European XFEL

MHz X-ray imaging with Silicon Pixel Detectors

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8th EIROforum School on Instrumentation ESO Headquarters, Garching, 17.05.2024

Outline

- The European XFEL beam
- Experiments at EuXFEL
- Detector Requirements
- How to deal with high dynamic range
 - Dynamic gain switching (AGIPD)
 - Non-linear response (DEPFET DSSC)
- MHz burst mode operation
 - Analog storage cells (AGIPD)
 - On-chip analog-to-digital conversion (DSSC)
- Raw data correction at European XFEL
- Conclusions





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Acknowledgment

- AGIPD Consortium (H. Graafsma)
 - DESY, PSI, Uni Bonn, Uni Hamburg
 - DSSC collaboration (M. Porro)
 - EuXFEL, DESY, PoliMi, Uni BG, Uni Heidelberg, pnSensor, MPG-HLL, INFN
 - European XFEL
 - Data Department (S. Aplin)
 - ► DET Group, CTRL, ITDM, EEE, DA
 - SPB/SFX instrument (A. Mancuso/R. Bean)
 - MID instrument (A. Madsen)
 - FXE (Ch. Milne)
 - HED (U. Zastrau)
 - SCS (A. Scherz)
 - SQS (M. Meyer)





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Introduction: European XFEL





Three main undulator systems (SASE 1, 2, 3)

- Supply seven scientific instruments
- SPB/SFX, FXE, MID, HED ('hard X-ray')
 - ▶ 6 keV < E < 25 keV
- SCS, SQS, SXP ('soft X-ray')
 - ▶ 0.25 keV < E < 3 keV

- 10 Hz train rate
- Bunch train internal structure
 - 2700 pulses for 600 μs
 - **4.5 MHz pulse rate** (~222 ns spaced)
 - Lasing pulses < 100 fs width</p>
- Pulses of ~ 10¹⁴ photons
 - Most experiments are pulse-resolved
 - Detectors need to cope with bunch train structure

Introduction: experiments

MHz XPCS to look at system dynamics Speckle patte Pulse structure on AGIPE 10000.000 ÌIIII. IIIIÌ 100 ms (10 Hz) X-ray pulse trains anoparticle suspension bed by the X-ray pulse Lehmkühler et al. PNAS 117:24110-24116(2020)



M. Frost et al., accepted by Nature Astronomy (2023)

X-ray scattering experiments



F. Büttner et al., Nat. Mater., 20, 30-37 (2021)



Sobolev, E. et al. Megahertz single-particle imaging at the European XFEL Commun Phys 3, 97 (2020)

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Serial femtosecond protein crystallography (SFX)



Wiedorn, M.O,. et al. Megahertz serial crystallography. Nat Commun 9, 4025 (2018)

Oversimplifying:

X-rays from pulse interact with sample (sample often destroyed) Interaction creates a 2D X-ray 'pattern' Contains physical information Detectors need to image this pattern

Detector requirements

The detector needs to cover as much solid angle as possible

- Reduced pixel pitch for spatial resolution
 - ► ~1 Mpix with ~200 µm pixel pitch
- The detector needs to cope with 4.5 MHz burst pulse rate
 - High detector occupancy
 - No event-driven readout
 - No time to read out the whole image in between pulses
 - Images have to be stored and then readout in between trains

Huge difference in signal in the same image

- The detector needs a wide dynamic range
- The same pixel needs to accurately detect:
 - ► Single photons
 - ► Tens of thousands of photons (~ 10⁴ ph/pixel)

European XFEL environment is harsh for the detector

- High doses are delivered (sometimes instantaneously)
 - Detector should be radiation tolerant as much as possible
 - Calibration constant need to be updated frequently



MHz Imaging detectors for EuXFEL

Detector	Specs	Gain Mechanism	Gain	Start of Operation
AGIPD	352 memory cells (analog) 200μm x 200μm sq. pixels 1-10 ⁴ 12 keV ph 3-20 keV Modular: 16 (1MPix) or 8 (0.5MPix) modules	3 gains with automatic switching	12000 g HG 6000 0 Integration time cik 1000	AGIPD1M (SPB/SFX): 2017 AGIPD1M (MID): 2019 AGIPD500K: 2020 (new gen.) AGIPD4M (SPB/SFX): 2024 (new. gen) AGIPD1M (HED): 2024 (new gen)
LPD	(3x)512 memory cells (analog) 500μm x 500μm sq. pixels 1-10 ⁵ 12 keV ph 7- 20 keV Modular: 16 module (1MPix)	3 parallel gain stages with on front-end selection	3000 1000	LPD (FXE): 2017
DSSC	800 memory cells (digital) $204\mu m \times 236\mu m$ hex. pixels N x 256 ph @ 4.5 Mhz N x 512 @ f \leq 2.2 MHz N \leq 1 for single ph sensitivity 0.5 - 6 keV Modular: 16 modules (1MPix)	Linear response (miniSDD), non-linear signal compression in sensor (DEPFET)	DEFFET Response on Fluresence Intensity	DSSC1M (SCS): 2019 DSSC DEPFET: 2024

Hybrid pixel detector technology

Detection component and front end readout are developed separately

- Pixellated sensor
 - Typically silicon in proportional mode
 - Other solutions possible e.g.:
 - CdZnTe, GaAs for higher photon energy detection
 - ► LGADs to improve S/N ratio at soft X-ray energies
 - ► DEPFET ...
 - Signal generated in sensor is read out by ASIC
 - ASIC is also pixellated
- Sensor and ASIC are connected on a pixel-by-pixel basis
 - Bump-bonding between contacts
 - ASIC output wire-bonded to rest of read out chain

Example of single AGIPD module:

Sensor 128 x 512 pixels 2 x 8 read-out chips connected to sensor via bump-bonding



ASIC side



High dynamic range requirement

High dynamic range adaptive gain: the AGIPD detector





- Charge-integrating pre-amplifier (pre-amp)
- Pre-amplifier with dynamic gain switching (DGS)
 - Three feedback capacitors C_f
 - ► Three gains (High, Medium, Low)
 - Threshold comparator at the output node of pre-amp
 - ▶ If signal above V_{thr} additional capacitor is switched in
- Correlated Double Sampling (CDS)





- Readout output stored in analog storage cell
- 'gain stage' also stored analogically
- To correct raw data
 - Pedestal value to subtract
 - Conversion factor into physical unit (*gain factor*)
 - Information about the the 'gain stage'
 - Six constants per pixel and per storage cell

Sztuk-Dambietz, J. et al. "Operational experience with Adaptive Gain Integrating Pixel Detectors at European XFEL" Front. Phys., Volume 11 – 2024 https://doi.org/10.3389/fphy.2023.1329378

Dynamic gain switching calibration



Fluorescence spectra for High Gain calibration

- "absolute" calibration: conversion factor from ADC units \rightarrow keV
- **Dynamic range scans for lower gains calibration** (Medium and Low)
 - Raw output as function of input signal
 - Linear fit of the response
 - "relative" calibration: fit slope $\mathbf{m} \rightarrow$ slope ratio \rightarrow gain factors ratio
- Pedestal estimated with 'dark' runs
 - Pre-amp forced switch for Medium and Low gain









Dynamic gain switching data quality



- Plenty of User Operation hours
 - 'stress test' of the goodness of calibration
- The dynamic gain switching has been proved working
 - A few issues have been identified
- Gain switching region may show issues
 - Intensities not mapped
 - Reliability of the pedestal determination
- Forced gain switch not always predictive
 Issues manifest in other detectors with dynamic gain switching architecture





Sikorski, M.; Ramilli, M. . et al. "First operation of the JUNGFRAU detector in 16-memory cell mode at European XFEL" Front. Phys., Volume 11 – 2024 https://doi.org/10.3389/fphy.2023.1303247



Dynamic gain switching data quality (cont'd)

Late gain switching

- Signal sampled while still settling
 - Artifact in corrected image
- Encountered in other DGS detectors
- Possible solutions
 - Increase exposure time
 - AGIPD, JUNGFRAU
- Inhibit late gain switching
 - ► GOTTHARD-II











High dynamic range with non-linear response: the DSSC detector



- Depleted P-channel Field Effect Transistor
 - ► Invented by J. Kemmer and G. Lutz in late 1980s at MPI Munich
- FET integrated on a fully depleted n-Si bulk
 - In-pixel signal amplification
 - Potential minimum for electrons between source and drain
 - Charge accumulation induces charge in gate
 - Change of current between source and drain proportional to charge
- The DSSC DEPFET potential valley extends towards the source
 - Extracted charge will eventually fill the Overflow Regions (OR)
 - Gating effect of charge in OR less pronounced
- The sensor response is not completely linear with extracted charge
 - For small amounts it maintains a linear response
 - For increasing amounts it will eventually deviate from linearity

Lechner, P. et al. "DEPFET active pixel sensor with non-linear amplification" (2012) art. no. 6154112, pp. 563-568 doi:10.1109/NSSMIC.2011.6154112

Aschauer, S.; et al. "First Results on DEPFET Active Pixel Sensors Fabricated in a CMOS Foundry a Promising Approach for New Detector Development and Scientific Instrumentation". J. Inst. 2017, 12, P11013–P11013 doi:10.1088/1748-0221/12/11/p11013



DEPFET: FET integrated on a fully depleted Si bulk



DEPFET response calibration

- Accurate calibration of the sensor response is needed
 Intensity scan of the whole dynamic range
 - Performed in Nov. 2022 with AI fluorescence setup
 - EuXFEL beam used to generate K emission from Al target
 - Intensity on AI target provided by Gas Monitor (GM)
 - ► DSSC module illuminated by AI fluorescence
 - Calibration idea:
 - Acquire the whole non-linear response (NLR) curve
 - Detector output as function of the GM output
 - Linear part \rightarrow absolute calibration
 - Used to intercalibrate with GM
 - Absolute calibration of detector response to flux
 - Do it for every pixel



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Non-linear response curve on pixel(10, 125)



DEPFET response calibration

Non-linear response of a DEPFET pixels(10, 125)



Maffessanti, S., Hansen, K. et al., "A 64k pixel CMOS-DEPFET module for the soft X-rays DSSC imager operating at MHz-frame rates". Nature Sci Rep 13, 11799 (2023) https://doi.org/10.1038/s41598-023-38508-9

A. Castoldi et al. "Qualification of the X-ray spectral performance of the DEPFET pixels of the DSSC imager", NIM A, 2023

Fit with phenomenological function

DEPFET DSSC 1 Mpix camera assembly





- DSSC equipped with DEPFET is being assembled at European XFEL
 - 3 out of 4 quadrants are in place
 - More DEPFET are being produced
- First users in 2025
 - European XFEL

MHz burst frame rate requirement

Coping with MHz frame rate: analog storage

- Detector cannot be read out in less than 200 ns
- Images have to be stored somewhere and read out in between trains
- AGIPD chose the analog storage cell solution
 - Each pixel is endowed with 352 capacitors
 - Each capacitor holds the output of one acquisition
 - Capacitor values is read out and passed on the (off chip) ADC in between trains
- This simple solution has some drawback
 - The footprint for all these storage cells is ~80% of the pixel area
 - The storage cells are appreciably different from each other
 - All the constants have to be produced for each storage cells
 - ► To calibrate one pixel 6 x 352 = 2112 constants are needed!
 - Other effects:
 - Cross talk
 - ► Charge leak

This simple solution requires substantial calibration effort to mitigate its effects





Coping with MHz frame rate: on-chip digitization





- DSSC opts for on-chip digitization of the signal
 - Signal passes amplification and filtering
 - Sample and hold stage
 - One capacitor stores the signal
 - ► The other has it read out and digitized by an analog-to-digital converter
 - ADC output stored in an SRAM with 800 images depth

Porro, M. et al. "The MiniSDD-based 1-Megapixel Camera of the DSSC Project for the European XFEL" April 2021, IEEE Transactions on Nuclear Science PP(99):1-1 https://doi.org/10.1109/TNS.2021.3076602

Coping with MHz frame rate: ADC calibration

- The on chip ADC has 8 at 4.5 MHz
 - 9 bit at frame rates ≤ 2.2 MHz
 - Limited resolution (AGIPD off-chip ADC has 14 bits)
- Differential non-linearity (DNL)
 - One of the main qualifiers for ADC performances
 - Deviation w.r.t. the ideal step of one LSB
 - Measure of the "actual bin width" of the ADC
- Can be measured by injecting voltage in ADC in a controlled way
 - In this way the output is characterized

DSSC DNL has been characterized with a 13 bit input DAC





Coping with MHz frame rate: DNL correction

- Fluorescence measurements on DSSC
 - Some bins are over/under sampled
- DNL correction may be relevant
 - Spectroscopic measurements
 - weight the occurrences *N* in the i-th bin
 - Marked improvement of the peak resolution
 - Drop of the error on gain value estimate

Characterization of the DNL can be necessary

This information is then used in offline analysis

$$N(i)_{corr} = \frac{N(i)}{DNL(i)+1}$$

PulXar Cu Ka spectrum (single pixel)





Calibration and raw data correction

Calibration effort at European XFEL

European XFEL aims to provide facility users with a fully corrected and calibrated dataset as the primary data product.

SRN 27.4, 35 (2014)



Keeping the calibration constants updated

- EuXFEL must provide the tools to achieve best data quality
 - Provide high quality corrected data
 - provide a reliable online preview
- We need to update the correction constants regularly
- **Quick to gather data: dark run constants**
 - Frequently updated (at least once per shift)
 - Pedestal and noise
 - Bad pixel classification (from pedestal and noise values)
 - Automatized procedure for acquisition and calculation
 - No need to expert supervision

Special calibration procedures

- Need expert contribution to acquire and process
 - ► Gain constants
 - ► NLR curves
 - ► DNL
 - ▶ ...
- Automation of procedures still on the way
- Updated when possible (e.g. during shutdowns)





Constants loaded in DB

Online correction

- Implemented in EuXFEL control software (Karabo)
 - Detector class specific
 - Basic correction only
 - Code optimized for speed
 - Run on high performance machines
- Accessible from GUI
- Output corrected image
 - Necessary for experiment tuning!

Offline correction

- Implemented in scripts
 - Detector class specific
 - Algorithm aims to most complete correction possible
 - Common mode correction
 - ► Clustering
 - ► Baseline shift compensation ...
 - Code written to handle large data volumes
- Correction triggered by Metadata Catalogue
 - Scripts run a SLURM jobs on Maxwell Cluster



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Summary

European XFEL is an X-ray user facility with challenging requirements for detector development

- MHz-level pulse rate in bursts
- Up to 10¹⁴ photons per pulse
 - High dynamic range required!
 - High doses delivered to the detector
- How we deal with high dynamic range
 - Dynamic gain switching (AGIPD)
 - Proven effective
 - Calibration issues
 - Non-linear response (DEPFET DSSC)
 - Calibration procedure successfully established
 - ► First user experiments will come soon
- How to deal with MHz-level frame rates
 - Analog storage cells (AGIPD)
 - Cumbersome calibration
 - On-chip analog to digital conversion (DSSC)
 - ► Get rid of all analog storage cells effects
 - Limited resolution (8 bits)

- Calibration constants updated when needed
 - Effort to automatize calibration
- Provide the infrastructure to correct raw data
 - Database to store the constants
 - ► Offline correction pipeline
 - Online correction pipeline

Backup

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Detectors for EuXFEL

Hard X-rays 6-25 keV



X-ray energy

Noise: 50 e- (HG) Dyn range: 1008 keV ph



Dyn range: 10⁴ 12 keV ph

JUNGFRAU x 18Irth (all hard X-ray inst.) ePix100 (MID, HED) Noise: 80 e- (HG)

pnCCD (SQS)

Soft X-rays 0.5-3 keV

European XFEL

10 Hz

Noise: 3 e-Dyn range: 1500-3000 1 keV ph

GOTTHARD-II (all instr.)



Strip detector Noise: 280 e- (HG) Dyn range: 10⁴ 12 keV ph Up to 2700 images/train



Noise: 350 e- (HG) Dyn range: 10⁴ 12 keV ph

DSSC (SCS, SQS)



Noise: 60 e-Dyn range: N x 256 ph @ 4.5 Mhz -N x 512 @ f≤2.2 MHz $N \leq 1$ for single ph sens.

Rate







4.5 MHz

R D





Detector integration in Karabo

- Karabo European XFEL's Control System framework for control, DAQ and monitoring
 - Distributed system of devices (physical and 'logical') that communicate with each other through a message broker
 - Devices are aggregated in topics (one topic per instrument)
 - GUI Client facilitates interaction and control of devices
- Tight coupling of controls and DAQ
 - DAQ is generic for all data source (e.g. detector, motors, sensors, etc)
 - Data is stored centrally, ensuring easy accessibility
- Integration of detectors in Karabo
 - Enables control of the detector and its infrastructure
 - Supports complex procedures, including detector startup and calibration data collection
 - Provides monitoring capabilities (e.g., temperatures, power, detector status) and 2nd level detector protection
 - Data online viewers offer near real-time experiment feedback

AGIPD1M detector system for SPB/SFX and MID instruments



1M AGIPD system

16 modules are mounted on four independently movable quadrants
Vacuum operation (P< 10⁻⁵ mbar)
Electronics/Control: two independent detectors: 'half 1' and 'half 2'
Readout: 16 independent detectors

Hybrid detector module Sensor: 128 x 512 pixels 500 μm thick silicon 2 x 8 read-out chips connected to sensor via bump-bonding Size: ~26 x 105 mm²





In ambient

In vacuum

Dynamic gain switching calibration



AGIPD Calibration for one operation mode

Da	rk data	Dynan s	nic range can	L	ow intensity X- ay fluorescence
Noise	Thresholds for gain encoding	Offset	Gain r (HG/MG,	atios MG/LG)	Absolute gain (HG only)
	Bad pixels mask	$\langle \rangle$	C.	rrected data	7
Calibration data Calibration constants	Constants G Bad pixel eva	eneration aluation	etante		

Data Type	Data Size	Measurement Time	Data Processing Time	Frequency
Dark Data	2.2 TB	5 mins	$\sim 10 \text{ mins}$	at least once per shift
Dynamic Range Scan - Pulsed Capacitor	8.2 TB	20 mins	$\sim 100 \text{ mins}$	6 months
Dynamic Range Scan - Current Source	21 TB	65 mins	\sim 180 mins	6 months
Fluorescence Data	15-20 TB	25-30 mins	up to 720 mins	6-12 months

Radiation hardness sensor design

- No bulk damage expected for E < 300 keV BUT
- Surface and interface damage:
 - Higher leakage current
 - Higher depletion voltage
 - Lower breakdown voltage
 - Charge losses at interface
 - Increased inter-pixel capacitance
- → Special high voltage design with 15 guard rings:
 - radiation tolerant up to 1GGy [■]
 - introduced additional non-sensitive area between detector modules [➡]



Distance from the last pixel to the edge of the sensor 1200 μm

JINST (2013) 8 C12015, DOI: 10.1088/1748-0221/8/01/C01015,

e-Print: arXiv:1210.0430 [physics.ins-det

DSSC Detector System Overview 2/2





DSSC











- Movable quadrants
- "service position' in the pic
- Total active area ~ 505 cm²
- Minimum insensitive area ~15%

IFDEPS 2024

NLR curves of DEPFET pixels



MHz X-ray imaging with Silicon Pixel Detectors Spectroscopic performance of DEPFET: Single photon detection F= 1.1 MHz, T_{int}=100 ns, T=18 °C



Full Format Readout ASIC

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M. Porro IFDEPS 2024

DSSC

130 nm CMOS Process with C4 bumps

- Gain and offset can be adjusted pixel-wise:
 - > 11 bits of coarse gain setting for ph. energy and input range selection
 - 6 bits of gain fine trimming (nominal accuracy 2%)
 - \blacktriangleright 4 bits for offset trimming (1.5 LSB range with 8% of granularity)

Pixel-wise fine gain trimming Pixel-wise coarse gain parameters keV $\frac{keV}{ADU} \propto C_{CSA} \cdot R_{V2I} \cdot C_{FCF} \cdot \frac{1}{t_{filt}} \cdot \frac{1}{C_{S\&H}}$ I_{ramp} Ĵclock