X-Ray Detector Simulation Pipelines for the European XFEL

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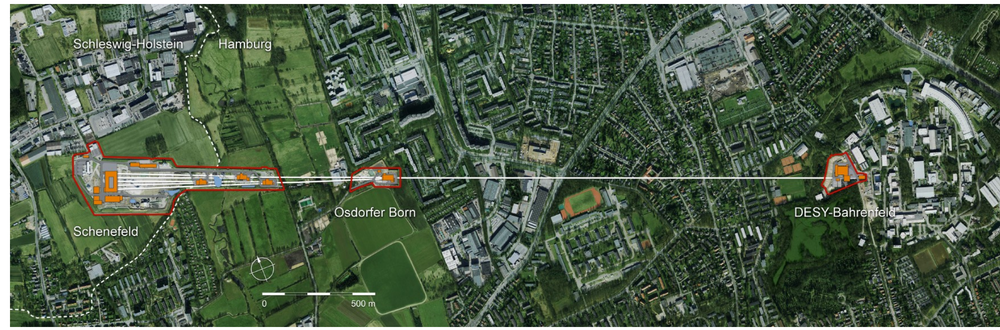
Freie Universität Berlin

UCL

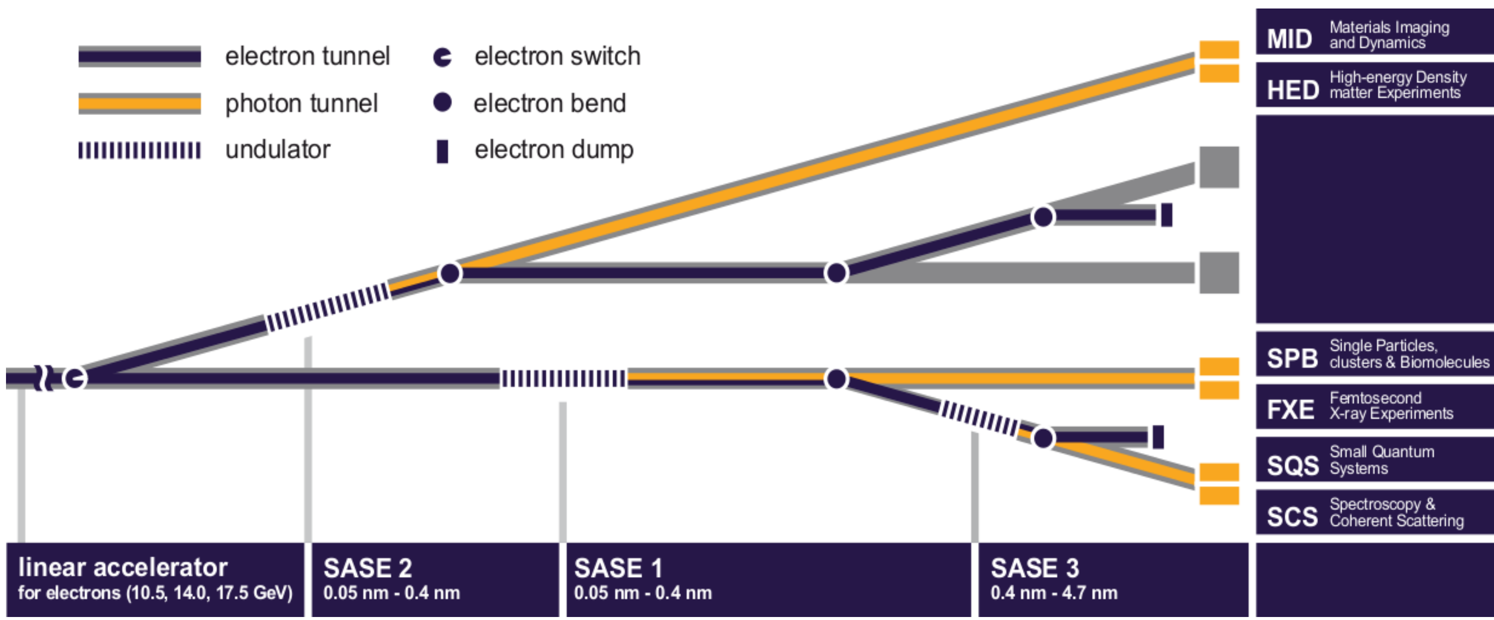
The European X-ray Free Electron Laser

- Driven by **superconducting LINAC** located in Hamburg, Germany
- Three photon paths service **six experimental stations** located in Schenefeld
- Photon energy ranges from **0.25 – 25.0 keV** (minimum wavelength: 0.05 nm)

Location in Hamburg, Germany

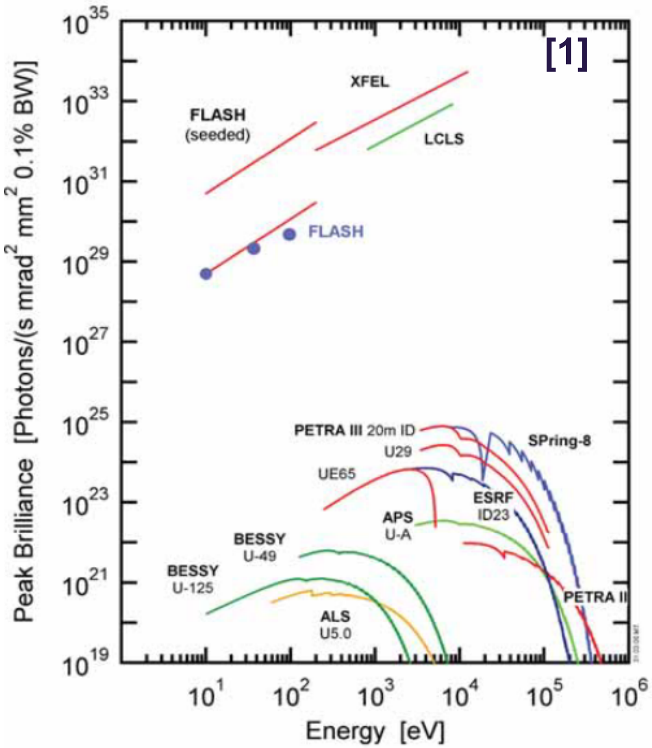


Experimental stations at the European XFEL

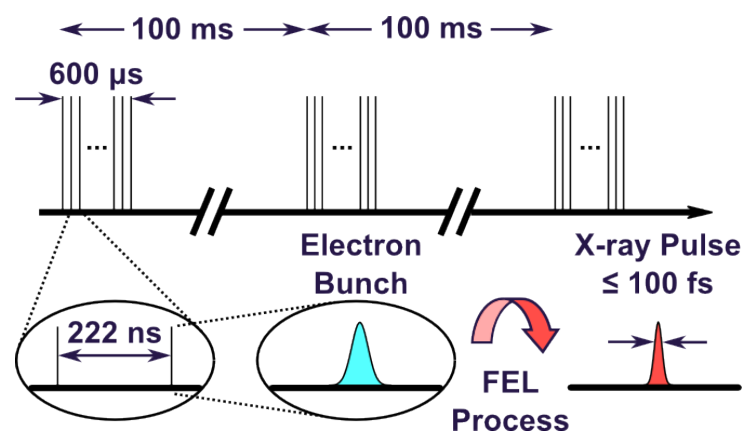


Images publicly available at **www.xfel.eu**

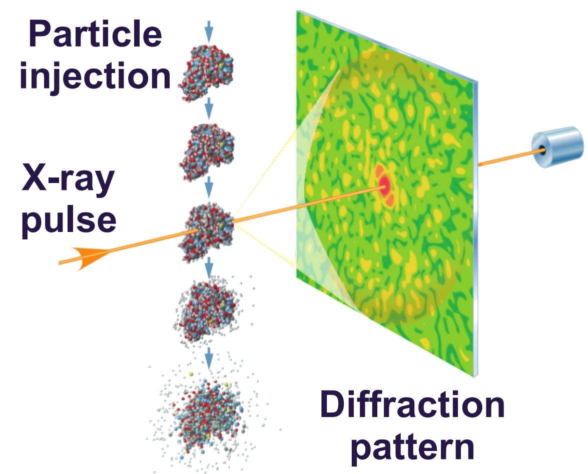
Exceptional Features of the European XFEL



Electron bunch time pattern (10 Hz repetition) [1]

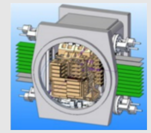
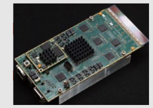
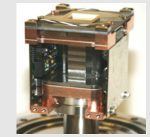
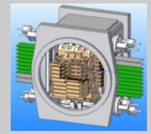
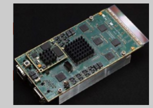
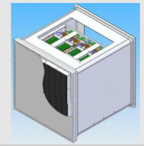
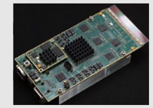
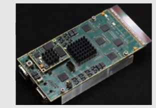
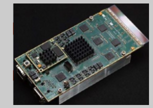
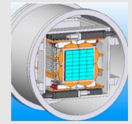
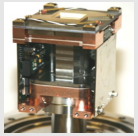
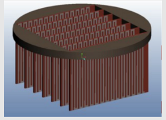
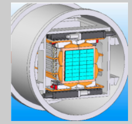
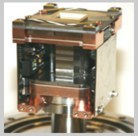
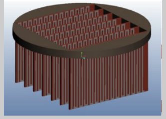
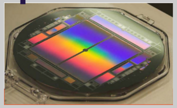


Schematic of an exemplary imaging experiment:



- **Photon beam properties**
  - Experiments can use **coherence** property of X-ray photons
  - High photon flux: up to **10^{13} photons per pulse**
- **Unique time structure**
  - 2700 electron bunches (200 ns seperation) produce 100 fs X-ray pulses
  - Allows study of dynamic processes (e.g. chemical reactions)

Detectors for XFEL Instruments

SASE 1 / SASE 2, 2.3 – 25 keV	Single Particles, Clusters and Biomolecules (SPB)	AGIPD 	Gotthard V2 	FastCCD 	
	Materials Imaging & Dynamics (MID)	AGIPD 	Gotthard V2 		
	Femtosecond X-ray Experiments (FXE)	LPD 	Gotthard V2 	Gotthard V1 	
	High Energy Density Matter (HED)		Gotthard V2 		
SASE 3, 0.26 – 3 keV	Small Quantum Systems (SQS)	DSSC 	FastCCD 	MCP 	
	Spectroscopy and Coherent Scattering (SCS)	DSSC 	FastCCD 	MCP 	pnCCD 

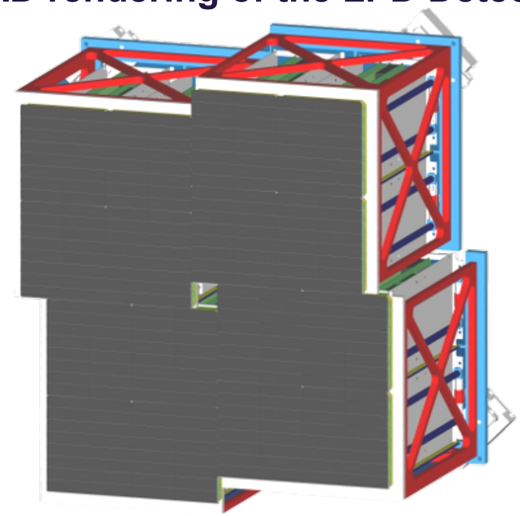
Slide from internal resources

European XFEL

Motivation and Requirements

- **Use cases**
  - Estimate detector performance
  - Aid in planning of experiments and analyzing results
  - As drop-in for real detector in processing/analysis pipelines
- Provide an **agile simulation environment** for the various X-ray detectors at XFEL
  - Extends A. Joy's **X-ray Camera Simulation Toolkit**
  - Accounts for the **variety of semiconductor X-ray detectors**
  - Modular physics simulations, separated into **three sub-simulations**

CAD rendering of the LPD Detector

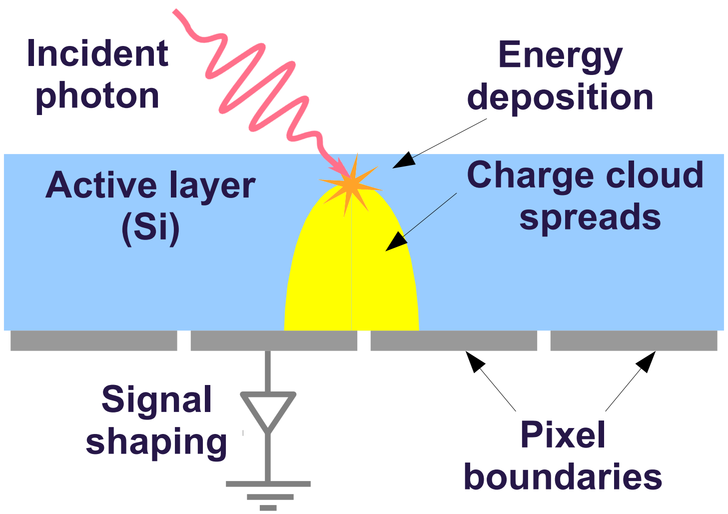


	LPD	AGIPD	DSSC	pnCCD	FastCCD
Pixels [µm] (Shape)	500 (square)	200 (square)	204 (hexagonal)	75 (square)	30 (square)
Dynamic range	$1x10^5$ at 12 keV	$1x10^4$ at 12 keV	$3x10^3$ at 1 keV, $1x10^4$ at >1keV	$1x10^3$ at 2keV; dE: 130eV at 5.9keV	$1x10^3$ at 500eV, dE: 400eV at 5keV
Total size [px]	1024 x 1024	1024 x 1024	1024 x 1024	200 x 128	1960 x 960
E_{ph} [keV]	1 - 24	3 - 13	0.5 - 6	0.1 - 15	0.25 - 6
Application	Integrating detector (e.g. SPB, MID, SCS)			+ Spectroscopic photon counting	

Thanks to **Matthew Hart** of the LPD consortium for providing the LPD rendering

Detector Simulation Layout

Divide the radiation detection process into three stages:

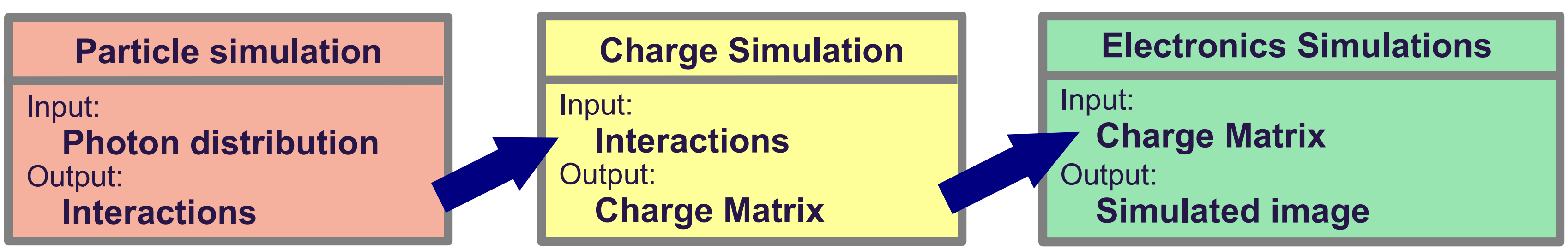


X-ray/matter interaction
- Energy deposition in the detector material
- Based on Geant4 v10.0, using Livermore models based on Evaluated Photon Data Library (EPDL)
- Validation for previous versions exist (Pia + Batij et al., nano5, 2009, …, 2015)

Charge carrier transport
- Drift due to bias voltage, lateral diffusion
- Carriers accumulate to a measurable signal

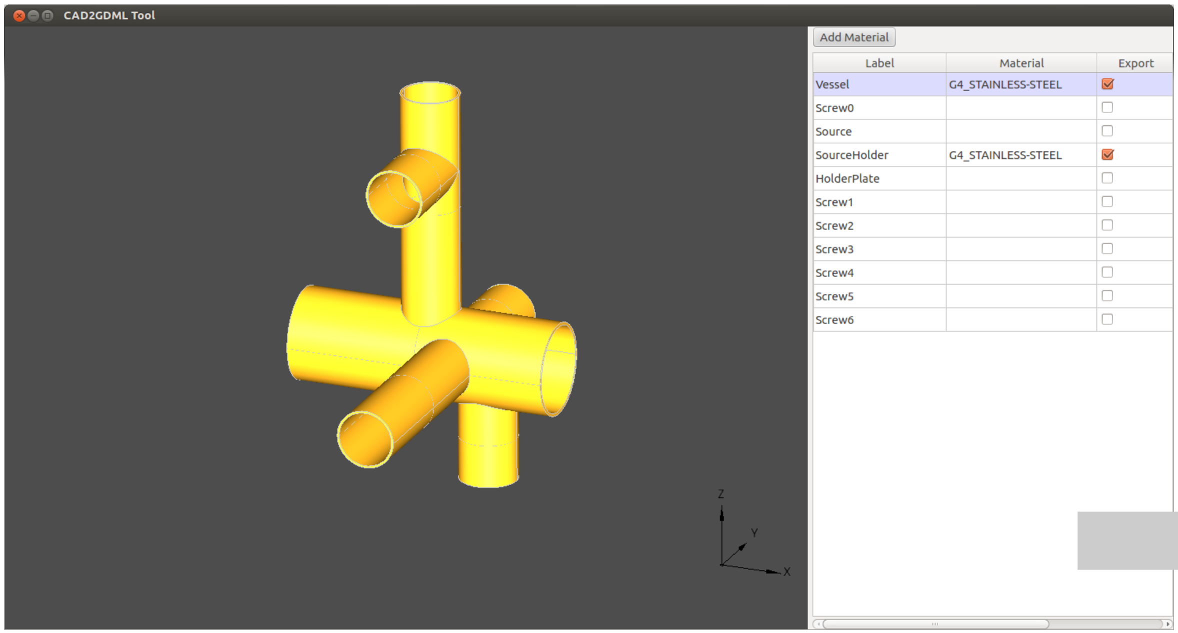
Detector electronics
- Amplify and shape the signal Electronics Simulation
- Phenomenological approach

Independent simulations run in so-called devices on the computing framework of EuXFEL. Together they form a **X-ray Detector Simulation Pipeline**.

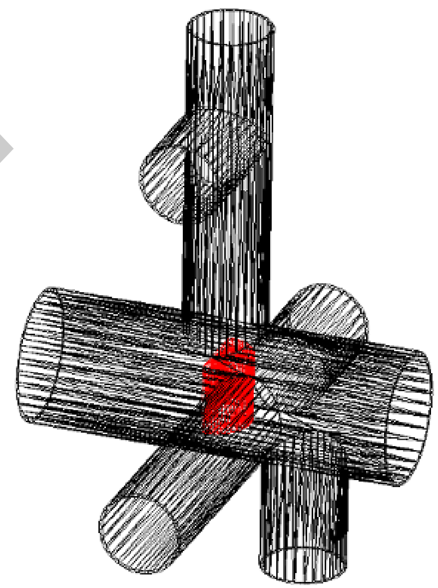


Geometry Modeling

A software tool to convert CAD drawings to Geant4 geometries has been devoped:



Geant4 wireframe rendering:



- Convert CAD step files to GDML (Geant4)
- Interface to specify materials
- Built with Qt4 and based on pythonOCC[1], a python wrapper of the openCascade[2] library

[1] http://www.pythonocc.org/
[2] http://www.opencascade.org/

Initial Validation: pnCCD Flat Field Measurements

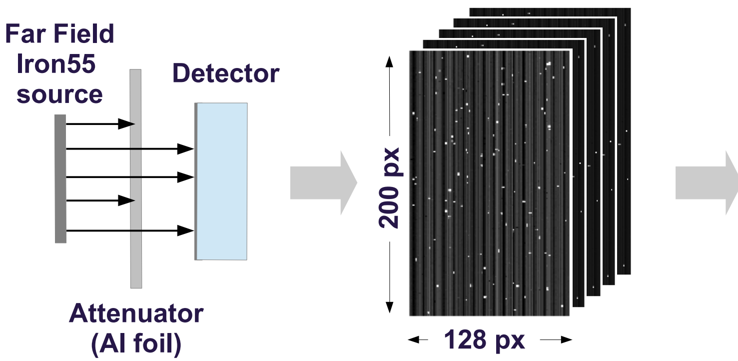
Particle Simulation
- Fe55 Source
- 4,800 Frames
- 2,300 Photons/Frame

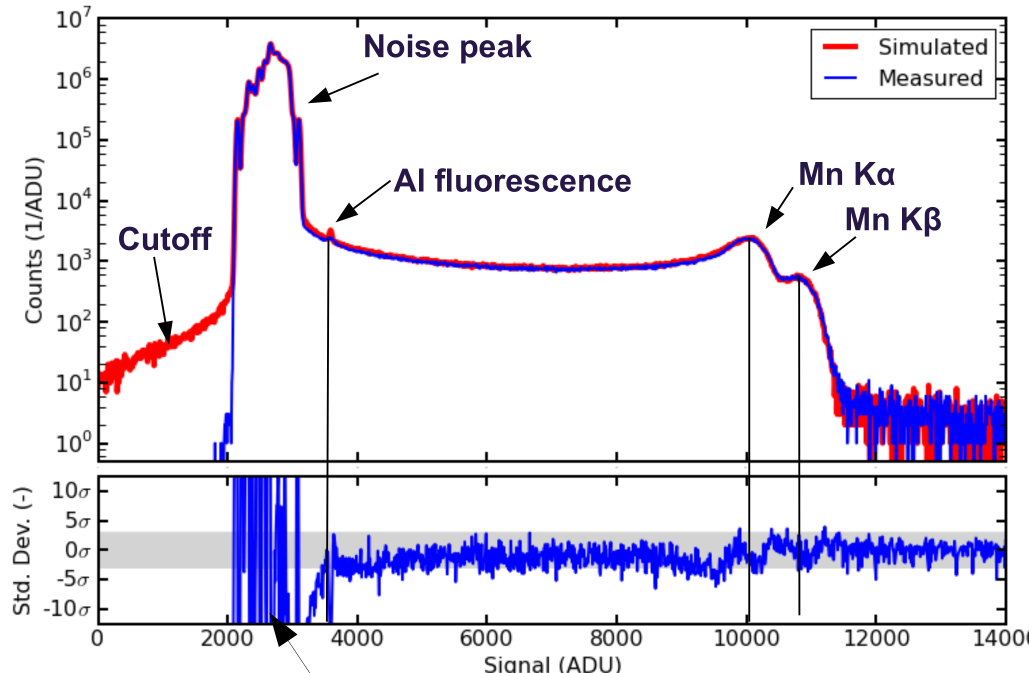
→ **Charge Simulation**
- 200x128 px (75 µm)^2
- 450 µm thickness
- T = 295 K, V_{bias} = 300 V

→ **Electronics Simulations**

CTI*→ ADC → Offset*→ Noise*

*Based on calibration data





$$\Delta y = \frac{y_m - y_s}{\sqrt{y_m}}$$

Simulation deviates strongly, minor shift on energy scale

- Source & attenuator yield **unique emission spectrum**, which is resolved by pnCCD
- In addition: **dark image datasets** show effects of the detector electronics & read-out
- Raw, uncorrected spectra, not normalized **3σ agreement simulation and measurement**
- Prominent spectral features coincide
- Deviations in the Noise peak

Data at courtesy of **pnSensor GmbH**

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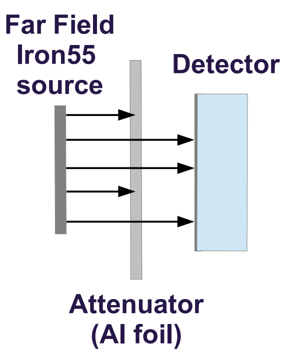
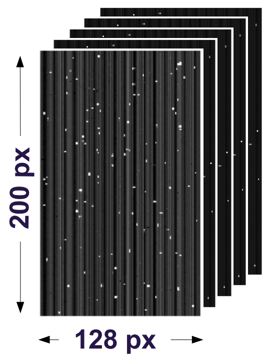
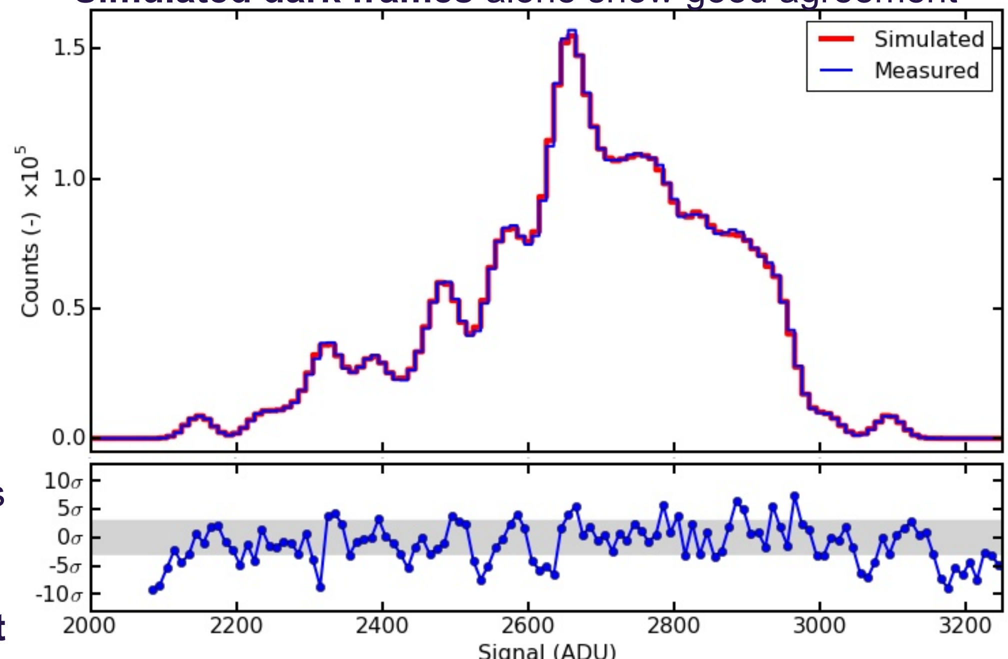




Simulated dark frames alone show good agreement



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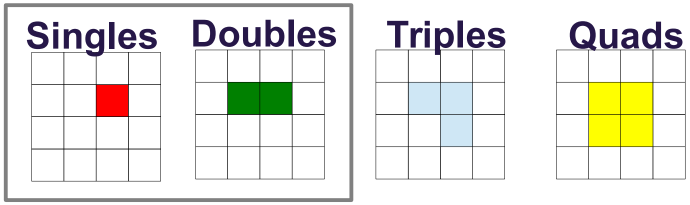
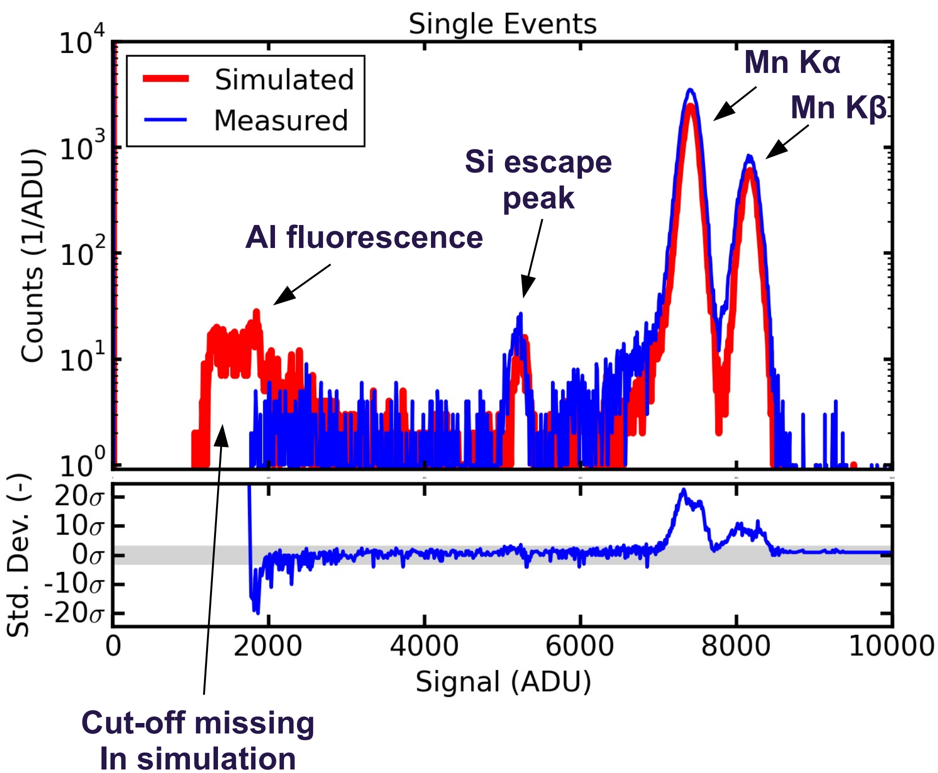
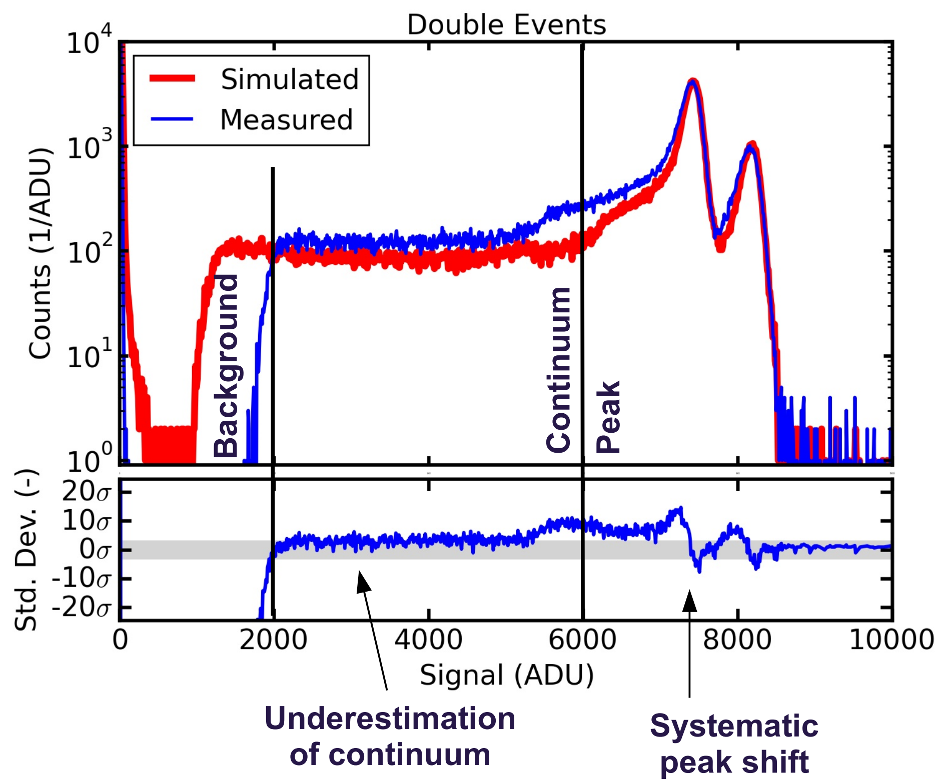
Data at courtesy of **pnSensor GmbH**

Charge Simulation Validation: Event Patterns

- Classification of **Events** by **Multiplicity** (Singles, Doubles, ..) considers **charge splitting effects**
- Data after offset & common mode correction
- Qualitative features match, quantitative disagreement in event numbers
- Current charge cloud model leads to underestimation → more validation measurements at APS beam time next week

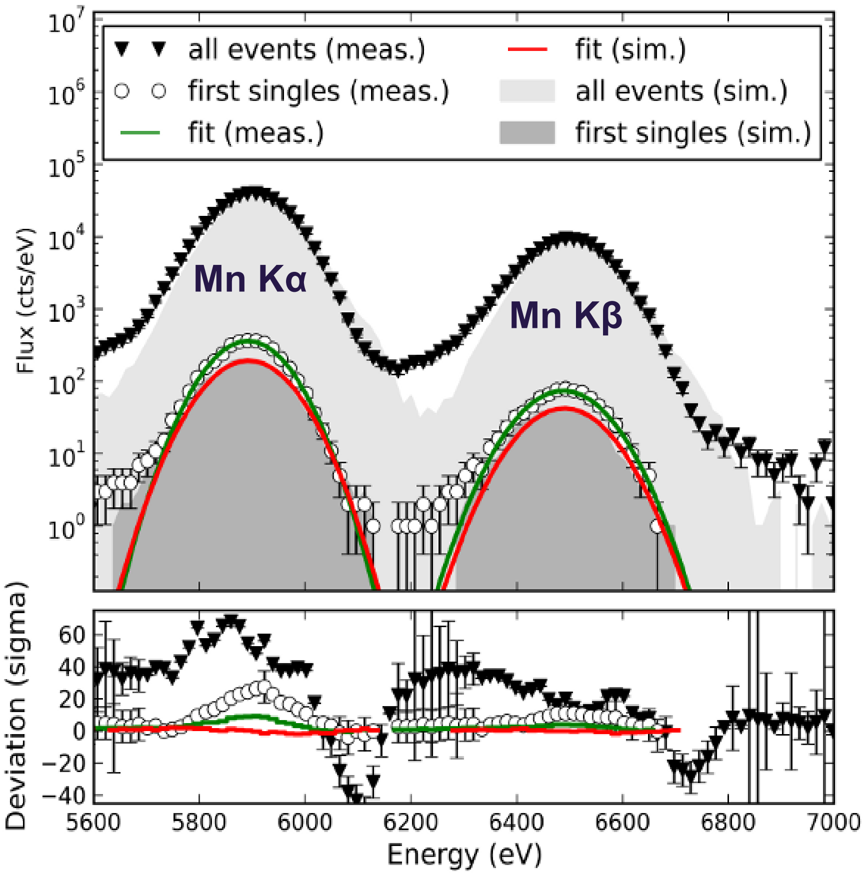






Fowler *et. al,* Nucl. Instr. Meth. Phys. Res. A 450 (2000) 75-87

Histograms of the Corrected Raw Data



Results published in [9]:
A. Joy, M. Wing, S. Hauf, M. Kuster, T. Rüter
X-CSIT: A Toolkit for Simulating 2D Pixel Detectors.
Journal of Instrumentation, 10(C04022), 2015

- Event pattern analysis: Charge simulation requires further investigation
  - Simulation has **fewer counts in continuum region**
  - Peaks **shift towards higher signal levels** in the simulation
  - Charge cloud shape/diameter underestimated
- Detector calibration
  - Emission spectrum and linear fit of corrected raw data yields **detector gain**
  - **Peak fits** give further indicators of simulation quality
- Correction and calibration allows **comparison with literature values**
  - Overall good agreement in peak energies
  - Mismatch in peak widths: related to **noise**
  - Mismatch in peak tails: related to **split events**

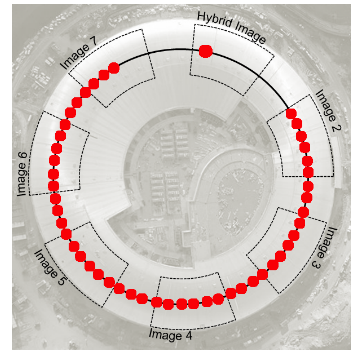
Peak		Simulated [eV]	Measured [eV]	rel. Dev.	XDB[7] [eV]
Mn Kα	Position	5893±3	5891±3	0.0002	5895.02
	FWHM	152±1	141±1	0.0688	
Mn Kβ	Position	6490±4	6488±3	0.0003	6490.45
	FWHM	159±2	158±2	0.0056	

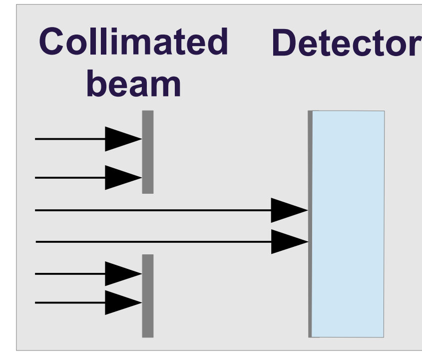
[7] **X-ray Data Booklet**: http://xdb.lbl.gov/

Simulating Megapixel Detectors for XFEL

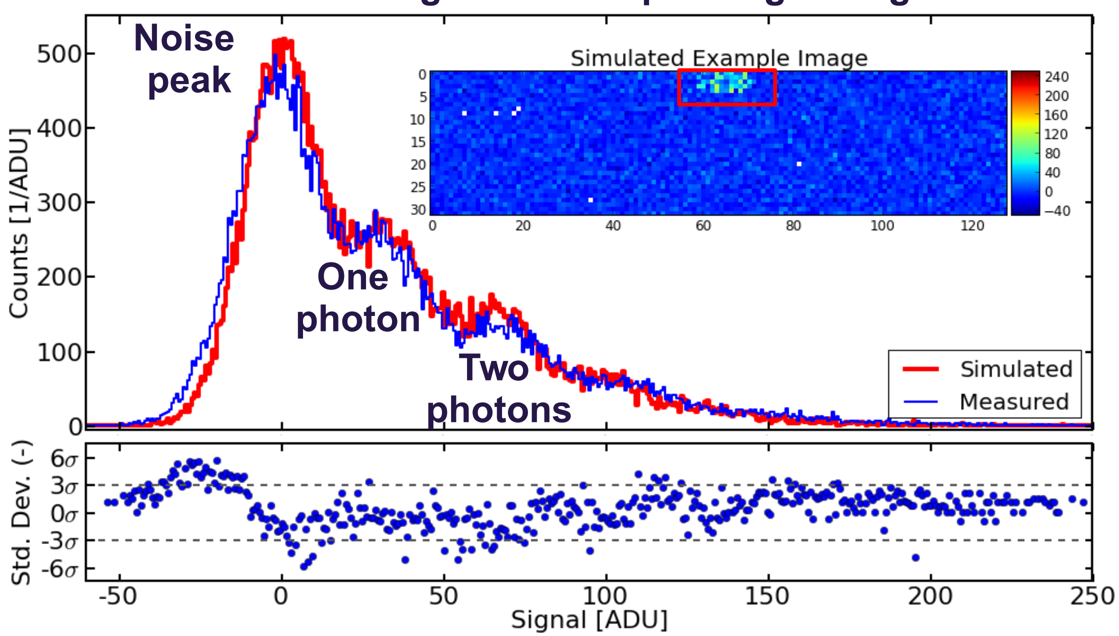
LPD Measurements at Diamond Synchrotron

- Monochromatic, attenuated & collimated **partial beam** (18keV in Hybrid Mode)
- Measured: 500 Frames (from single memory cell)
- Simulated: 500 Frames with 150 Photons each
- Electronics: ADC, Offset, Noise, Common Mode

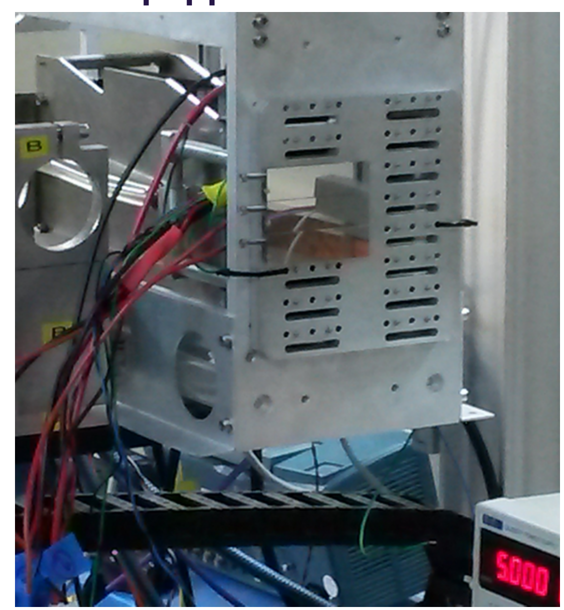




Comparison of measured and simulated data shows 3-6σ agreement depending on region:

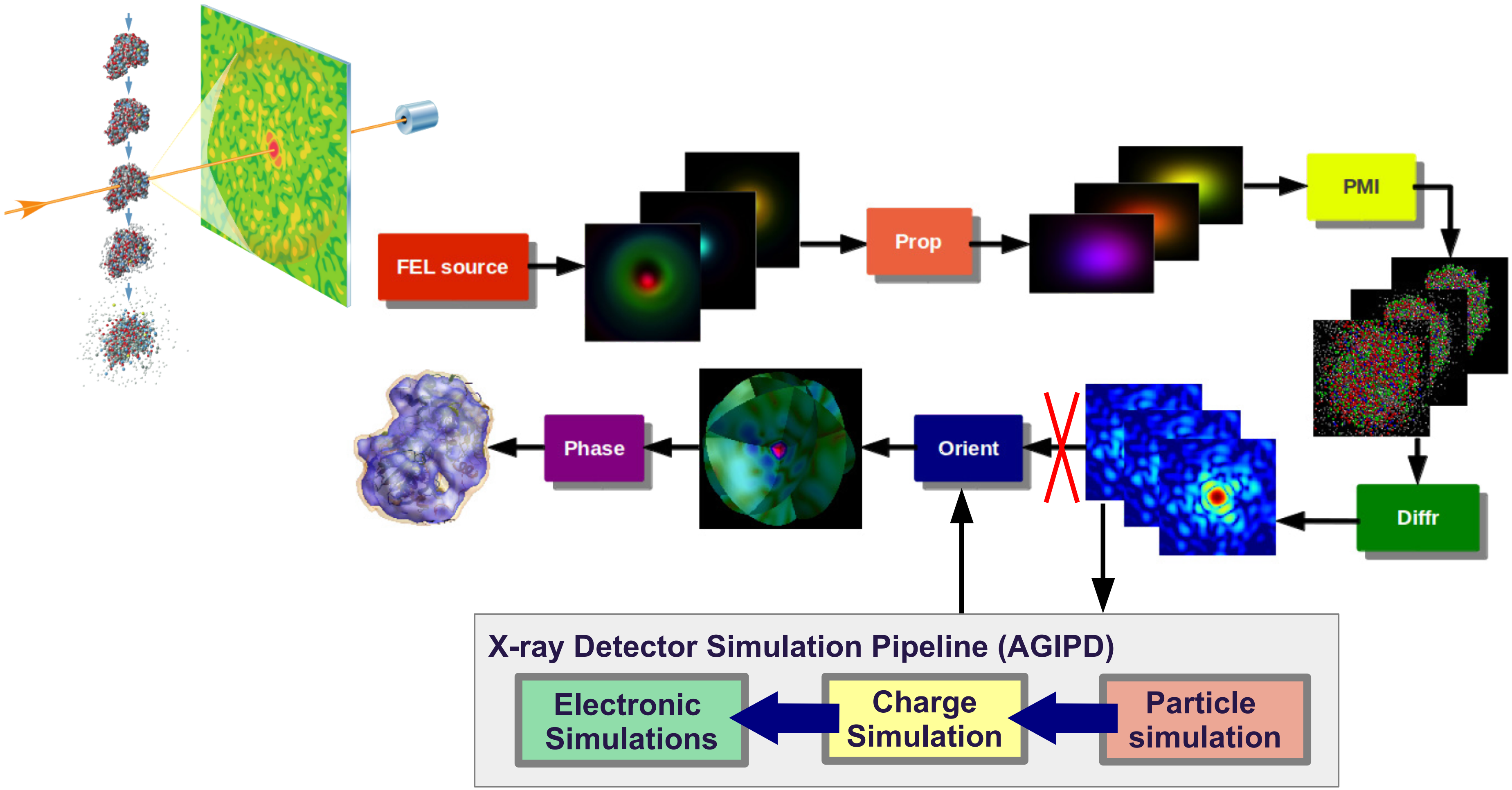


LPD supermodule equipped with 3 tiles



Special thanks to **P. Lang and the LPD Consortium** for providing the dataset

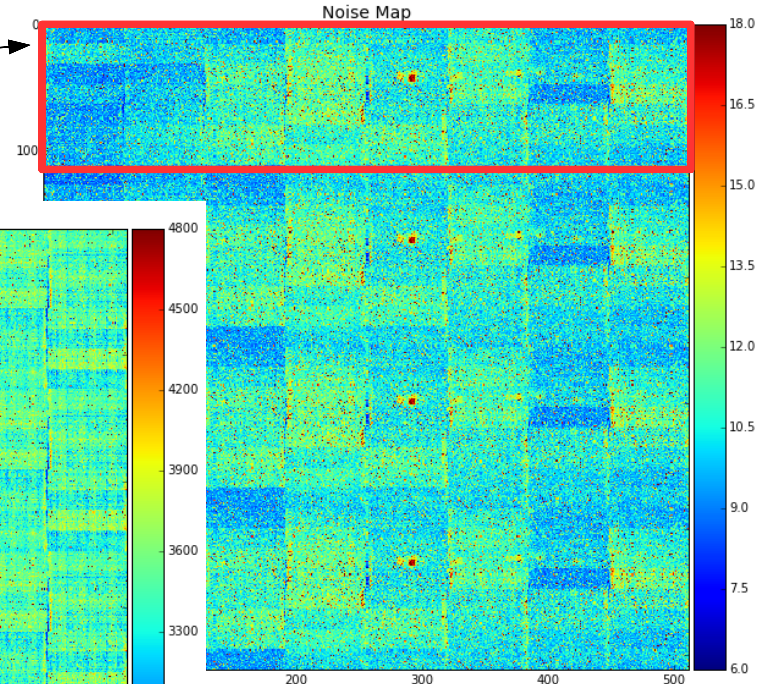
Integration into SPB Instrument Simulation

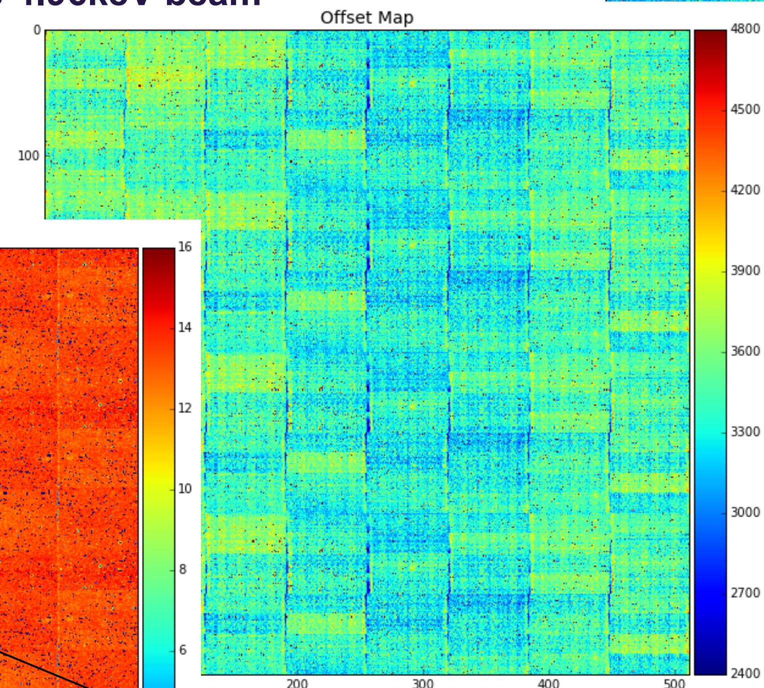


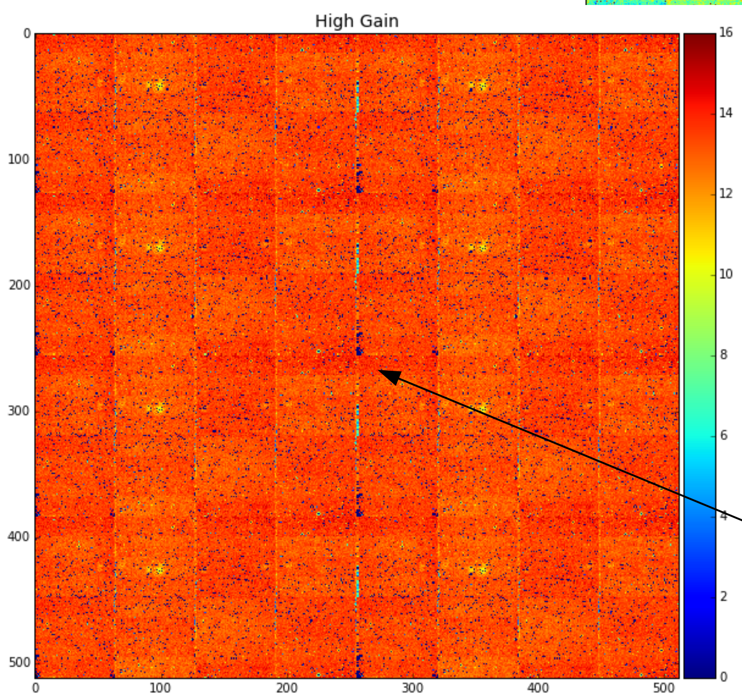
In preparation: C. H. Yoon et. al. *simS2E: A multi-physics framework for modelling a complete single particle imaging experiment at an X-ray Free Electron Laser*

AGIPD Calibration Data & Simulation Configuration

- Noise, offset and gain map, all values in ADU
- Calibration data from single module (512x128 px) and **repeated to match size**
- Module was operated at **4.5MHz** at **20˚C**
- Diffraction experiment uses **4.96keV beam**
- **Using calibration data measured by AGIPD consortium**







Zero gain corresponds to dead pixels

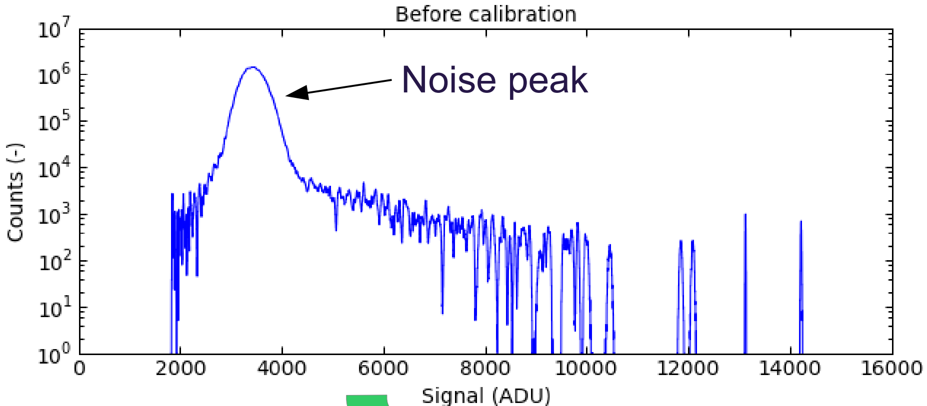
Gain interpolated for non-optimal operating conditions

Thanks to **J. Sztuk-Dambietz** and the AGIPD consortium for providing the data

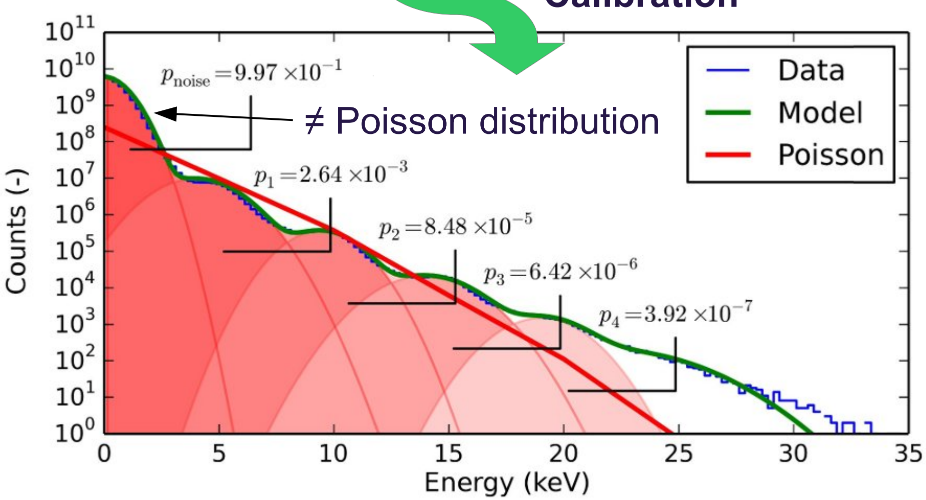
AGIPD Simulation of 2NIP: Initial Results

- 2NIP: Nitrogenase iron protein
- Computed for 200,000 frames using PyDetLib

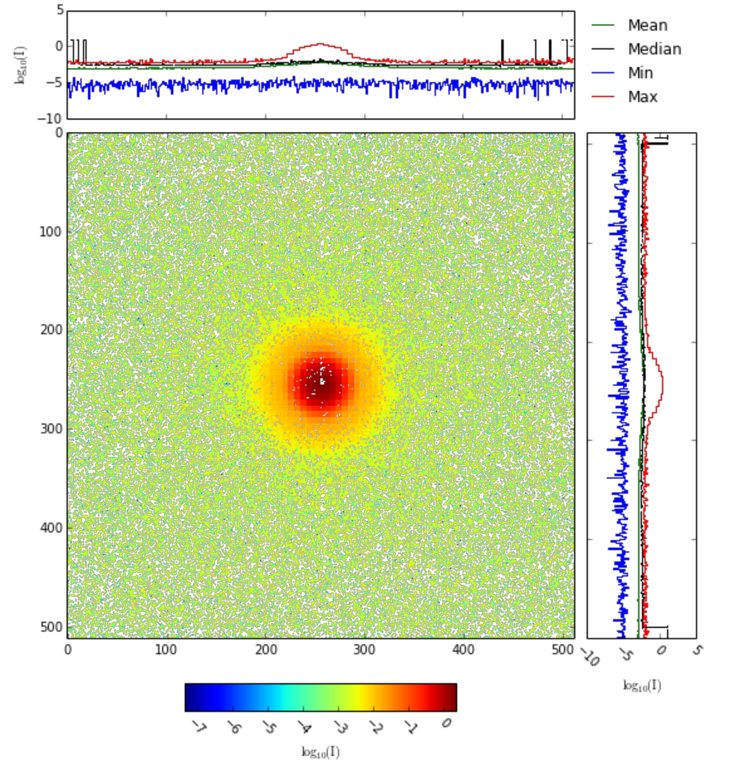
Spectra before and after calibration



Calibration



Mean image after calibration (dead pixels are masked, log scale)

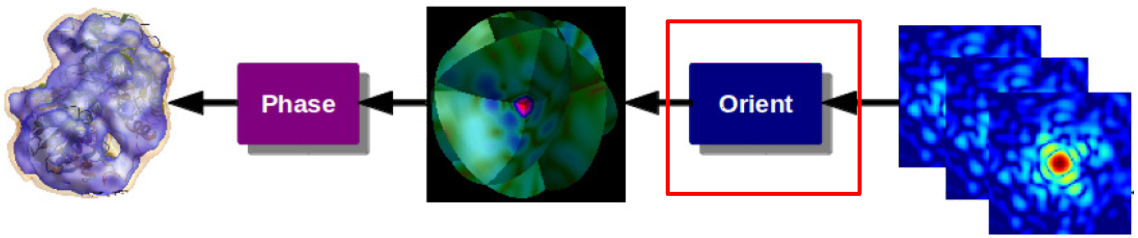


Problem: Peak separation 4δ but at 0.25 Mpixel still ~ 100 false positives if single photons to be included → Events best given as probabilities.

$$p'_k = kp_k \Big/ \sum_{i=0}^{N} p_i \qquad p_k(x) = A_k \exp\left(-\frac{(x-\mu_k)^2}{2\sigma_k^2}\right)$$

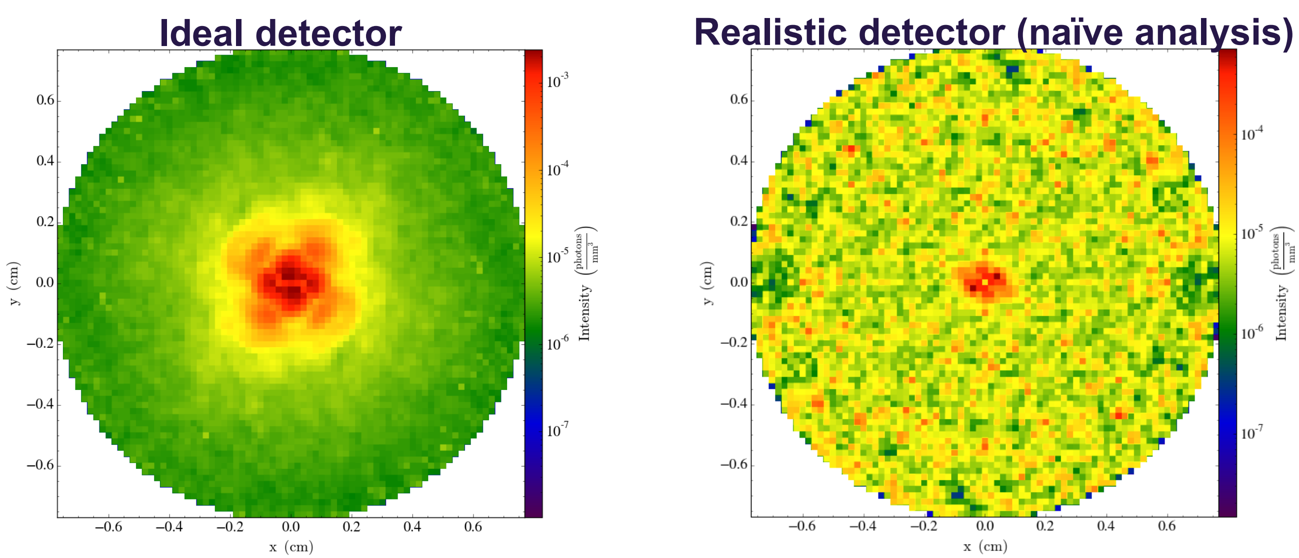
AGIPD Simulation of 2NIP: Initial Results

- Simulated images are **random orientations** of 2NIP particles → for **reconstruction need to be oriented** using EMC (Expand – Maximize – Compress) algorithm (Elser & Loh, 2009)



- EMC assumes photon intensity at each point of diffraction volume is Poisson-distributed → allows for shot noise, doesn't like false positives.

Maximum density slices through diffraction volume



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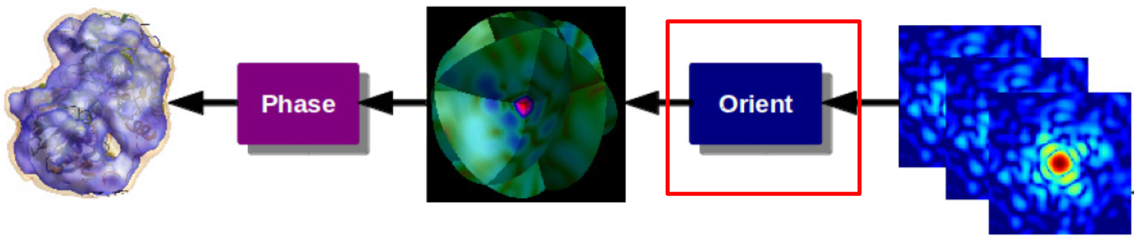

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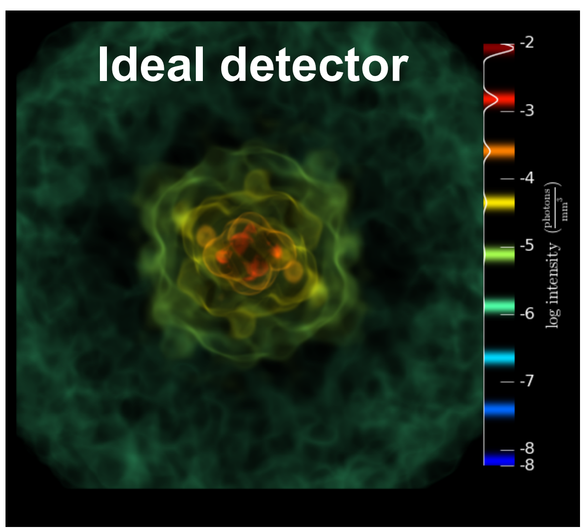
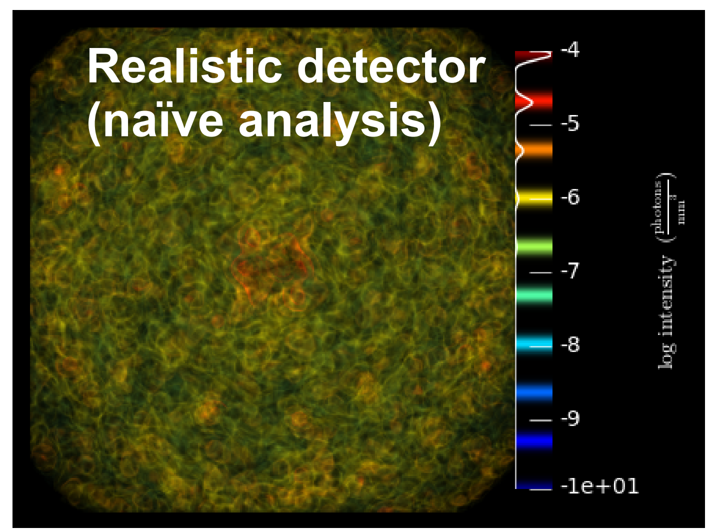
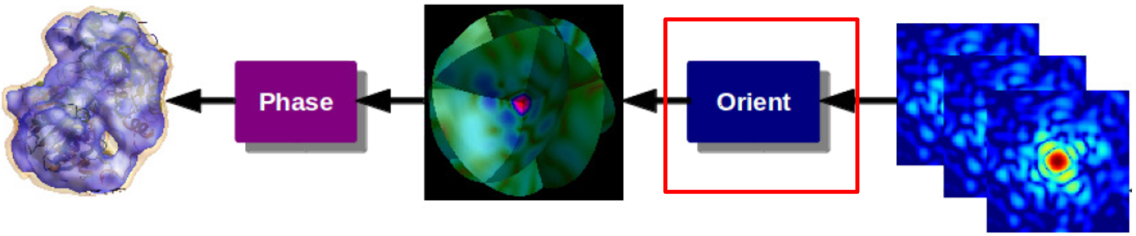
Diffraction volume (log. intensity)





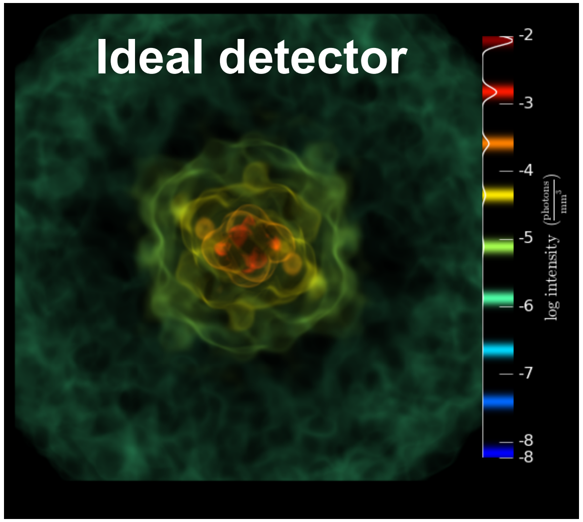
AGIPD Simulation of 2NIP: Initial Results

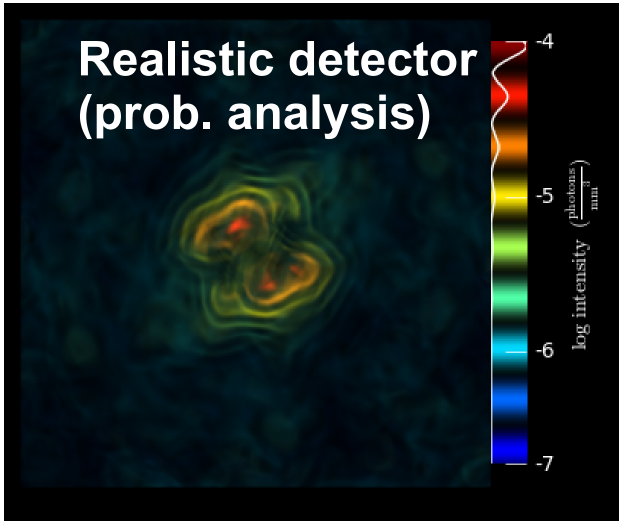
- Simulated images are **random orientations** of 2NIP particles → for **reconstruction need to be oriented** using EMC (Expand – Maximize – Compress) algorithm (Elser & Loh, 2009)



- EMC assumes photon intensity at each point of diffraction volume is Poisson-distributed → allows for shot noise, doesn't like false positives.

Diffraction volume (log. intensity)





Conclusion & Outlook

- **Drop-in detector simulation environment is available in EuXFEL's computing framework**
- **Conducted successful initial tests for two detector systems**
  - pnCCD: Simulation reproduces essential features of data from flat field measurement
    - 3σ agreement between measured and simulated attenuated Fe55 spectra
    - Shortcomings in split charge continuum
    - Testbed for further investigations: Small pixel size (75 µm) allows investigation of charge sharing effects
  - LPD: Low photon regime resolved with 3-6σ agreement
- **X-ray Detector Simulation Pipeline employed in start-to-end simulation of experiment end station**
  - Noticeable divergence from ideal detector → **exploring experimental limits requires realistic detector model**
  - Simulated scenario at low end of AGIPD specification (high T, low Eph)
  - Does advanced data preprocessing before EMC help?
- **Outlook**
  - Develop towards user-accessible tool
  - Further study detector effects (roll, tilt, electronic settings)