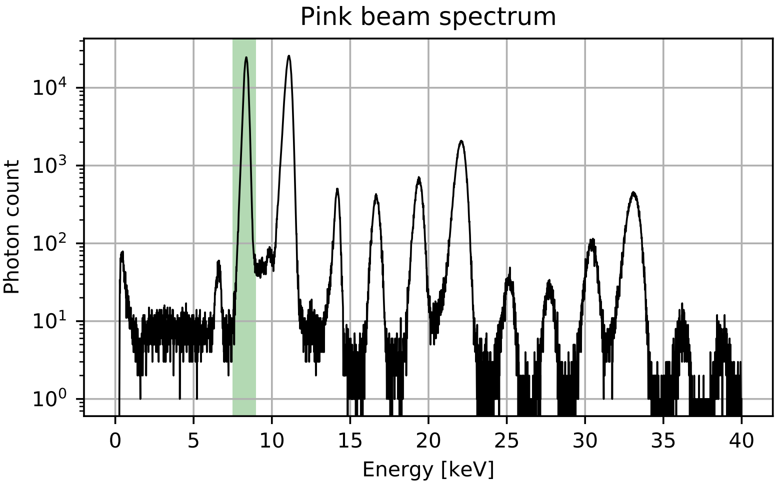

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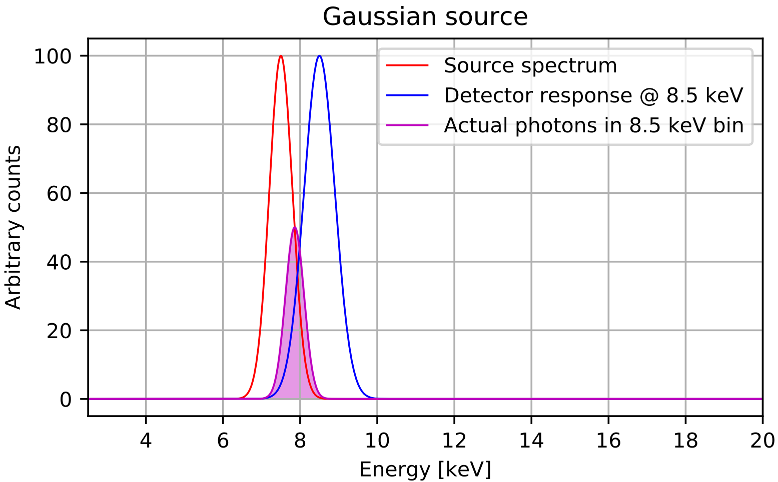

ENERGY CORRECTION

Solution

Deconvolute detector response using overlapping gaussians approximation:

$$\overline{E}_{\text{actual}} = \frac{\sigma_B^2 \cdot (E_{\text{bin}} - \mu_B)}{\sigma_B^2 + \sigma_D^2} + \mu_B$$

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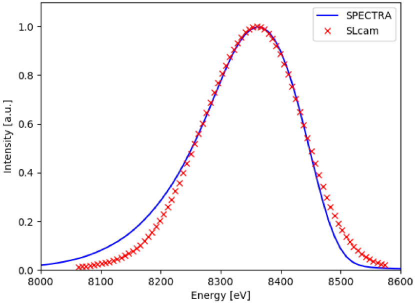

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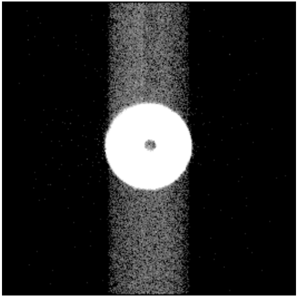
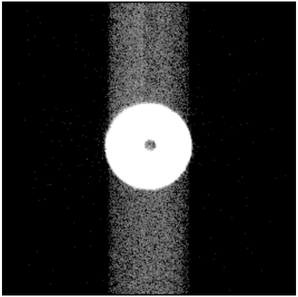
CHALLENGE 2: CCD READOUT EFFECT



Problem

- Misplaced events due to CCD shift
- Similar intensity as diffraction patterns

CHALLENGE 2: CCD READOUT EFFECT



Possible solutions

1. “Flatfield” correction, difficult due to low counts
2. Central Beam Attenuator (CBA): reduce required dynamic range

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UGCT SPECTRAL

CONCLUSIONS

Software

- Used reliably for multiple week-long experiments
- HEXITEC family now included
- Talking about loan of Mönch detector

Hyperspectral Ptychography

- First ever combination of ptychography with hyperspectral imaging
- Providing coherence using detector instead of source works
- Extracting a K-edge profile from a single acquisition is possible

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THANK YOU!

Matthieu N. Boone
Sander Vanheule
Luc Van Hoorebeke

Silvia Cipiccia
Darren Batey

International Workshop
22nd iWoRiD
on Radiation Imaging Detectors

07-11/06/2020
Ghent, Belgium

Frederic Van Assche
frederic.vanassche@ugent.be

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DLS beamtimes MG22099-1, MT20987-1 and MG23140-1

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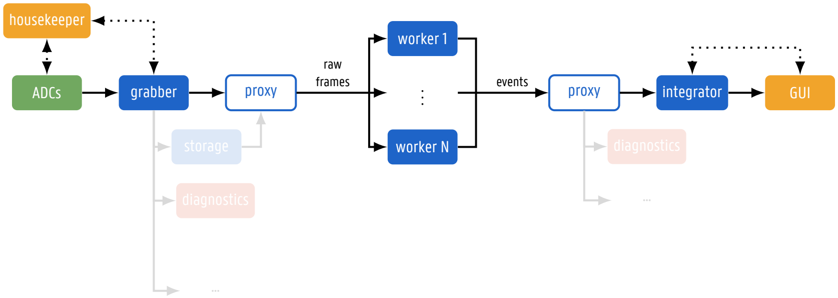
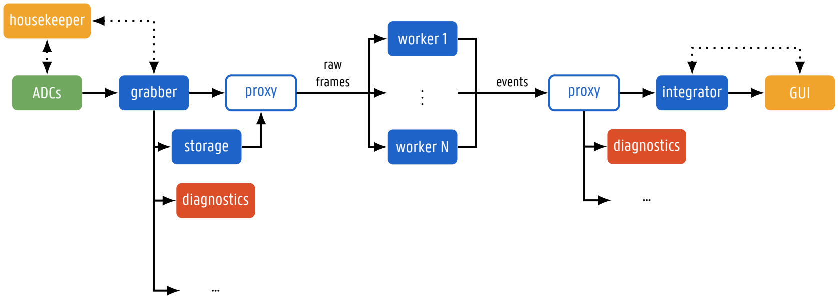
ARCHITECTURE

CENTRE FOR X-RAY TOMOGRAPHY



ARCHITECTURE



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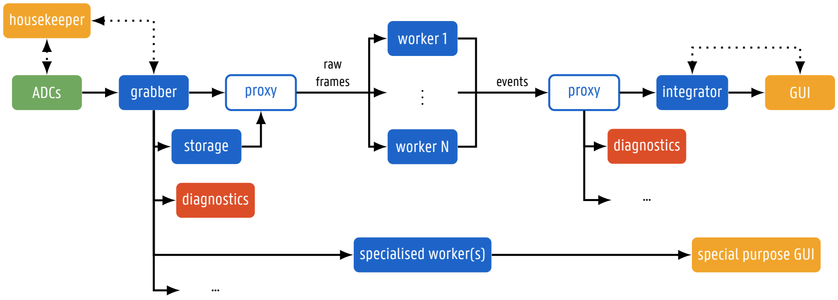

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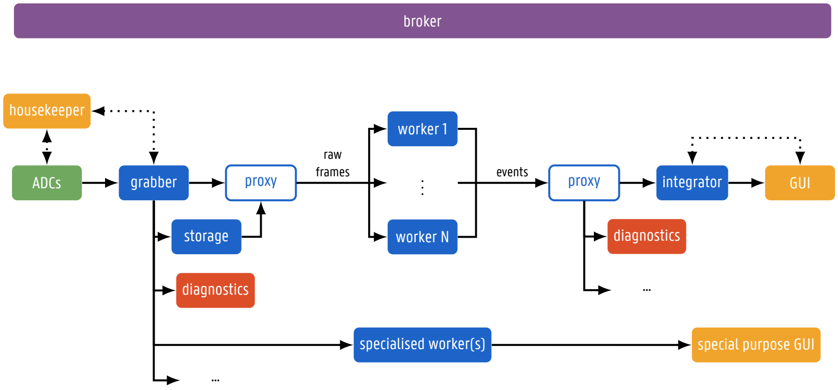

BASIC PROCESSING STEPS

1. Frame conditioning (CCD artefacts, dark current, bad pixels, ...)
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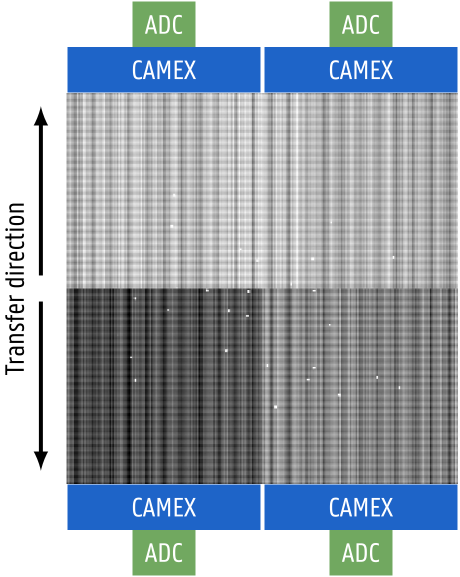
RAW FRAMES



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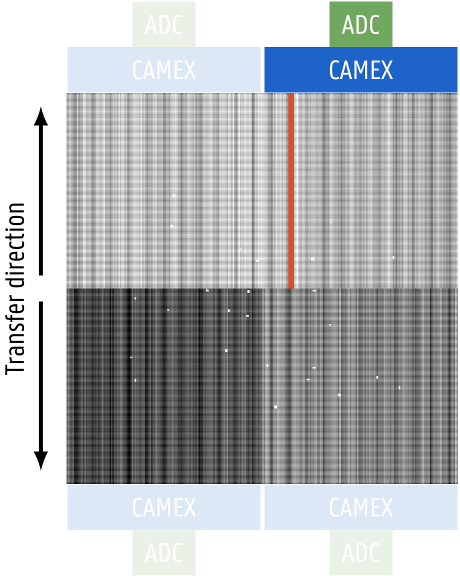
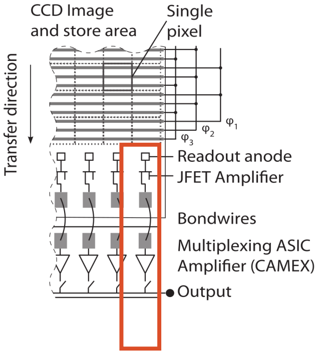

ADC
ADC
CAMEX
CAMEX
Transfer direction
CAMEX
CAMEX
ADC
ADC


CCD Image
and store area
Single
pixel
Transfer direction
φ1
φ2
φ3
Readout anode
JFET Amplifier
Bondwires
Multiplexing ASIC
Amplifier (CAMEX)
Output

RAW FRAMES

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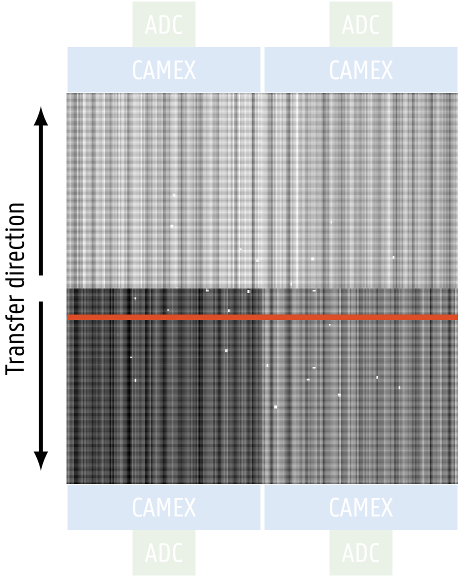


"Common mode"

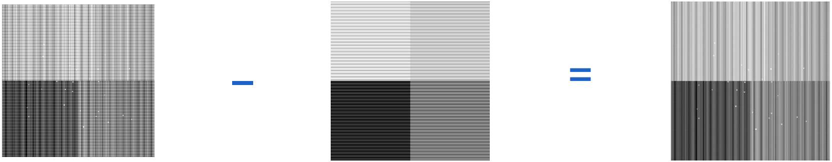
- Time-dependent "rolling pattern"
- Almost periodic
- Cause
  - Power supply ripple?
  - Clock jitter?
  - Clock mismatch?

Must be corrected in every frame

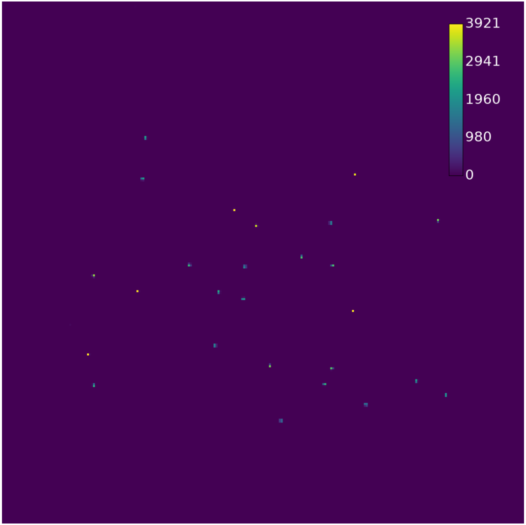
COMMON MODE REDUCTION

Iterative algorithm

1. Calculate μ and σ of line
2. Remove pixels $> 2\sigma$
3. Recalculate μ without excluded pixels
4. Repeat until converged (μ no longer decreasing)



CORRECTED FRAMES



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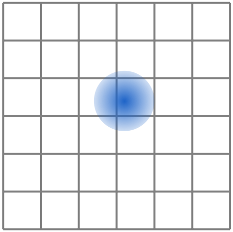
CLUSTER RECONSTRUCTION

CENTRE FOR X-RAY TOMOGRAPHY

Flood fill algorithm

1. Incident photon creates a charge cluster
2. Charge cluster gets trapped in one or more pixels
3. For each pixel all eight neighbours are checked
4. Neighbours above threshold are collected into an event
5. Event is stored with a total charge and center-of-mass location



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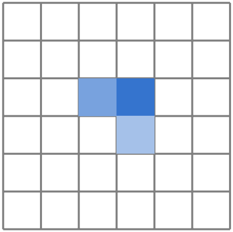

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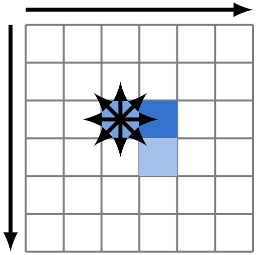

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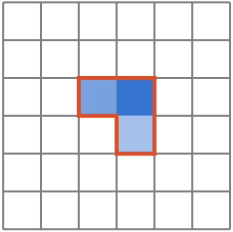

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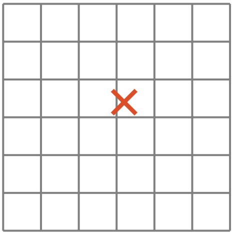
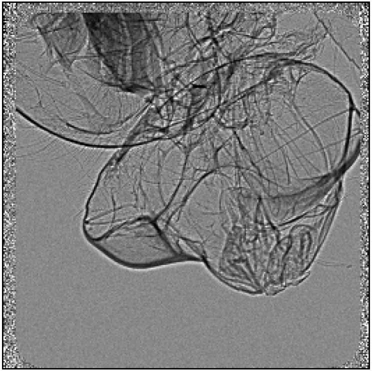
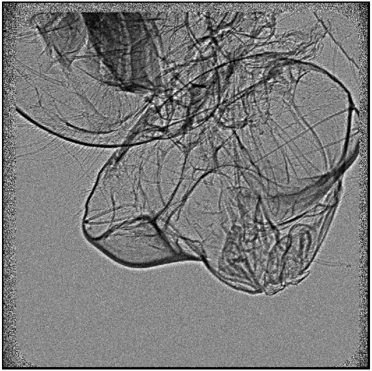


SUPER-RESOLUTION

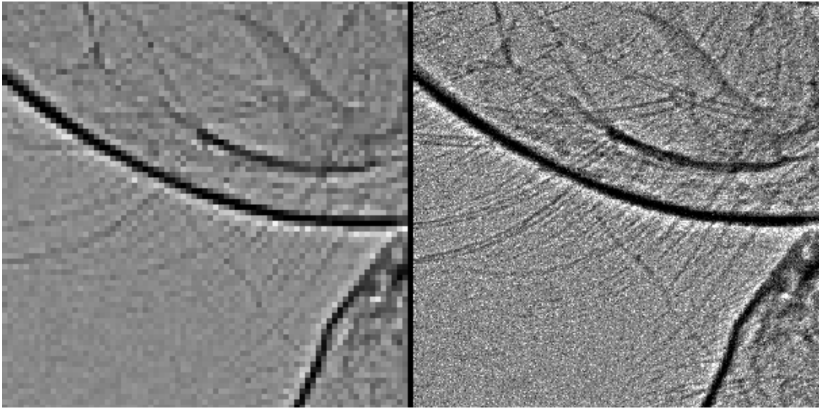


Physical detector pixels



4x4 super-resolution

SUPER-RESOLUTION



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