PAUL SCHERRER INSTITUT

Xiangyu Xie :: Postdoc :: Photon Science Detector Group :: Paul Scherrer Institut

Hybrid Pixel Detector development at PSI & Enhanced spatial resolution via DL for electron microscopy

University of Science and Technology of China :: 2023.12.29

About me …

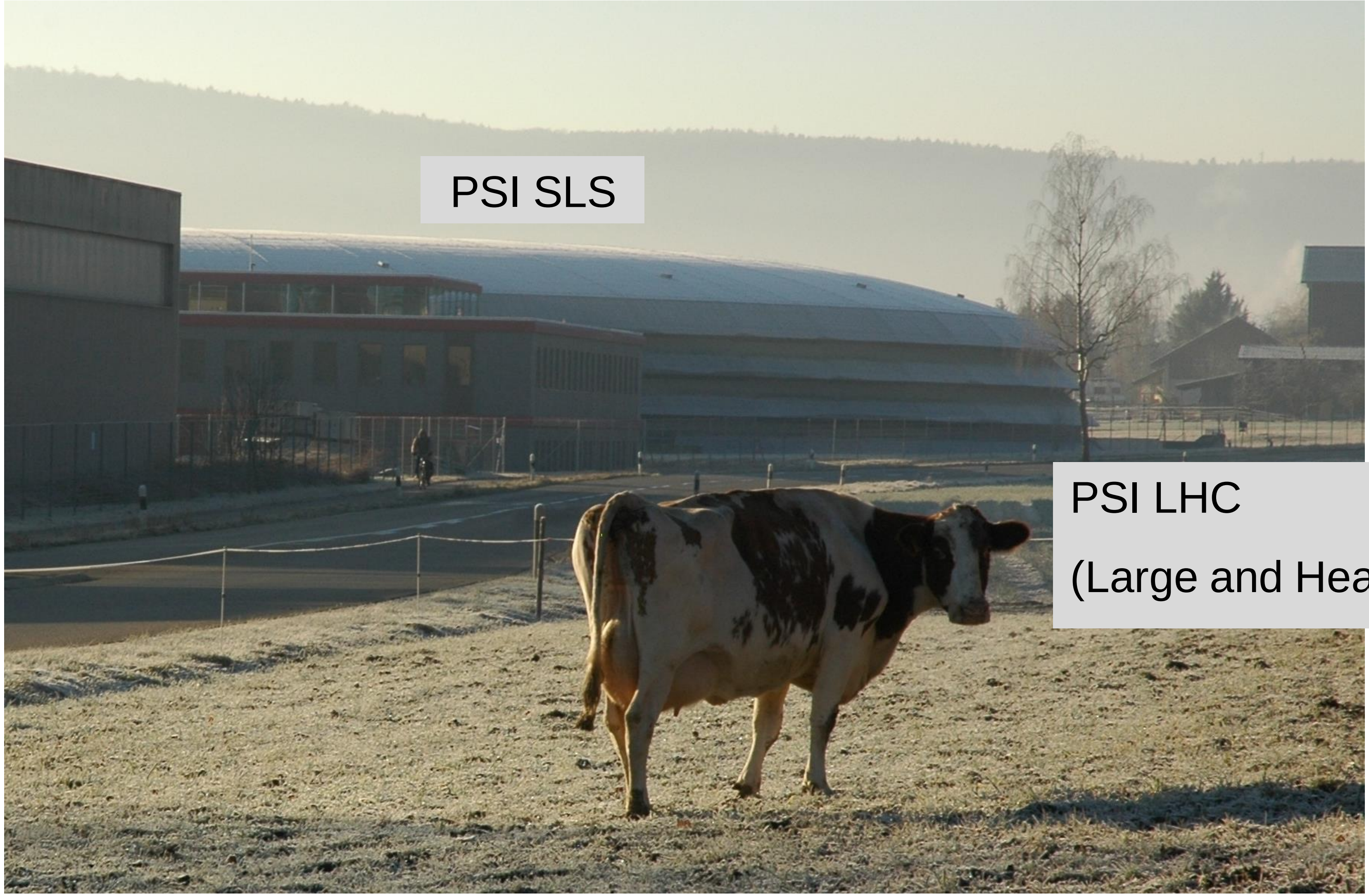
- Education
  - 2013-2017: BS, Physics, minor in Microelectronics, *University of Science and Technology of China*
  - 2017-2022: Ph.D., Experimental Particle Physics, *University of Science and Technology of China*
- Work experience
  - 2022-present: postdoctoral researcher, Photon Science Division detector group, *Paul Scherrer Institut*
- Research interest
  - Detector R&D, deep learning for detectors

Outline

- Hybrid pixel detector development for photon science at PSI
  - PSI and Photon Science detector group
  - Hybrid pixel detector developments at PSI

- Enhanced spatial resolution of MÖNCH via deep learning for electron microscopy
  - Sample preparation
  - Neural network design
  - Results evaluation

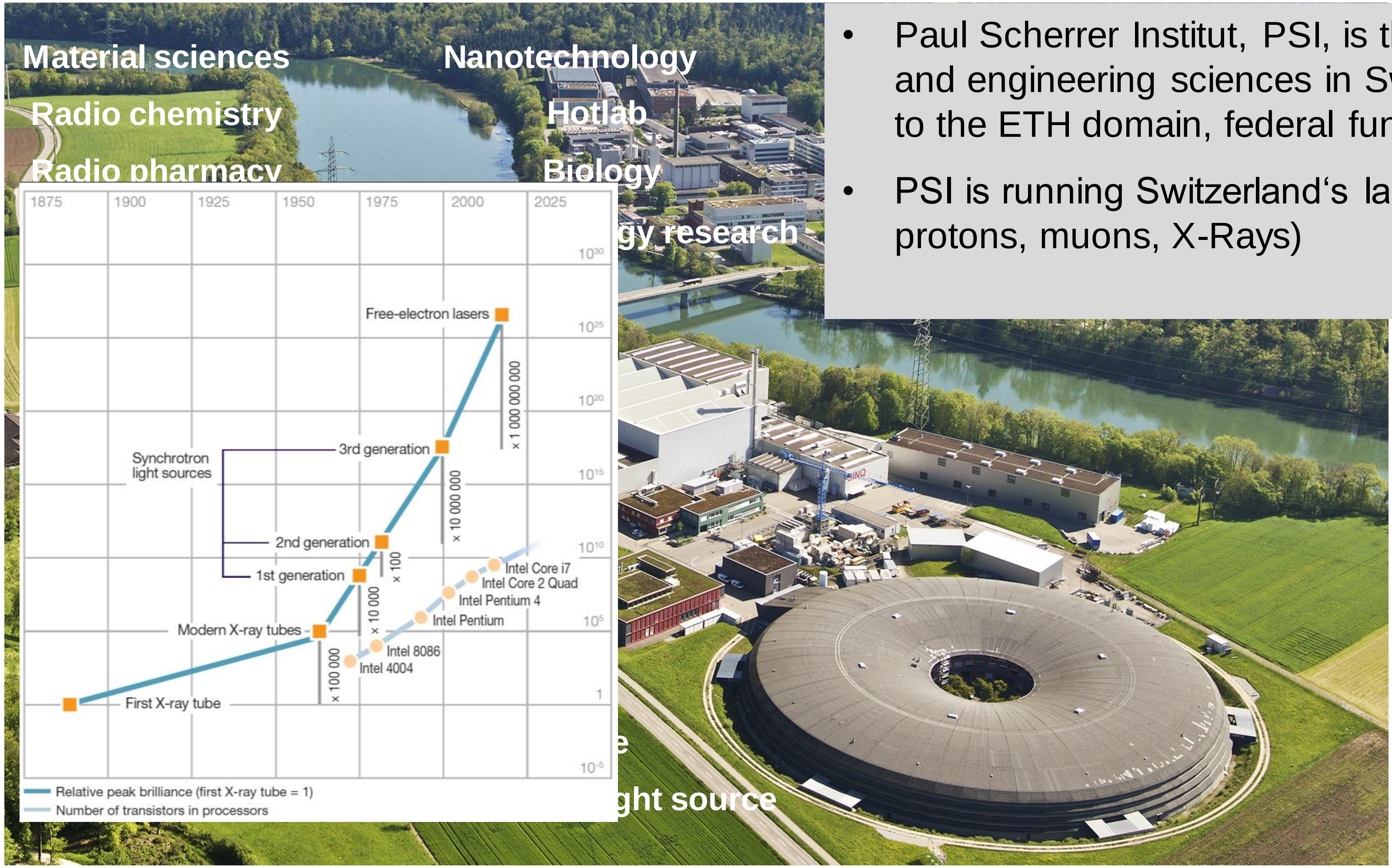
LHC at PSI



(Won 3rd prize in
SLS photo contest
Courtesy: Roberto)

Paul Scherrer Institut

- Paul Scherrer Institut, PSI, is the largest research center for natural and engineering sciences in Switzerland (2100 employees), belongs to the ETH domain, federal funded
- PSI is running Switzerland‘s large research facilities (neutrons, protons, muons, X-Rays)



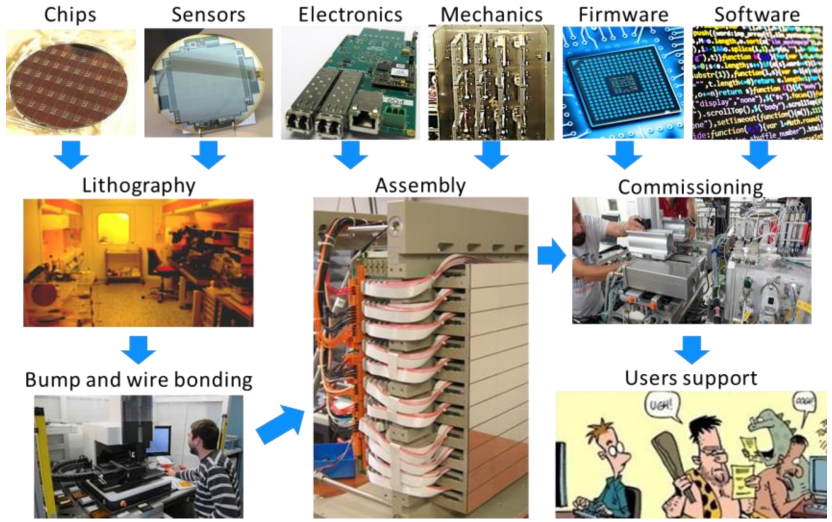
Synchrotron: SLS Swiss Light Source

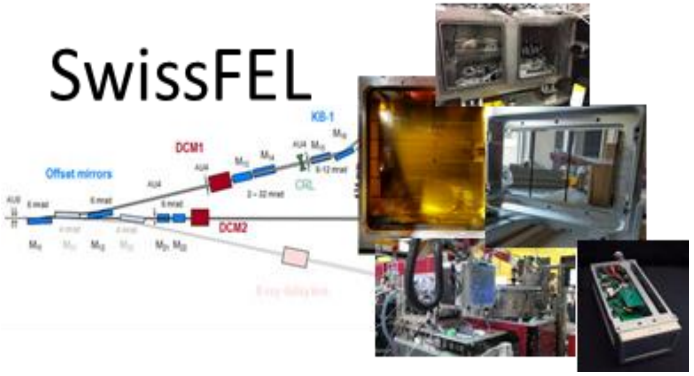
2.4 GeV, 288 m circumference, ~20 beamlines

XFEL: SwissFEL, 740m long

Photon Science Division detector group

- Develop detectors for the SLS and SwissFEL
  - Detector R&D
  - Design and production
  - Characterization and commissioning
- Other applications: electron microscopy

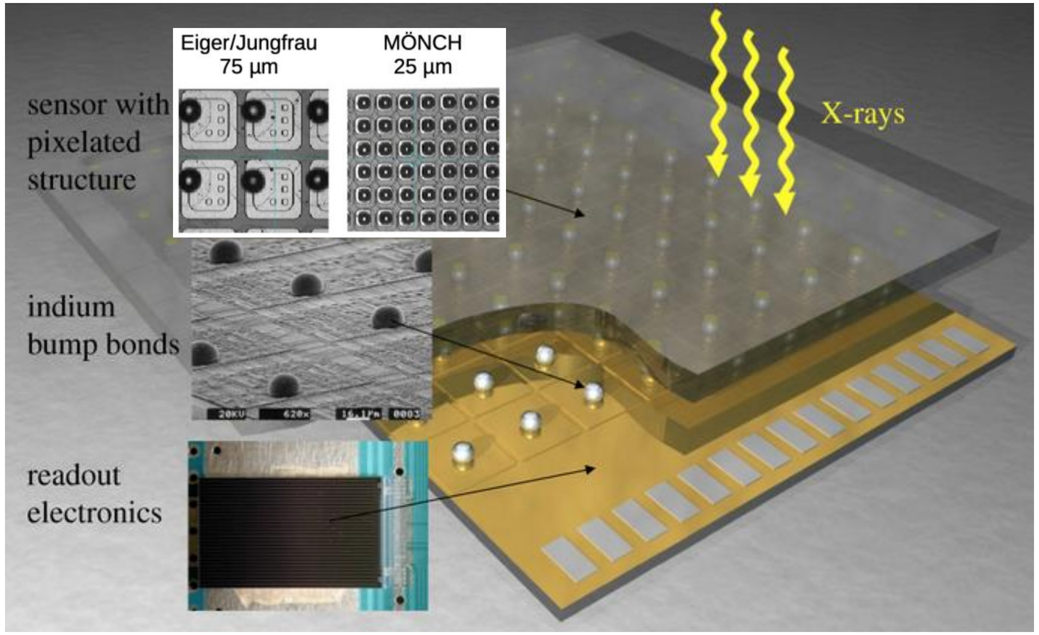




Hybrid Pixel Detector

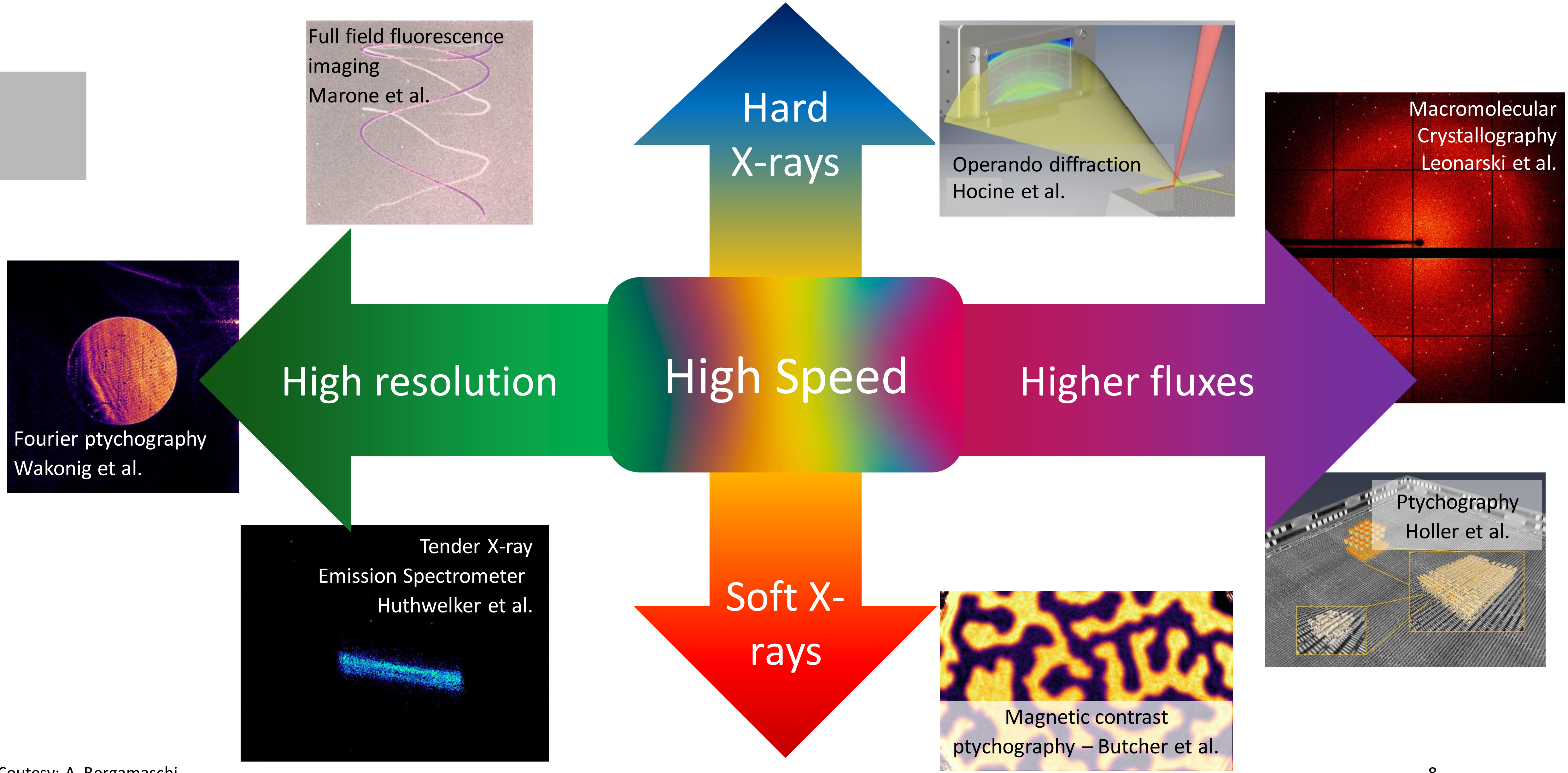
- Semiconductor sensor
  - Direct conversion
- Versatile readout ASICs
  - Fast signal processing
  - Fast readout
  - Radiation hardness
- Bump/Wire-bonding
  - Minimum pixel pitch $\approx 25\ \mu m$
  - Noise due to input capacitance

Hybrid pixel detector



→ Sensor & ASICs can be optimized independently
→ Can be customized according to applications

Challenges


Full field fluorescence imaging
Marone et al.
Hard X-rays
Operando diffraction
Hocine et al.
Macromolecular Crystallography
Leonarski et al.
Fourier ptychography
Wakonig et al.
High resolution
High Speed
Higher fluxes
Ptychography
Holler et al.
Tender X-ray Emission Spectrometer
Huthwelker et al.
Soft X-rays
Magnetic contrast ptychography – Butcher et al.

Sensor developments

- Inadequate silicon sensor performance at “low” and “high” photon energies

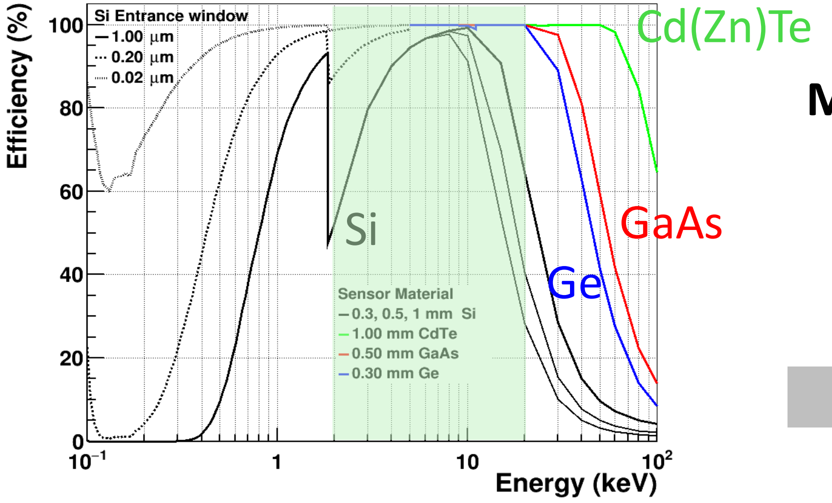
Soft X-rays (250 eV – 2 keV):

- low quantum efficiency of Si

Two technological developments

- thin entrance window
- inverse Low Gain Avalanche Diode (iLGAD) sensor

Efficiency *vs.* photon energy



High-energy photons (> 20 keV):

- limited stopping power of Si

Material under investigations

- CdZnTe
- CdTe
- GaAs

Performance of high-Z sensors

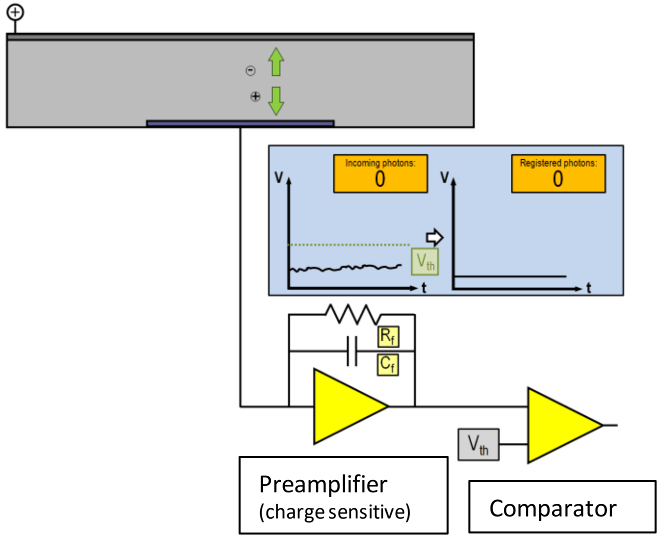
	Energy resolution	Stability	Afterglow	Dark current	Availability
High flux -500V CdZnTe	☺	☺	☺	☺	☹
Schottky -500V CdTe	😐	☹	☹	☺	☺
GaAs:Cr -300V	😐	😐	☹	☹	☺

Photon counting *vs.* Charge integrating detectors

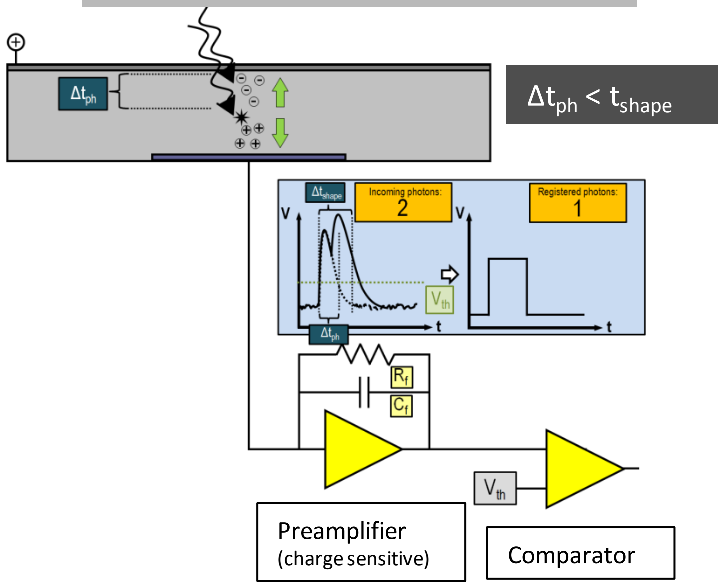
Single photon detection

Multiple photons

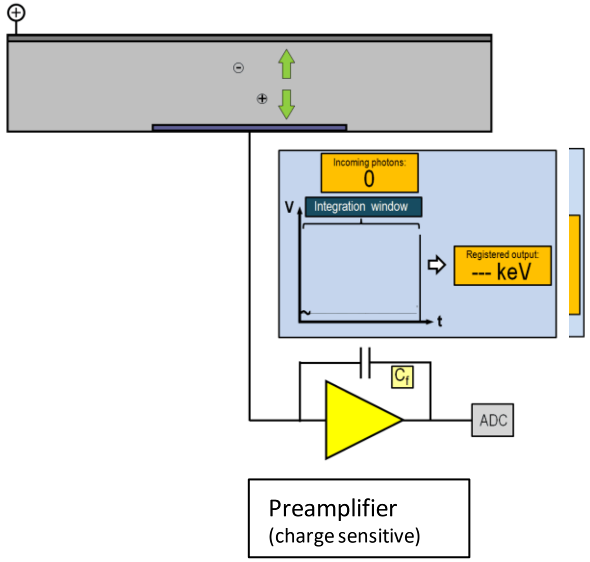
Single Photon Counting



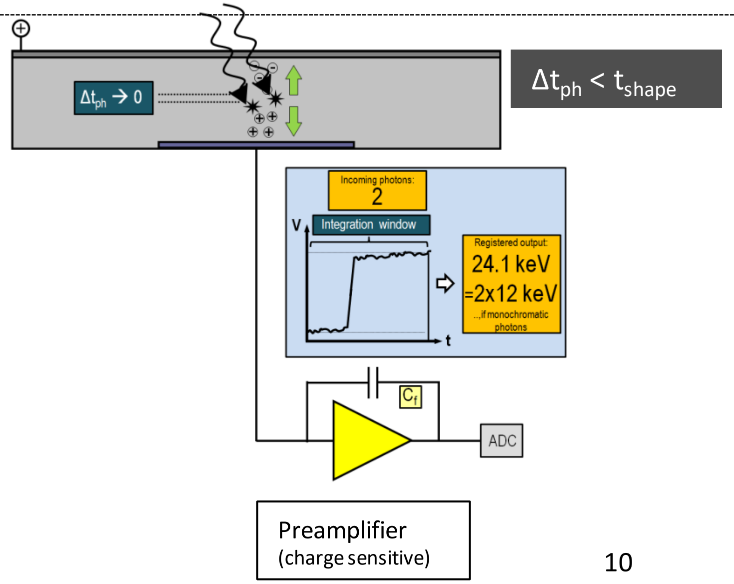
- \+ Readout of digital info
- \+ 'Noise free' operation
- \+ (Almost) unlimited dynamic range
- \- Minimum detectable energy
- \- Count-rate limitation (pile-up)



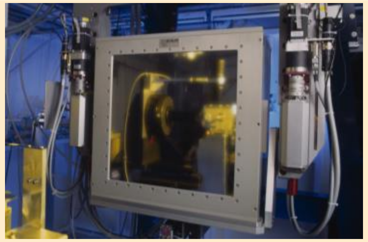
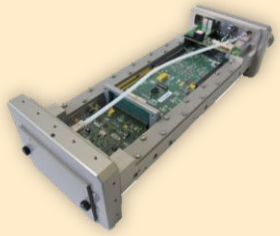
Charge Integrating



- \+ Energy for each photon
  (Low flux, Polychromatic)
- \+ Practically no count-rate limitation
  (High flux, Dynamic Gain)
- \+ Measurement of charge sharing
  (Position interpolation)
- \- Calibration procedure challenging
- \- Integration of leakage current

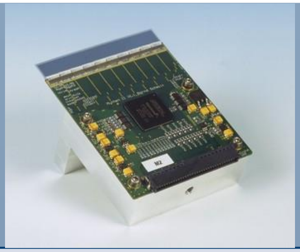
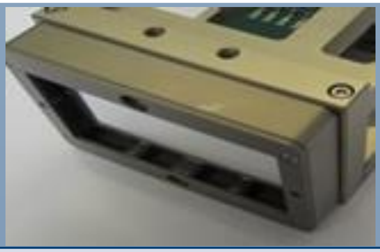
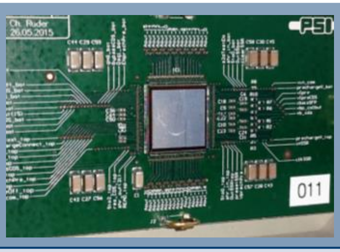


Detector portfolio: Photon counting

	MYTHEN-3	PILATUS	EIGER	MATTERHORN
				
Technology	UMC 110 nm	UMC 250 nm	UMC 250 nm	UMC 110 nm
Status	Modules available	Commercially available[1]	Commercially available[1]	Prototyping phase
Pixel size	50 µm (Strips)	172 x 172 µm^2	**75 x 75 µm^2**	**75 x 75 µm^2**
Maximum system size	120° (=48 modules)	**6M** (=42 x 43 cm^2)	**9M** (=23 x 23 cm^2)	
Minimum threshold	< 4 keV	< 2 keV	< 2.5 keV	
Count rate capability	>2 MHz/Strip (10% deviation, Standard)	0.5-1.0 MHz/Pixel (10% deviation)	0.2-0.7 MHz/Pixel (10% deviation)	
Maximum frame rate	**300 kHz (8-bit)**	300 Hz/Module	**23 kHz (1-bit)**	

1) PILATUS and EIGER are commercially available at Dectris.

Detector portfolio: Charge integrating

	GOTTHARD-2	AGIPD[1]	JUNGFRAU	MÖNCH
				
Technology	UMC 110 nm	IBM 130 nm	UMC 110 nm	UMC 110 nm
Status	Modules available	Modules available	Modules available	Prototyping phase
Pixel size	50 / 25 µm (Strips)	200 x 200 μm^2	**75 x 75 μm^2**	**25 x 25 μm^2**
Maximum system size	10 / 20 ASICs	1Mpixel	16Mpixel	
Noise (r.m.s.)	~ 270 e^- ENC @ 4.5 MHz	< 322 e^- ENC < 214 e^- ENC (HG)	**< 100 e^- ENC (G0) < 55 e^- ENC (HG0)**	
Dynamic range	**< $1\cdot10^4$ x 12.4 keV (3 gain stages)**	**< $1\cdot10^4$ x 12.4 keV (3 gain stages)**	**< $1\cdot10^4$ x 12.4 keV (3 gain stages)**	
Maximum frame rate	**400 kHz (cont.) 4.5 MHz (burst)**	**< 5 MHz (burst*) * 352 frames**	**2.4 kHz (cont.) < 1 MHz (burst)**	

1) Common development with University of Bonn, University of Hamburg and DESY

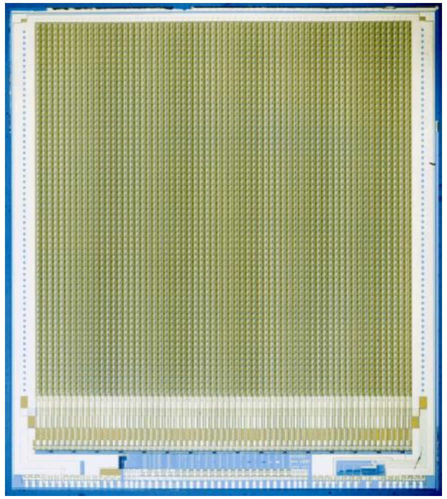
The birth of hybrid pixel detectors for Photon Science

CERN

Alice1LHCb

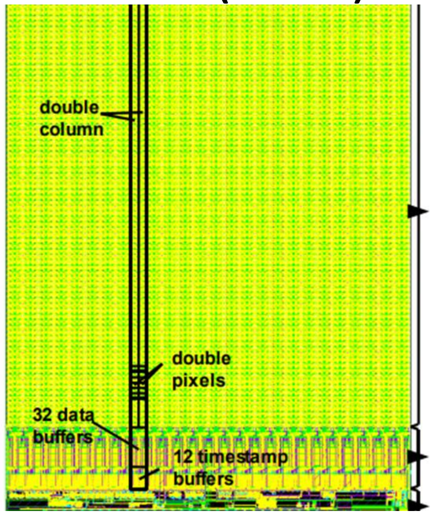
M. Campbell
E. Heine
X. Llopart

Medipix 1



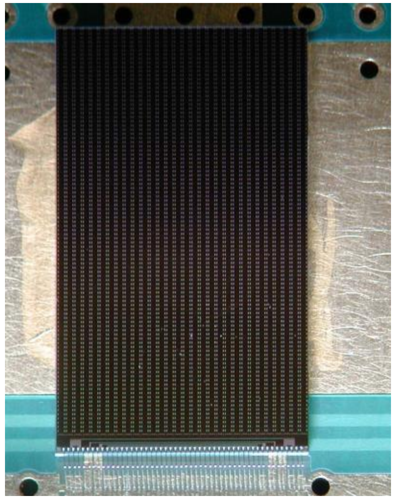
PSI

PSI46 (CMS)



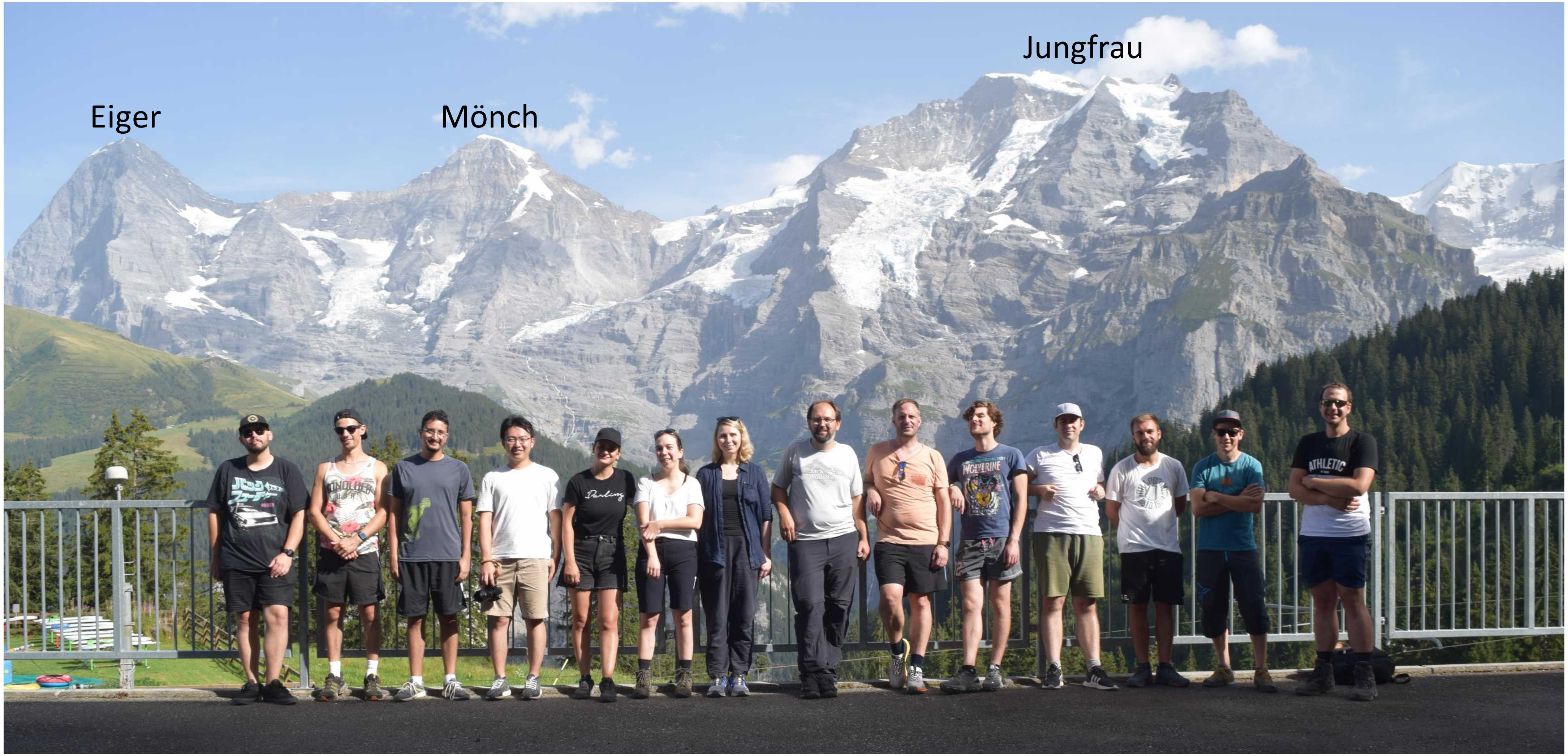
R. Horisberger
F. Van Der Veen
C. Broennimann

Pilatus I



Group members

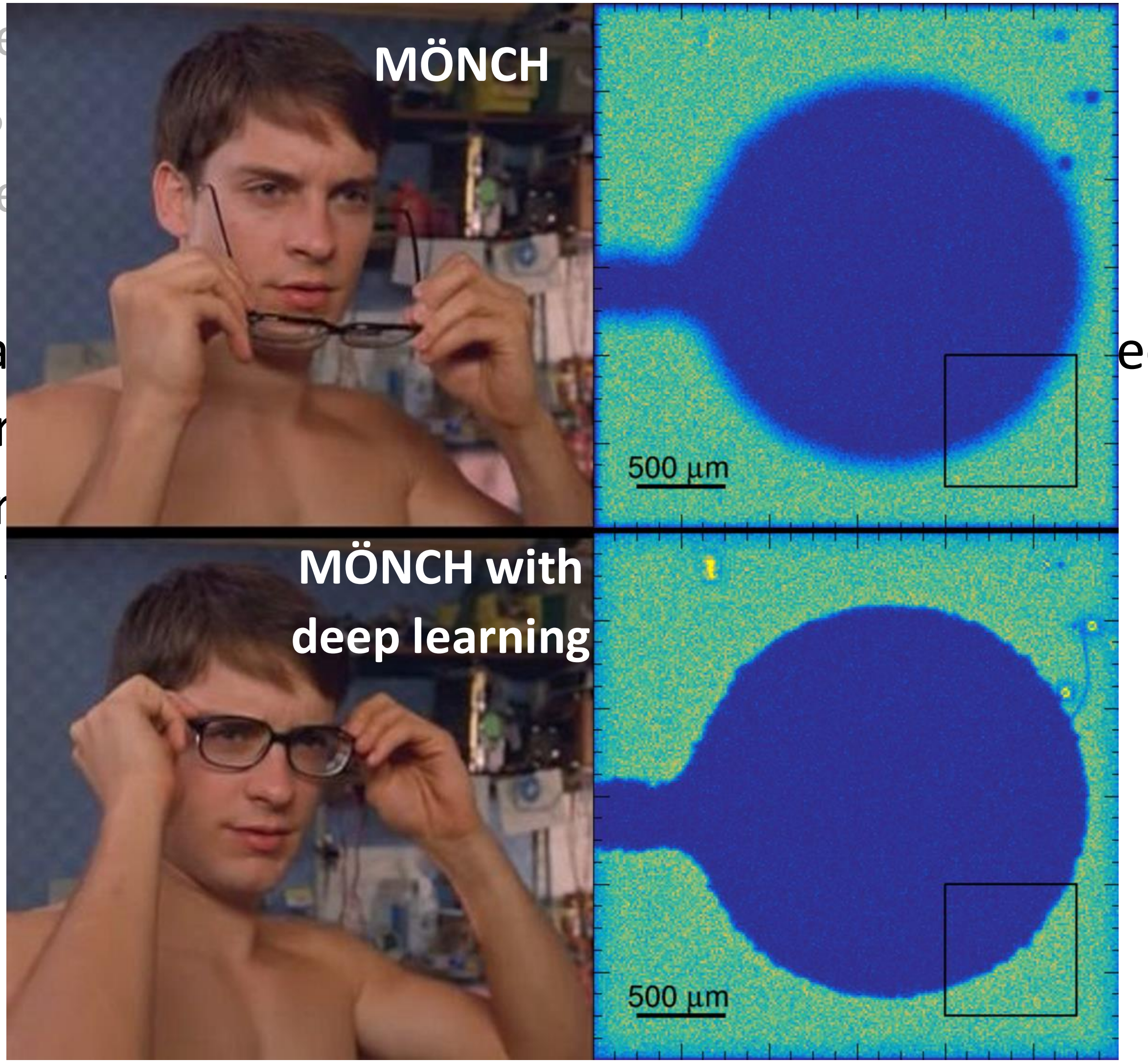
August 2023



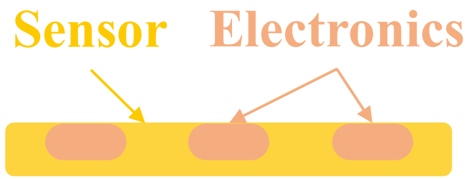
Missing: Anna, Bernd, Jiaguo, Aldo, Christian, Carlos, Davide, Dhanya, Roberto, Konstantinos…

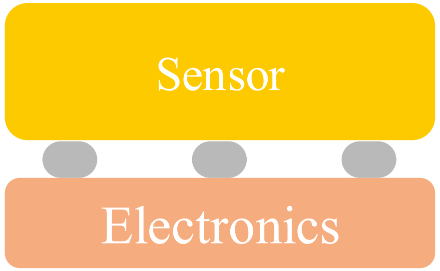
Outline

- Hybrid pixel dete
  – PSI and the PS
  – Hybrid pixel de
- Enhanced spatia ectron microscopy
  – Sample prepar
  – Neural networ
  – Results evalua



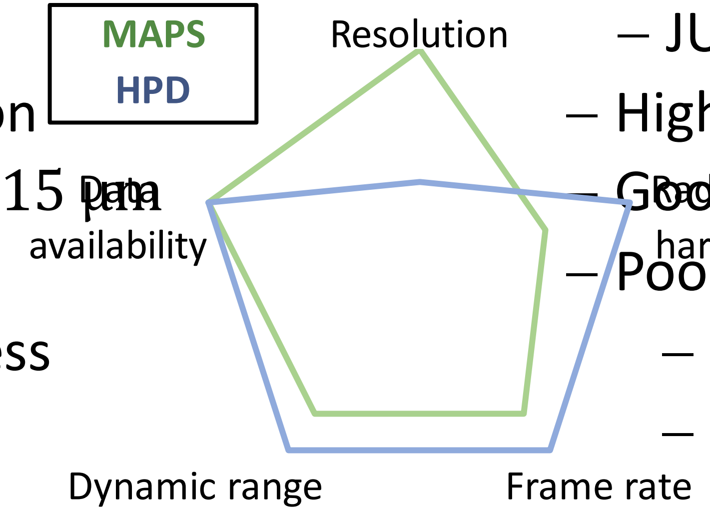
Direct Electron Detector for Electron Microscopy, the “resolution revolution”





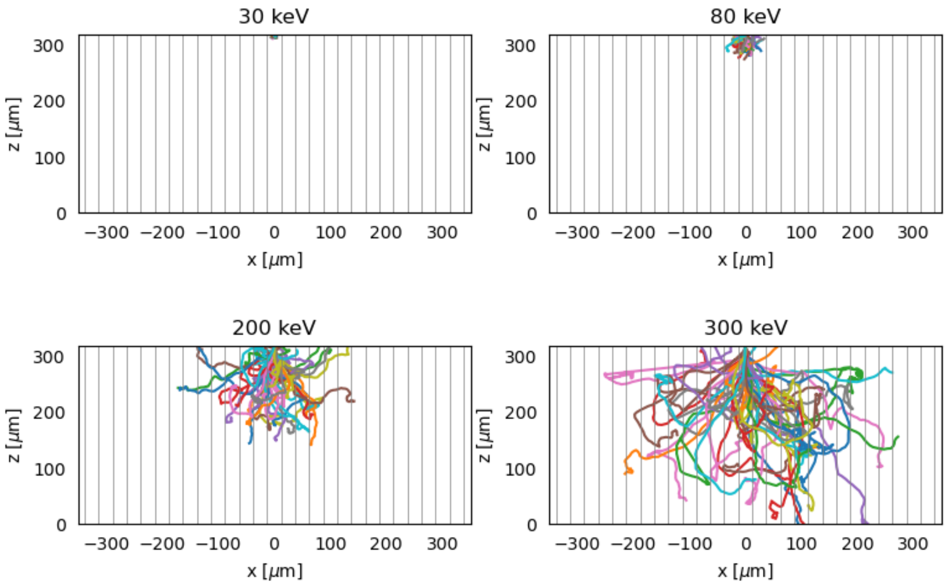
- Monolithic Active Pixel Senor (MAPS)
  - Widely applied for (cryo-)imaging and diffraction measurements
    - K2, Falcon…
  - Good spatial resolution
    - Pixel size usually $< 15\ \mu m$
  - Limited frame rate
  - Poor radiation hardness

- Hybrid Pixel Detector (HPD)
  - Getting popular for diffraction measurements
    - JUNGFRAU, Medipix…
  - High dynamic range and frame rate
  - Good radiation hardness
  - Poor resolution
    - Large pixel size usually $\geq 55\ \mu m$
    - Electron multiple scattering

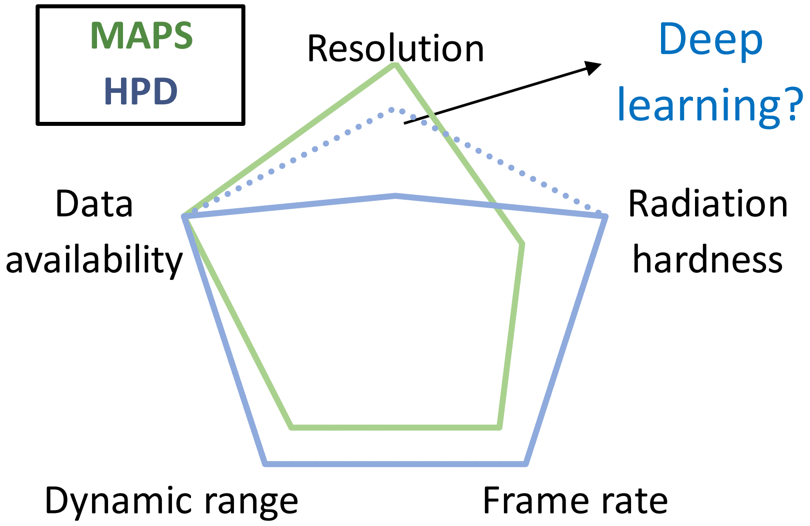


MÖNCH, towards a universal detector for diffraction and imaging

- MÖNCH, a HPD with much smaller pixel
  - **25 μm** pitch size
  - 400×400 pixels per tile
  - Charge integration, 14 bit, up to 6 kHz
- Lateral track due to multiple scattering
  - Poor resolution for e^- with $\mathrm{E} > 80\mathrm{keV}$



- **Deep learning** to reconstruct position
  - From the complex pattern to learn
    - Nature of energy deposition
    - Charge diffusion
  - Aim at subpixel resolution



Project members

- Funded as a Swiss Data Science Center(SDSC) project

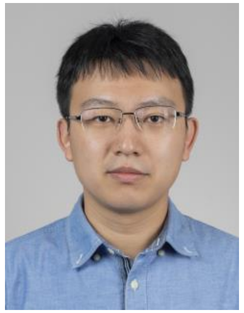
SDSC hub @ PSI

Dr. Carl Remlinger

PSI
Electron Microscope Facility group


PSI
Photon Science Division
Detector group

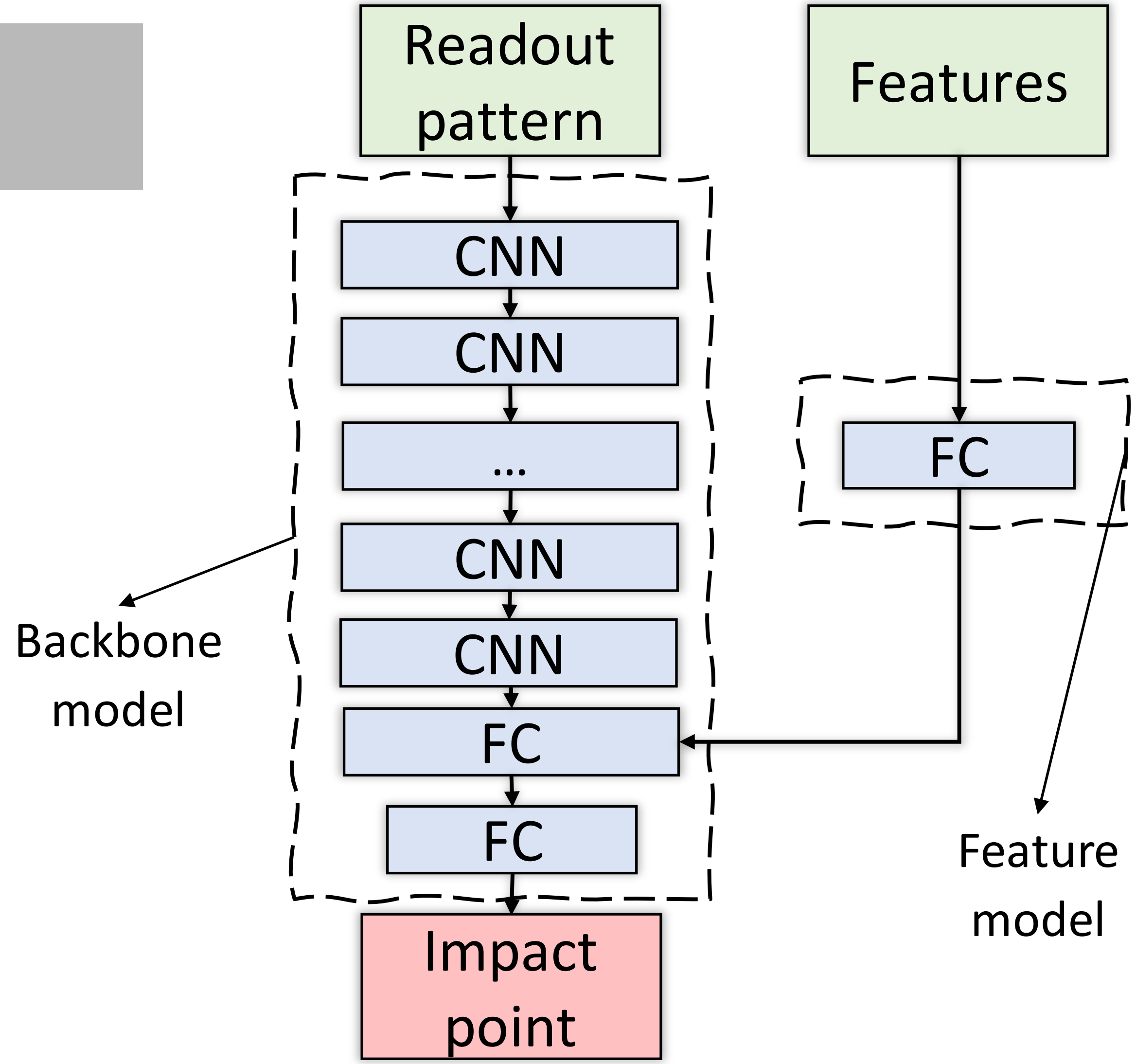


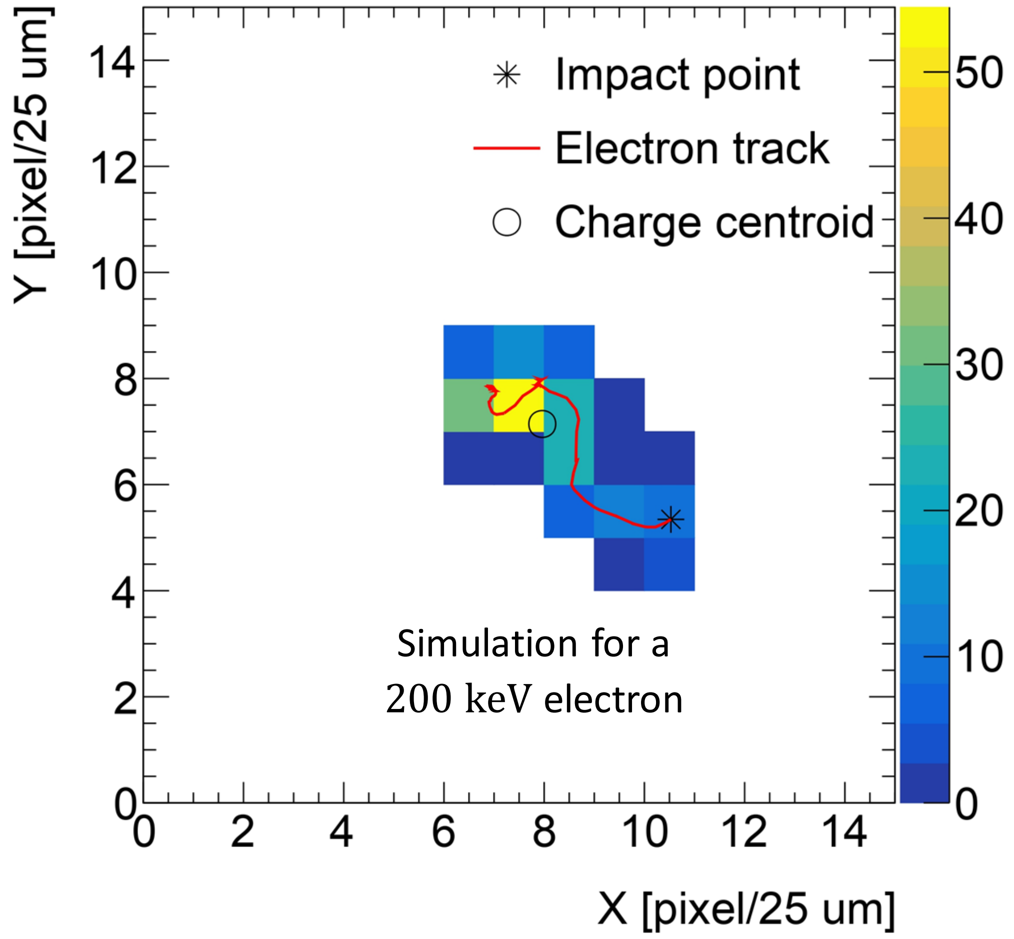
Project overview

- Deep learning development
  - Neural network candidate models
    - A baseline model (results discussed in this report)
    - Auto-encoder
    - …
  - Samples preparation
    - Simulation and experimental
    - Key: the ground truth impact point
- Characterization
  - Spatial resolution
  - Detective quantum efficiency
  - Standard sample imaging
- Deployment & dissemination
  - Data processing pipeline(WIP)

Baseline neural network model



- Input: readout pattern and features



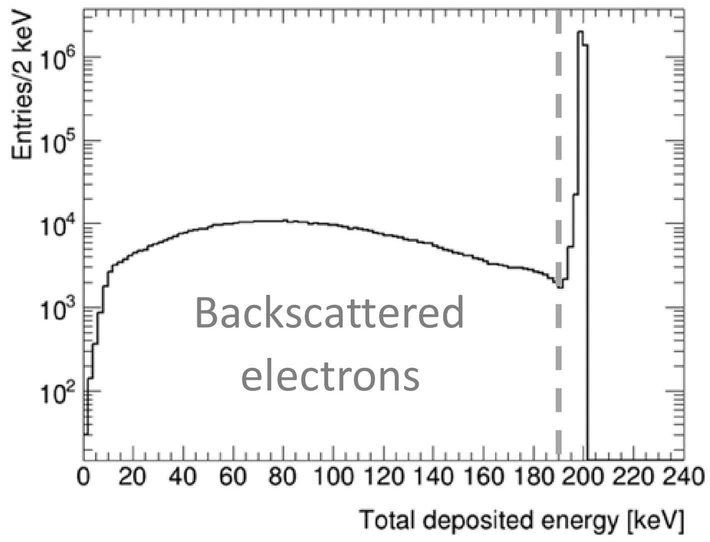
tures

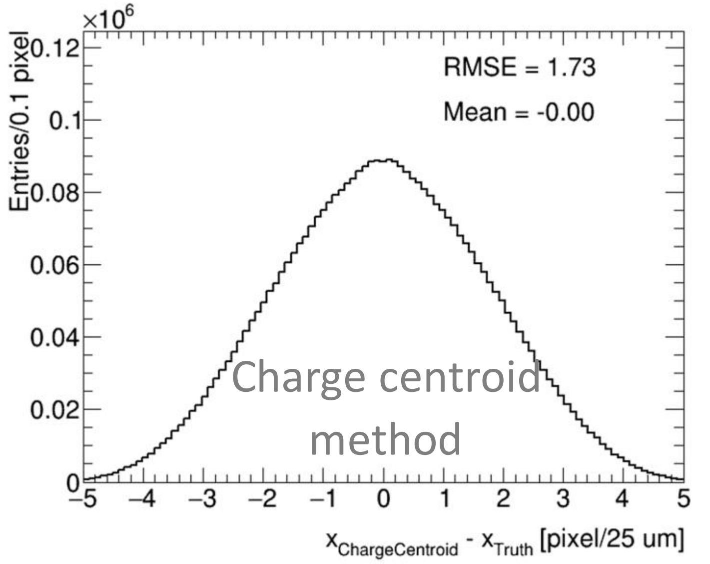
gy ...

) GPU

Simulation-based: samples analysis

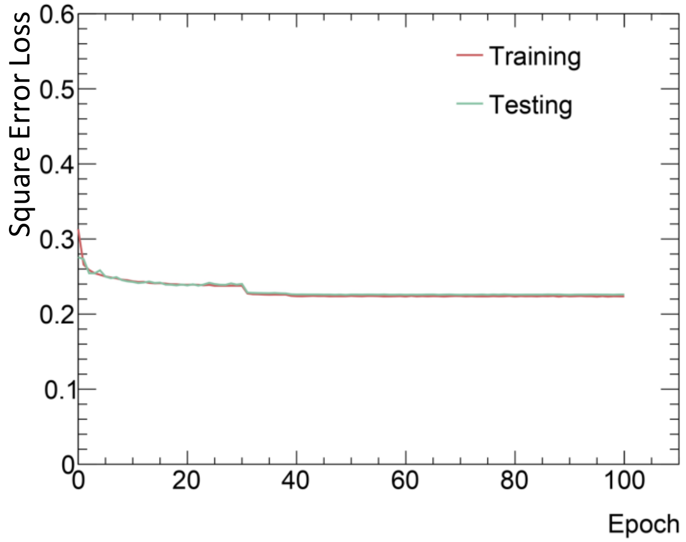
- Simulation setup
  - Geant4 + charge diffusion model
    - 320 μm silicon sensor
    - $V_{\text{bias}} = 90$ V
    - Start with 200 keV electrons
  - Total samples: 4M
    - 70%/30% for training/testing
- Simulation analysis
  - ~15% backscattered electrons
  - Charge centroid gives $\sigma_x = 1.73$ pixel

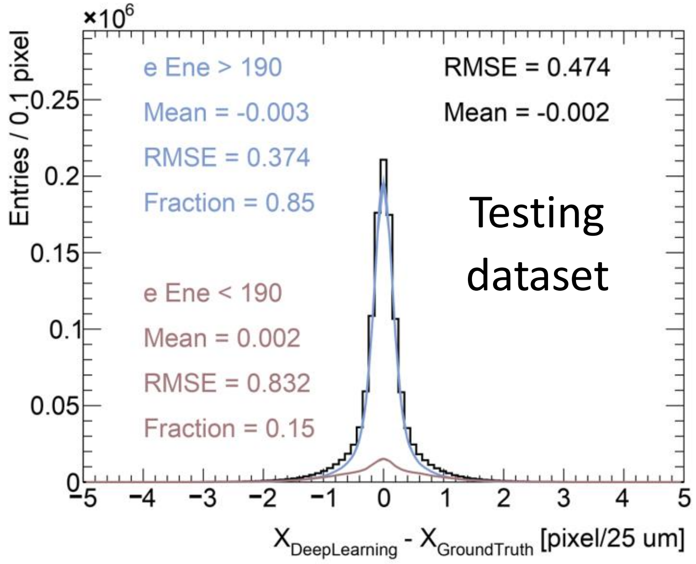




Simulation-based: training and results

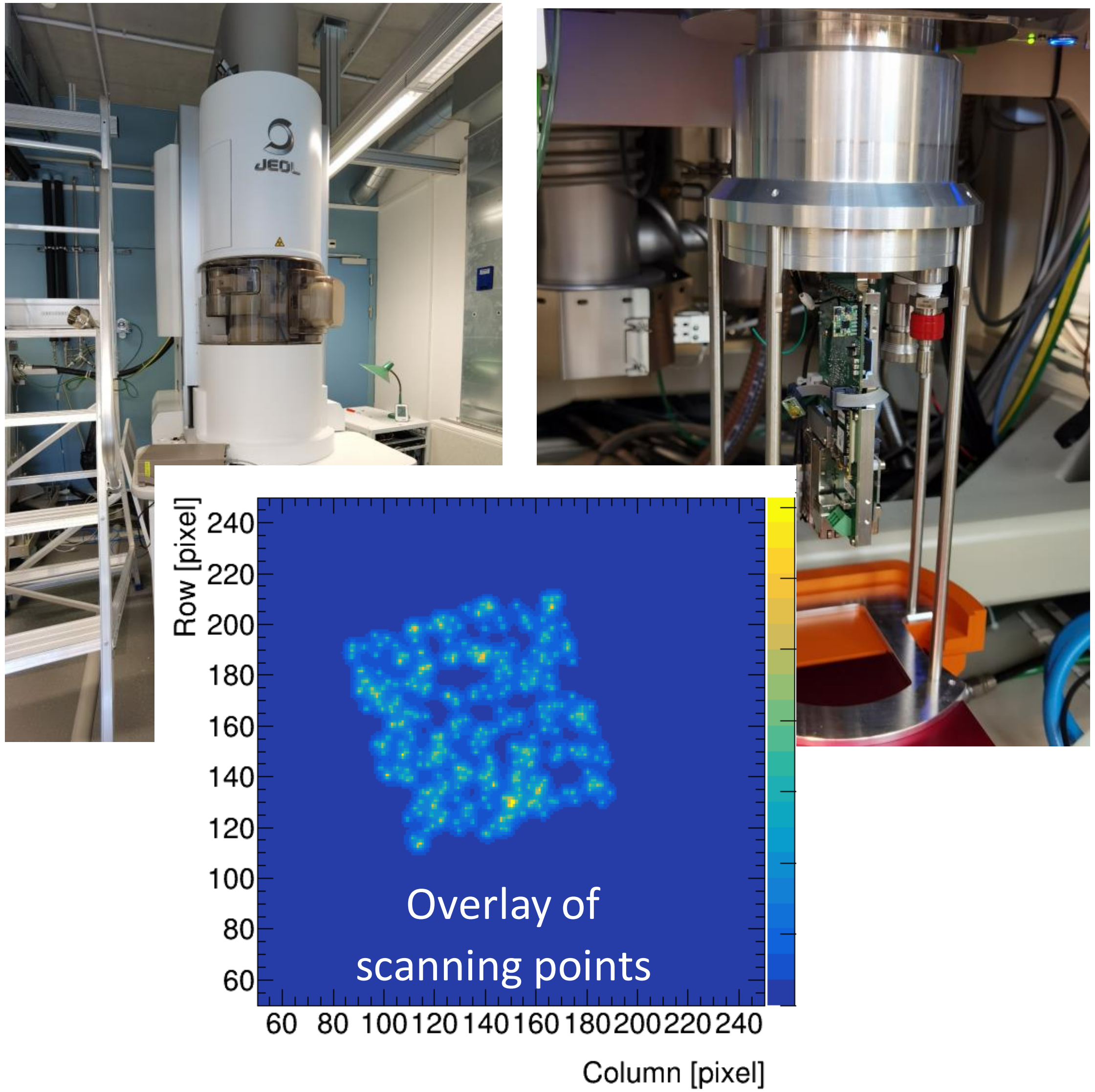
- Training setup
  - 100 epochs/iterations
  - Data augmentation
    - Rotation and flipping
    - Training label smoothing
    - Synthetic noise ($\sigma = 0.18$ keV)
- Simulation-based results
  - No significant overfitting
  - Deep learning gives $\boldsymbol{\sigma_x = 0.47}$ pixel
    - Fully deposited e^-: $\sigma_x = 0.37$
    - Backscattered e^-: $\sigma_x = 0.83$





Experiment-based: data taking setup

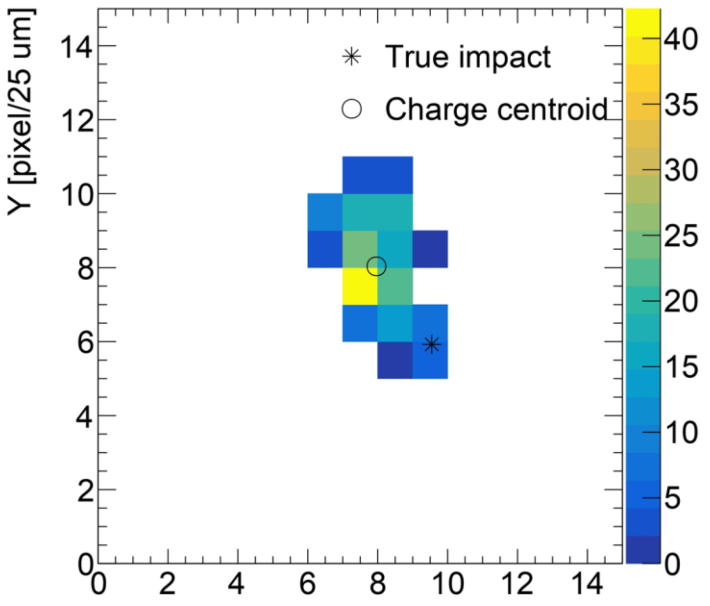
- EM: Jeol JEM ARM200F
  - 200 keV beam
  - Customized alignments
  - Narrow beam (~μm)
- Detector: MÖNCH v0.3
  - One tile; 400×400 pixels
  - $V_{bias} = 90$ V
- Ground truth impact points obtaining
  - EM randomly scans with longer dwell time (~s)
  - 430 scan points × 10,000 frames
  - **Unbiased ground truth position:** $\bar{x}, \bar{y}$

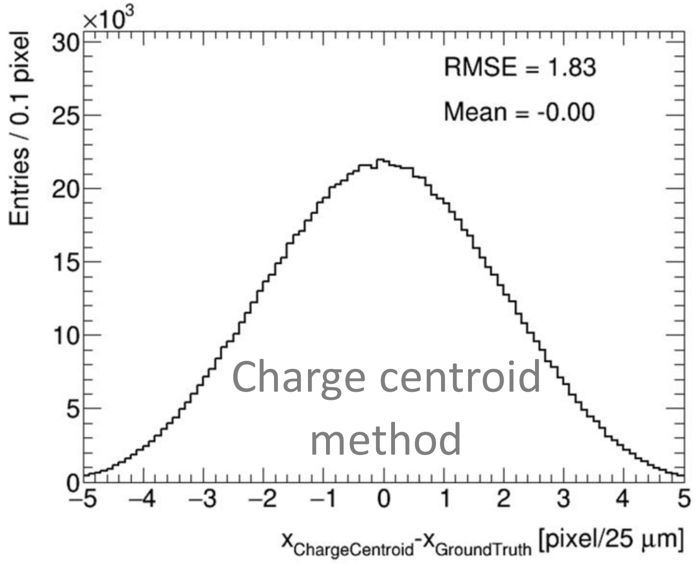


Experiment-based: sample analysis

- Frame level
  - Mask malfunction region
  - Pedestal subtraction
  - Energy conversion
- Cluster finding and selection
  - Adjacent pixels over a threshold of $5 \times \text{Noise} \approx 0.9\ \text{keV}$ (g2_lc_hg mode)
  - $20\ \text{keV} < \text{E}_{\text{cluster}} < 220\ \text{keV}$
  - Outlier filtered

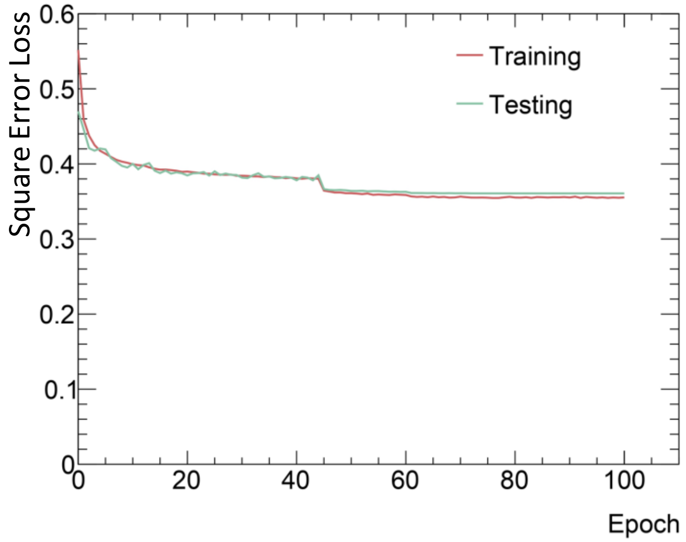
- Total samples: $\sim$1M
  - Charge centroid gives $\sigma_x = 1.83$ pixel



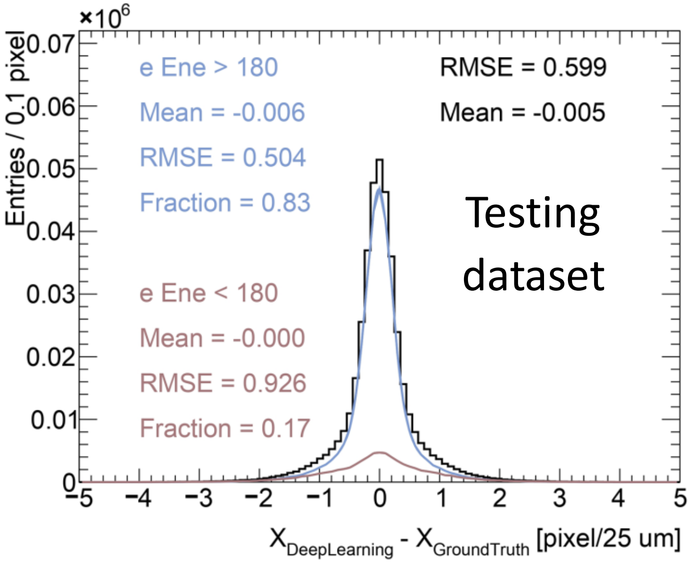


Experiment-based: deep learning results

- Training setup
  - 100 epochs
  - Data augmentation
    - Rotation and flipping
    - Training label smoothing



- Experiment-based results
  - No significant overfitting
  - Deep learning give $\boldsymbol{\sigma_x = 0.60}$ **pixel**
- Independent knife-edge measurements
  - Sample processed by the trained model
  - Edge spread function gives $\boldsymbol{\sigma_x = 0.58}$ **pixel**



Preliminary MTF and DQE results (200 keV)

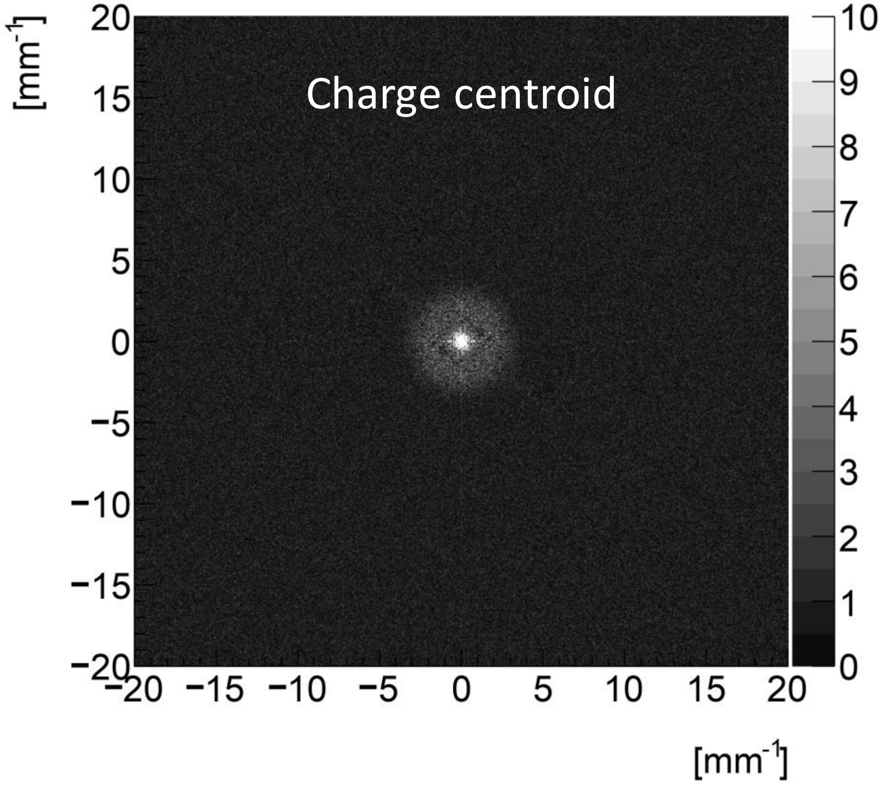
$$\mathrm{MTF}(\omega) = \mathcal{F}[\mathrm{PSF}(x)]$$

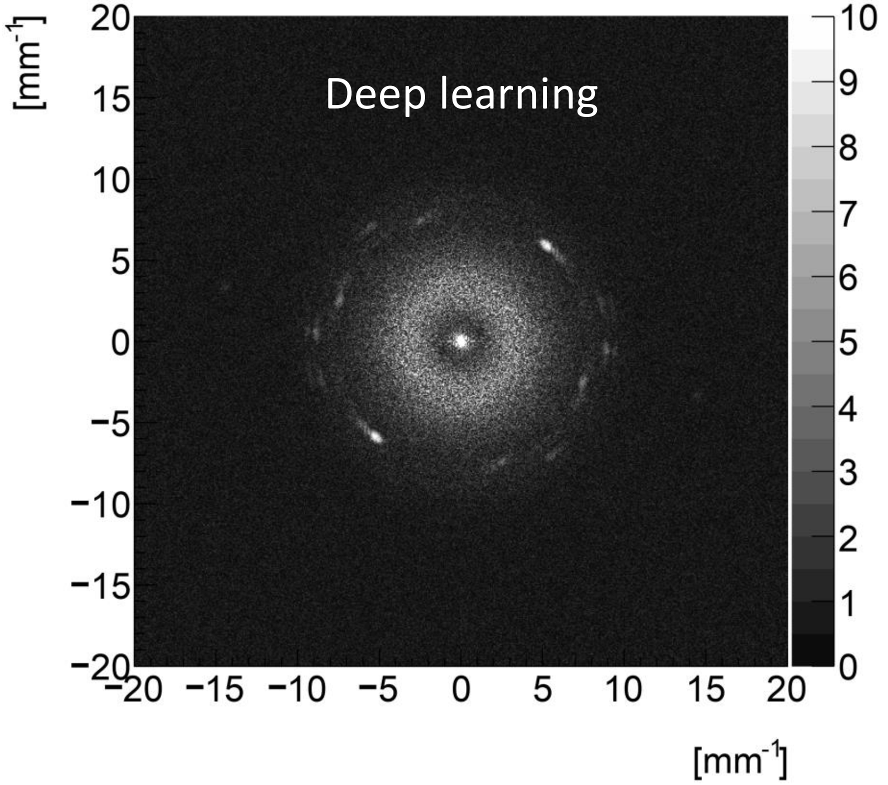
$$\mathrm{DQE}(\omega) = \mathrm{MTF}^2(\omega)\frac{d_n^2}{n\mathrm{NPS}(\omega)}$$

Flux = $\sim 10\ e^-/s/\mathrm{pixel}$

Results from the experimental data

- TEM sample with continuous carbon and gold nanoparticles





With deep learning, we can see the ring corresponding to 2.35 Å atom arrangements

Summary

X Xie et al, *enhancing spatial resolution in MÖNCH for electron microscopy via deep learning,* JINST (accepted)

- Significant improvements in spatial resolution on MÖNCH, via deep learning

@ 200 keV	**Charge centroid**	**Deep learning + super resolution**		
		Simulation based model	Experiment based model	Knife-edge with experi. model
σ_x [pixel]	1.83	0.70	0.60	0.58

- Promising performance for energies lower than $200\ \mathrm{keV}$
- Outlook
  - Detector calibration
  - Simulation development
  - Challenge: large MÖNCH module

Backup

PAUL SCHERRER INSTITUT PSI

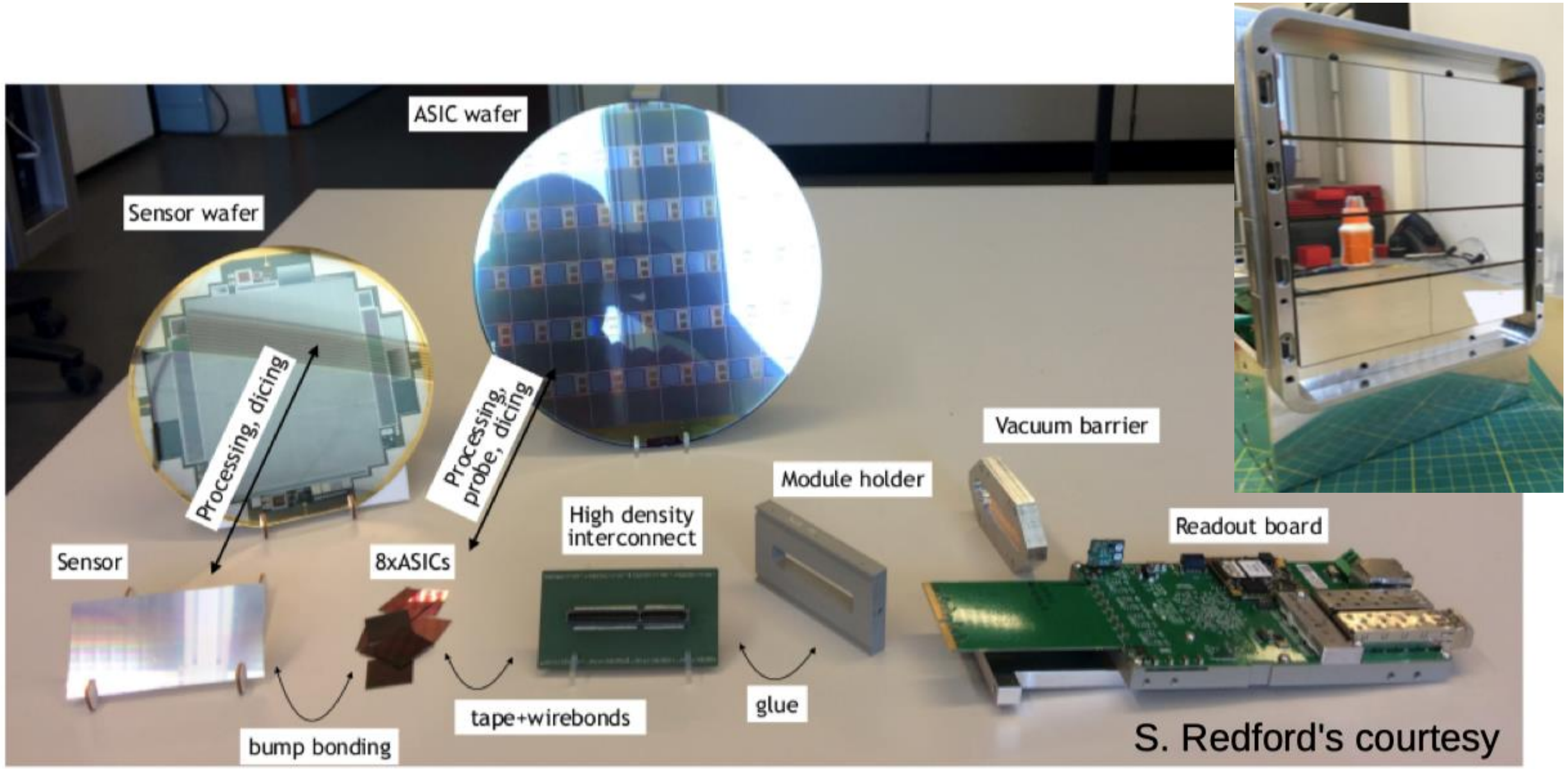
Design and build detectors in-house

Work done at PSI:

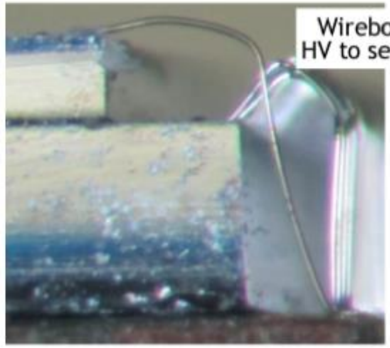
- sensor design
- ASIC design
- readout boards
- flip-chip bonding
- wire-bonding
- mechanics
- assembly
- firmware
- control software

+

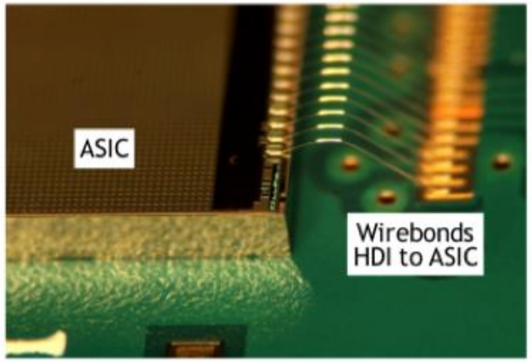
- calibration
- integration/commissioning
- user support/interface

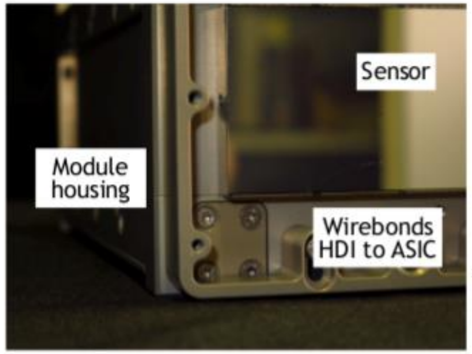


Sensor
bump bonding
ASIC

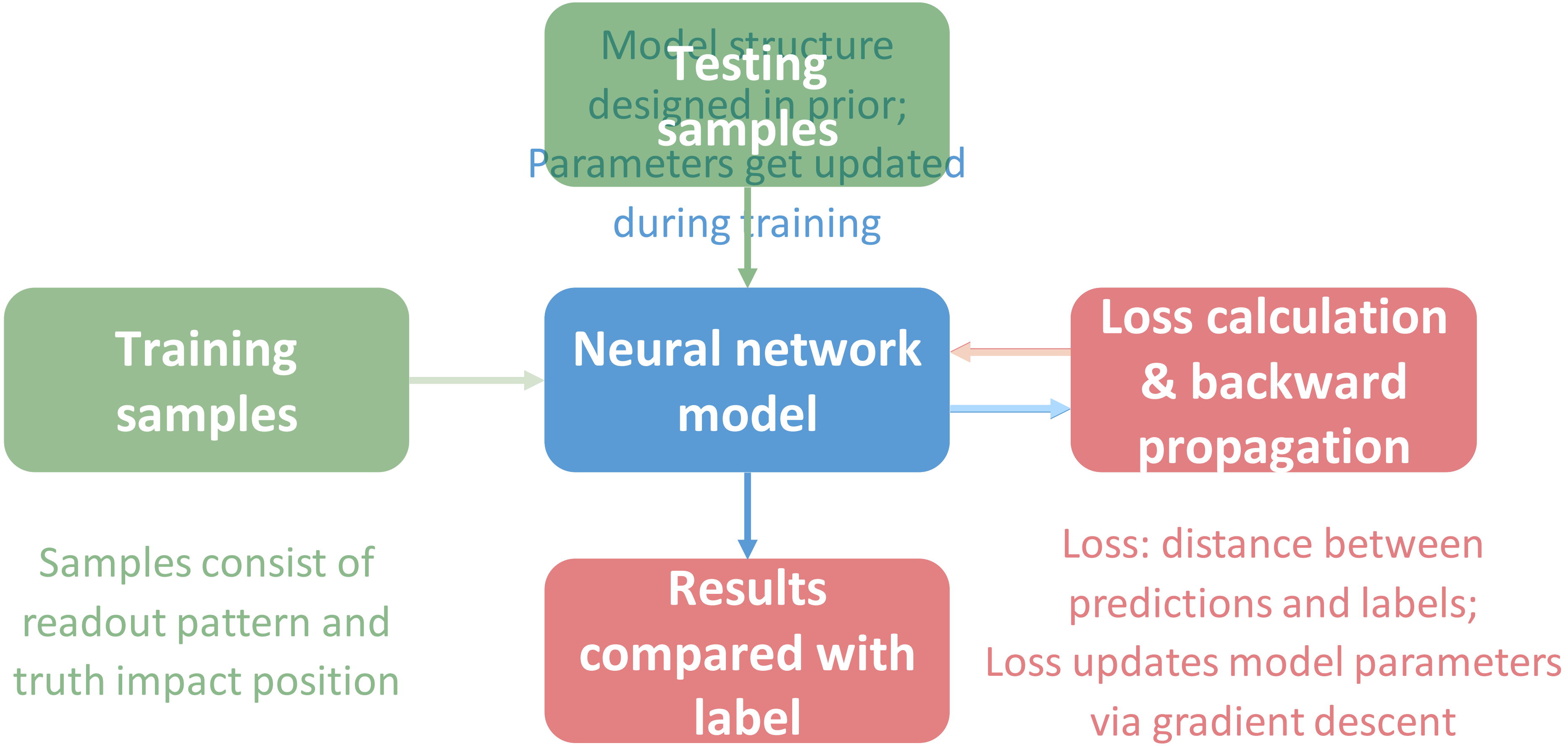


Wirebonds HDI to ASIC



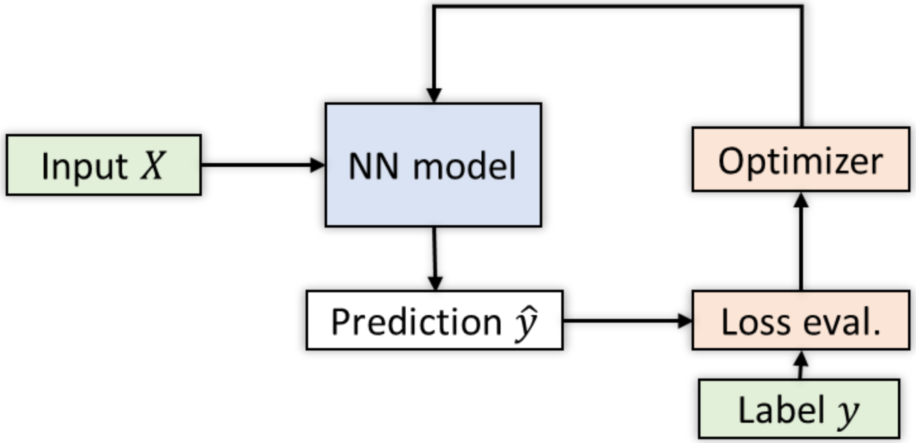


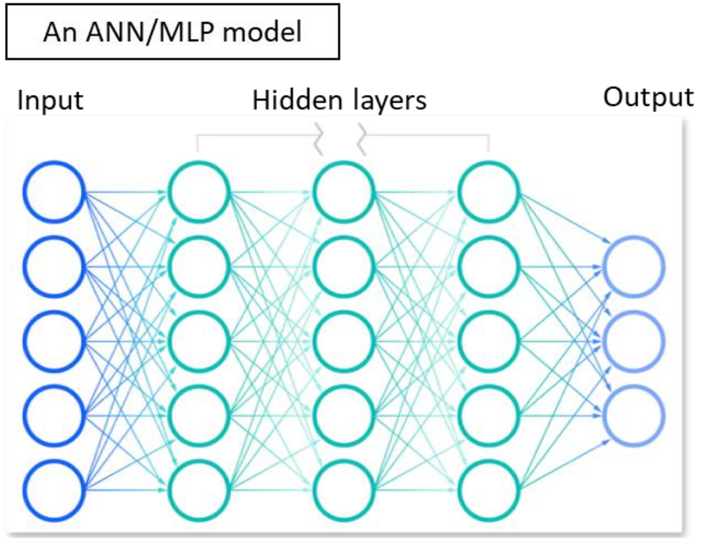
Deep learning workflow



Backup Deep learning components

- Dataset
  - Inputs X: signal waveforms, images, texts …
  - Labels y: time, position, cat/dog …
    - Known as ground truth in supervised learning
- Neural network model
  - Composes of inter-connected neuron layers
  - Each neuron layer has
    - Weight $W^{[l]}$, bias $B^{[l]}$
    - Activation function g
- Loss function + optimizer
  - Loss function F to evaluate loss J
    - F: RMSE, cross-entropy …
    - J: difference between predictions and labels
  - Optimizer: the pilot to update the model

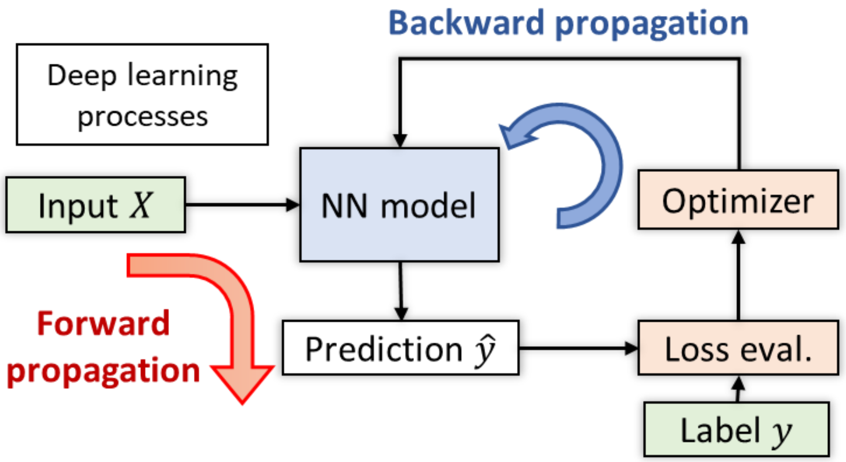


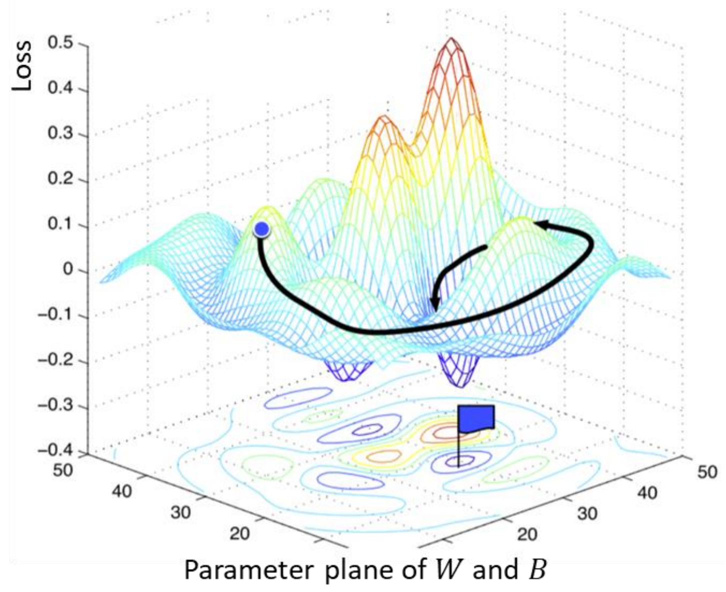


Backup: Deep learning training processes

- Forward propagation:
  - $Z^{[l]} = B^{[l]} + W^{[l]}A^{[l-1]}$
  - $A^{[l]} = g(Z^{[l]})$
- Backward propagation:
  - Loss evaluation: $J = F(\hat{y}, y)$
  - Optimizing: $W \leftarrow W - \alpha \frac{\partial J}{\partial W}, \frac{\partial J}{\partial W} = \frac{\partial J}{\partial A}\frac{\partial A}{\partial Z}\frac{\partial Z}{\partial W},$

    α: learning rate, usually $0.001 < \alpha < 0.1$
- Targets
  - To optimize the model to minimize loss
  - To predict well for untrained data, i.e., good generalization ability





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Backup: CNN kernel

10	10	10	0	0	0
10	10	10	0	0	0
10	10	10	0	0	0
10	10	10	0	0	0
10	10	10	0	0	0
10	10	10	0	0	0

Image in gray scale

*

1	0	-1
1	0	-1
1	0	-1

Kernel for vertical detection

=

0	30	30	0
0	30	30	0
0	30	30	0
0	30	30	0

Results

- Kernel
  - At early stages, CV experts manually designed kernel
  - In ML, dozens of kernels could be automatically formed during training
- Combination of results distinguish pattern in complex images