X-CSIT: a toolkit for simulating 2D pixel detectors

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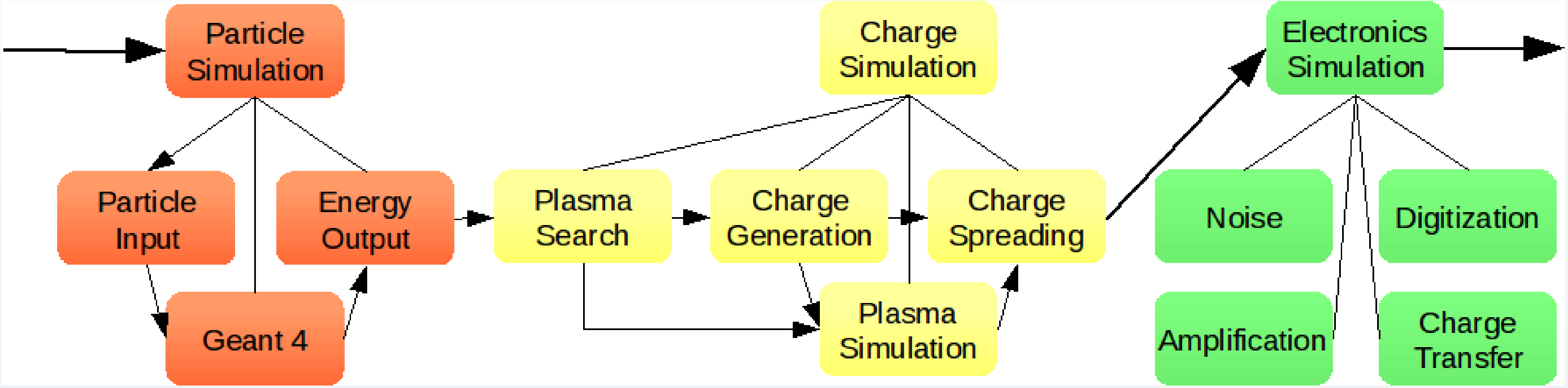
European XFEL

- X-ray Free Electron Laser starting in Hamburg, principally 3-24keV
- XFEL will use a range of 2D pixel detectors for imaging with various sizes and specifications
- A common simulation of these detectors was desired to
  - Predict detector performance and the effect of radiation damage
  - Aid planning experiments and analysing results

	LPD	AGIPD	DSSC	**pnCCD**
Pixels	500µm square	200µm square	204µm hexagonal	**75µm square**
Depth	500µm	500µm	500µm	**300µm**
Dynamic range	1×10^5 at 12 keV	1×10^4 at 12 keV	6000 at 1 keV	**Spectroscopic mode**
Dynamic range profile	Triple gain profile	Pre-amplifier chosen gain	DEPFET non-linear gain	**Linear**
Sensor size	32x128 pixels	512x128 pixels	256x128 pixels	**200x128 pixels**
Energy range	12 keV optimal, 1-24 keV	3-13 keV	0.5-6 keV optimal, 0.5-24 keV	**0.1-15 keV**

Objectives of X-CSIT

- X-CSIT (X-ray Camera Simulation Toolkit) is designed to provide a single common simulation framework for the detectors at XFEL
  - At XFEL, X-CSIT will be integrated into Karabo, which will provide simulations to users as well as handling concurrent processing
- To provide a common simulation while accounting for the variety of detectors, X-CSIT needs to be highly adaptable
  - This adaptability also lends itself to use with other groups and detectors
- The toolkit provides highly modular physics simulations dependent on user provided detector definitions, separated into three sub-simulations



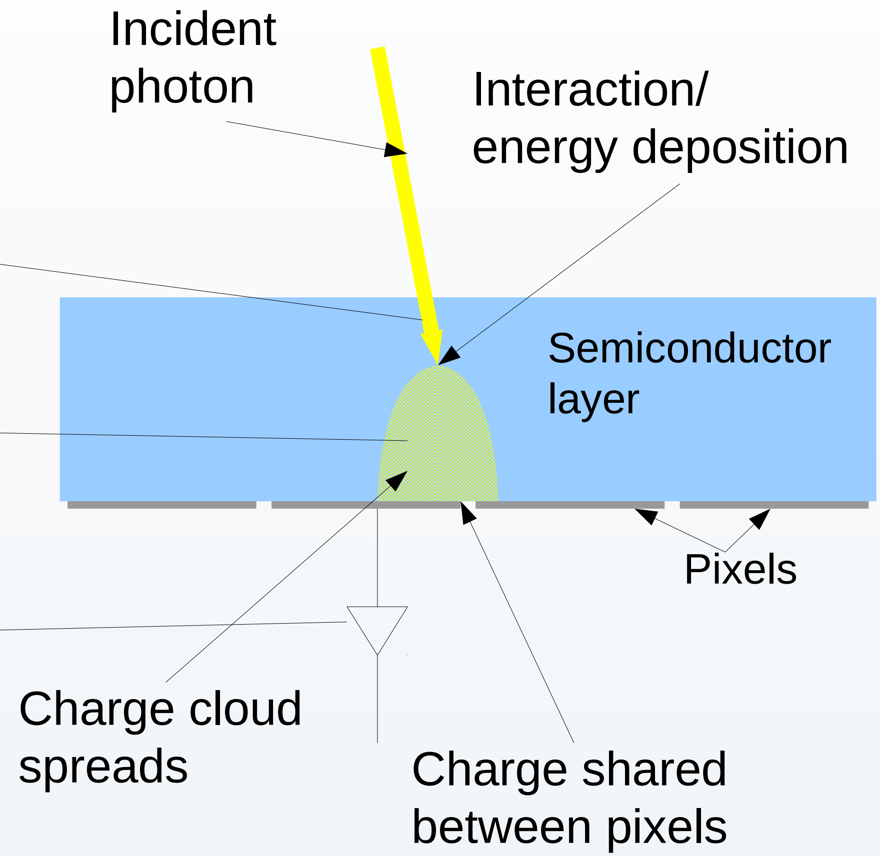
Toolkit Details - Physics

- X-CSIT uses three sub-simulations to cover three different physical regions

Particle Simulation
Photon interaction in semiconductor later and energy deposition

Charge Simulation
Spread of electron cloud in electric field as it travels to pixels

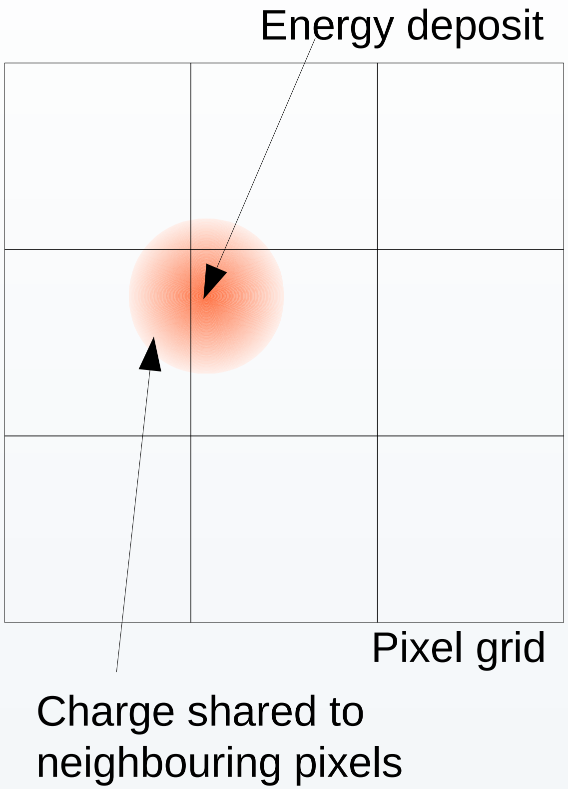
Electronics Simulation
Response of detector electronics to collected signal, including ASIC and Front End Modules

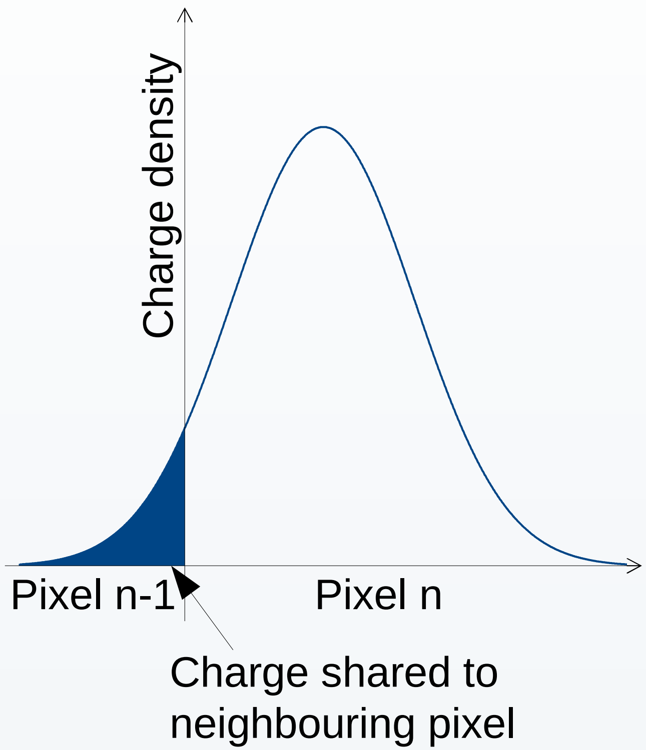


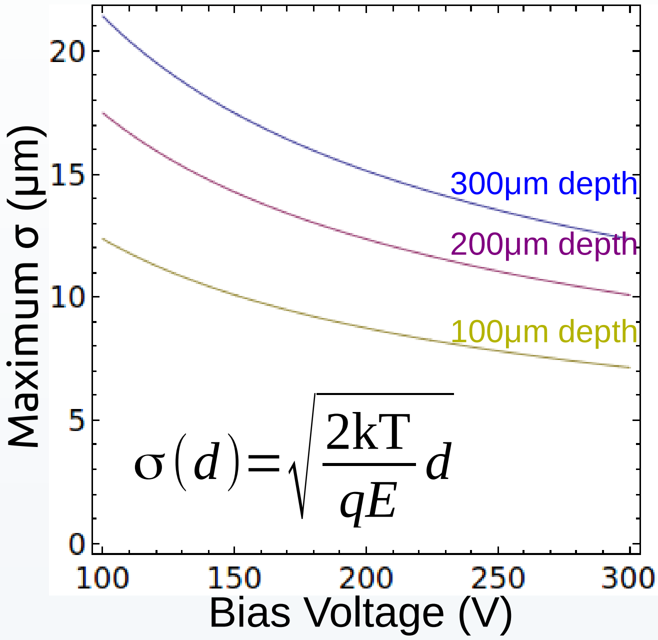
Toolkit Details – Sub-simulations

Particle Simulation	Charge Simulation	Electronics Simulation
Geant4 version 10.0, fully packaged within the particle simulation	Statistical model	Set of modular devices simulating an electronic component, e.g. amplification, digitization
	Drift+diffusion Simulation:	
	For most events, only drift+diffusion is simulated, charge clouds act independent of each other	
Simulates photo electric effects, Compton and Rayleigh scattering, Fluorescence and Auger emissions	Gaussian spread with a width going as the root of the depth	These devices are chained together to form a functional representation of a circuit
	Plasma Simulation:	
	At high electron-hole densities plasma effects can occur, increasing spread and collection time	Empirically driven based on expected performance or calibration data
Livermore physics list validated down to 250eV	Well studied in heavy-ion detectors, less so in X-rays	Karabo integration will add GUI tools to layout the modules
	Simulation will be written based on investigation done at XFEL next year	

Toolkit Details – Charge Simulation







$$\sigma(d) = \sqrt{\frac{2kT}{qE}d}$$

Charge diffusion produces a 2D Gaussian spread over distance, when this crosses a pixel boundary charge sharing occurs

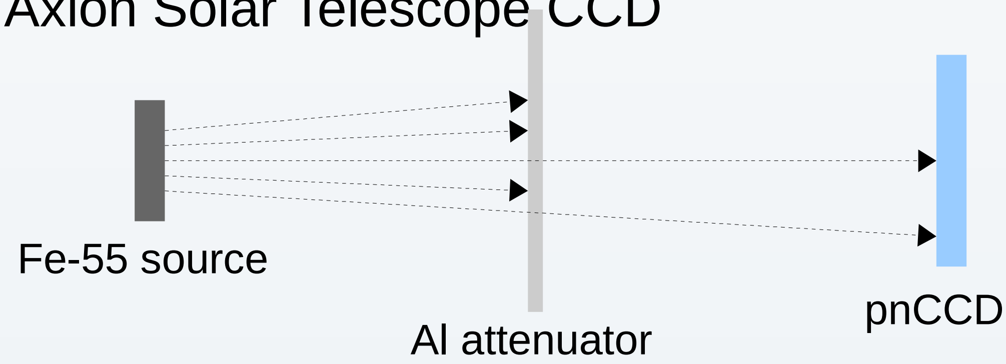
This is approximated with two orthogonal 1D Gaussians, which then use the cumulative distribution function to find the charge crossing a boundary

The width of this spread depends on interaction depth and the electric field due to the bias voltage

R.F. Fowler et al. Nucl. Instr. And meth. A 477 (2002) 226

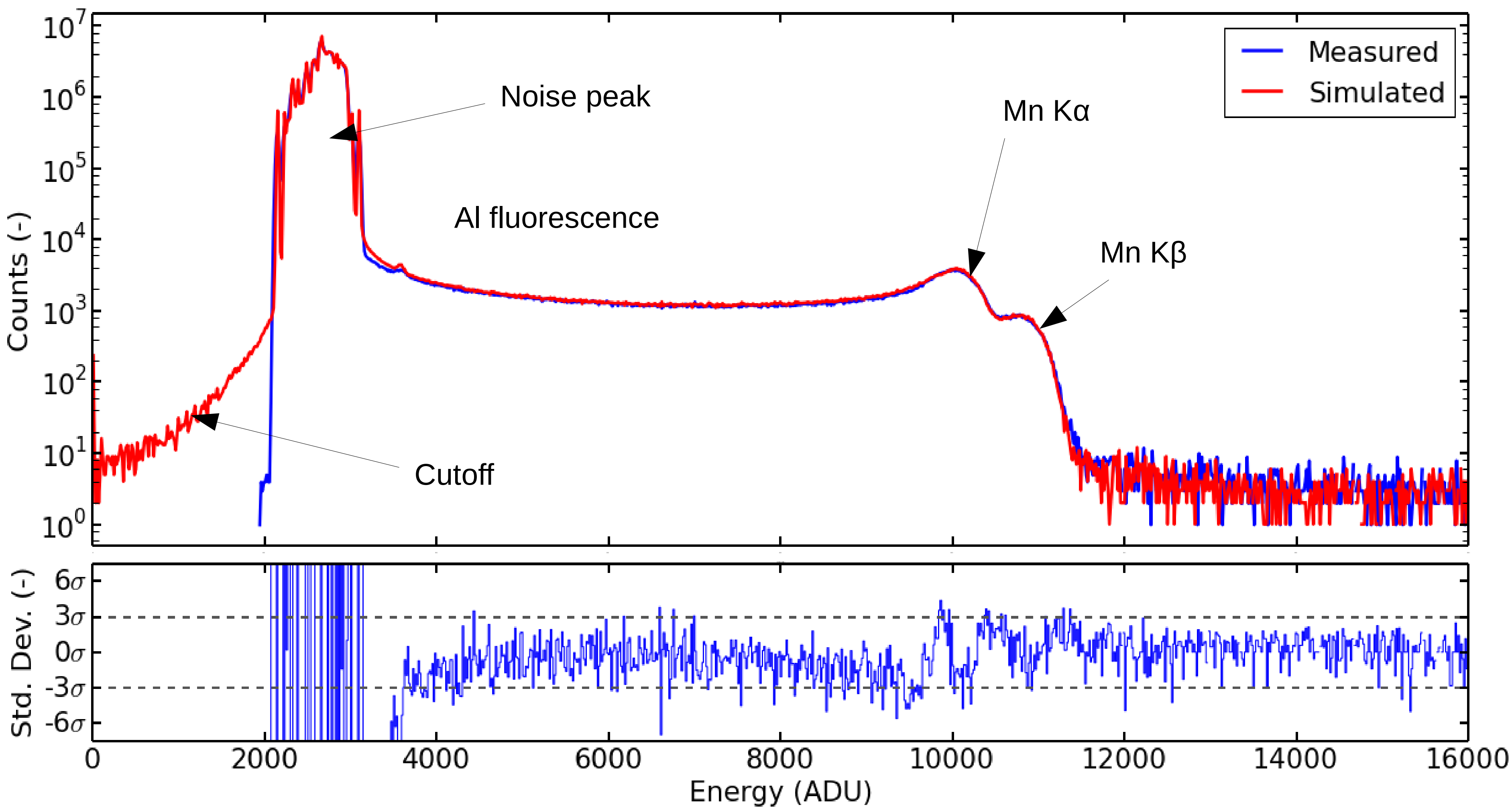
Initial Testing

- X-CSIT will require testing and validation before it can be released or made available to users at European XFEL
- A simulation of a pnCCD has been created using X-CSIT so that data taken with a Fe-55 source by a pnSensor GmbH can be used for initial testing
  - This has 200x128 pixels, a 75 micrometer pitch, 300 micrometer depth and an entrance window
- The data sets from the pnCCD and from the simulation were then run through the same analysis pipeline which has been validated for the CERN Axion Solar Telescope CCD

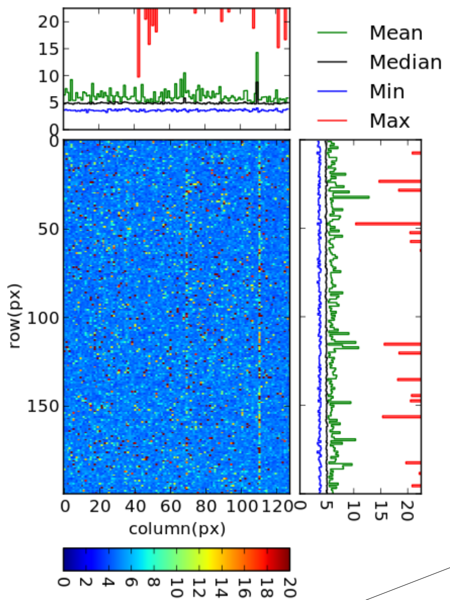


Testing - pnCCD

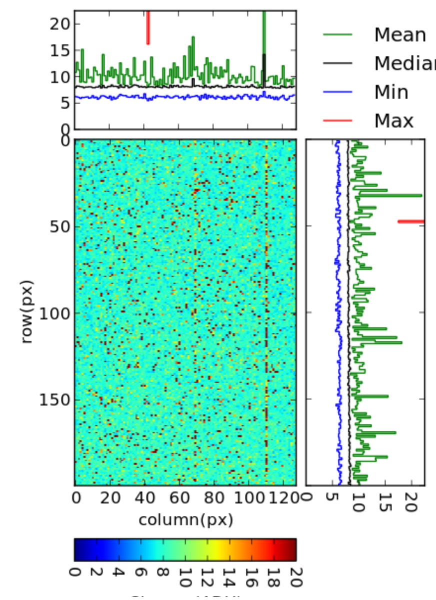
- Raw, uncorrected histogram
- Good, 3σ agreement between data and measurement



Testing - pnCCD

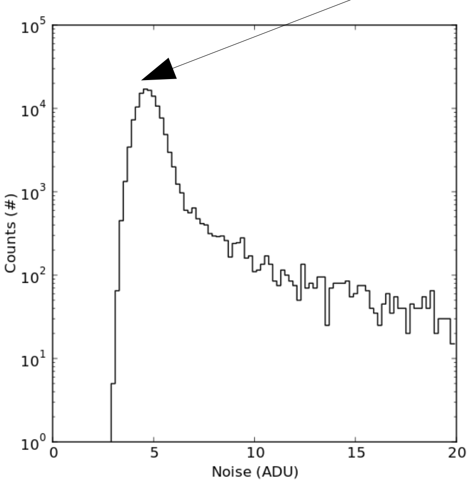


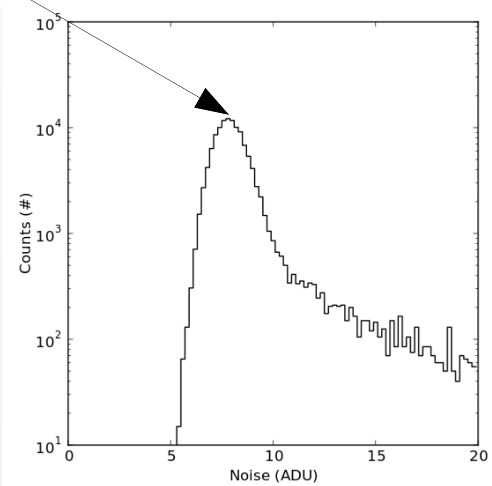
Noise map and histograms from simulated (Left) and measured (Right) dark frames



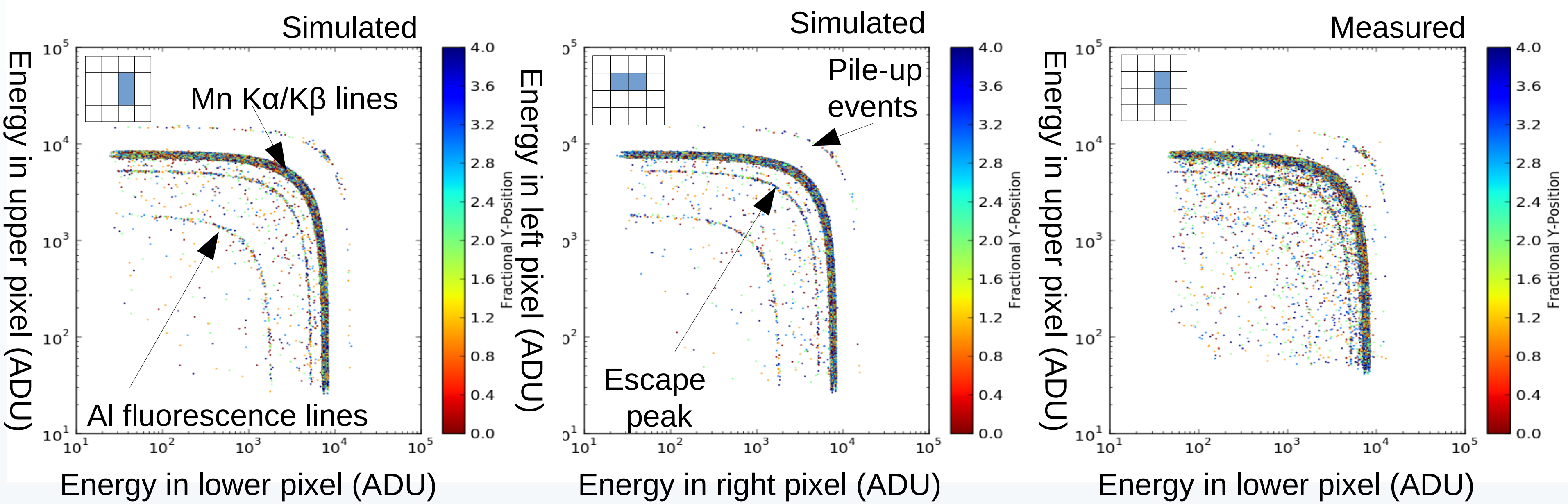
This discrepancy is responsible for the bad matching of the noise peak in the previous histogram

The measured dark frames were not perfectly shielded



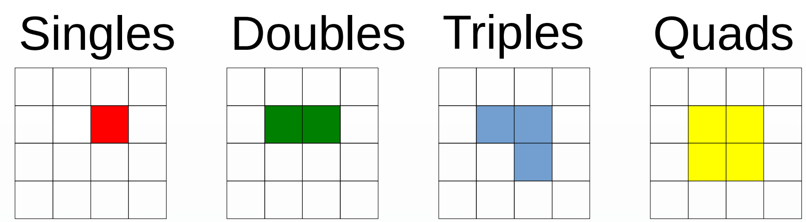


Testing - pnCCD

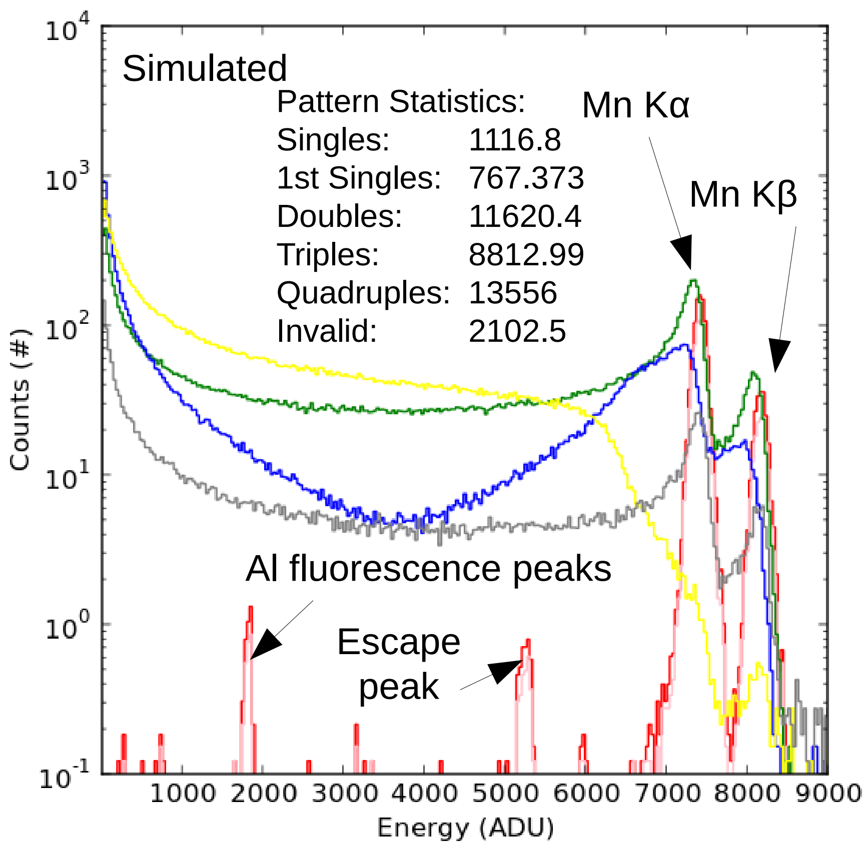


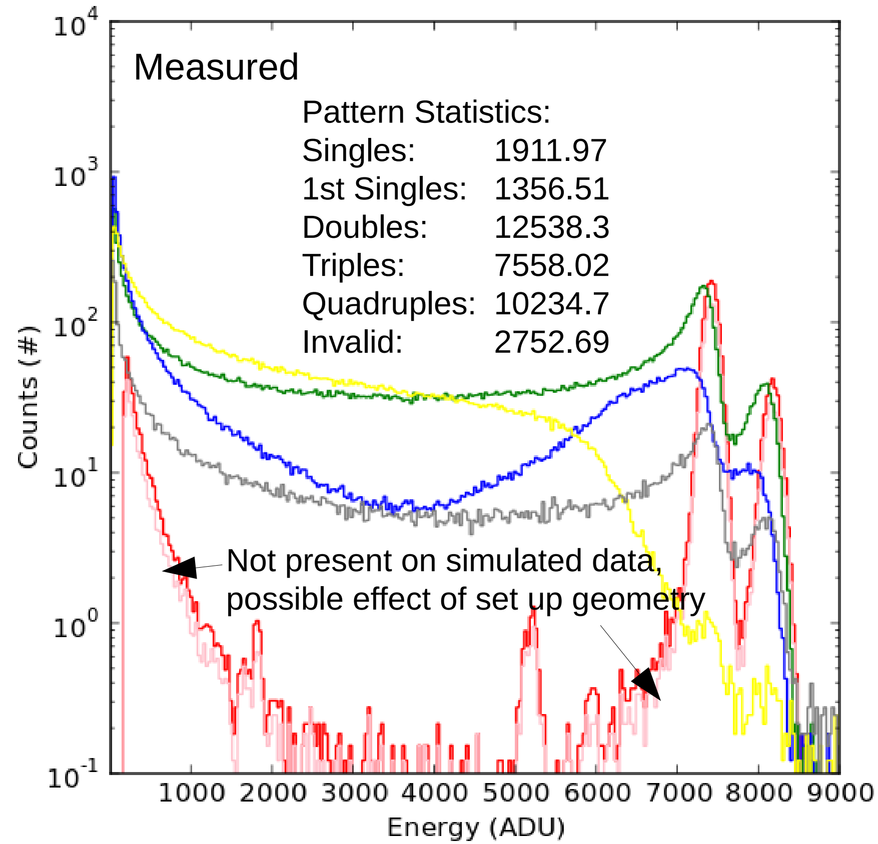
- Scatter plots of energy in adjacent pixels that were analysed to be from a single event
  - Offset and common mode corrected
- Simulated plots are symmetrical and show similar features to each other
- Isotropy between partners and in space
- Simulation plots also show similar features to the measured plot, although the simulation lacks background

Testing - pnCCD

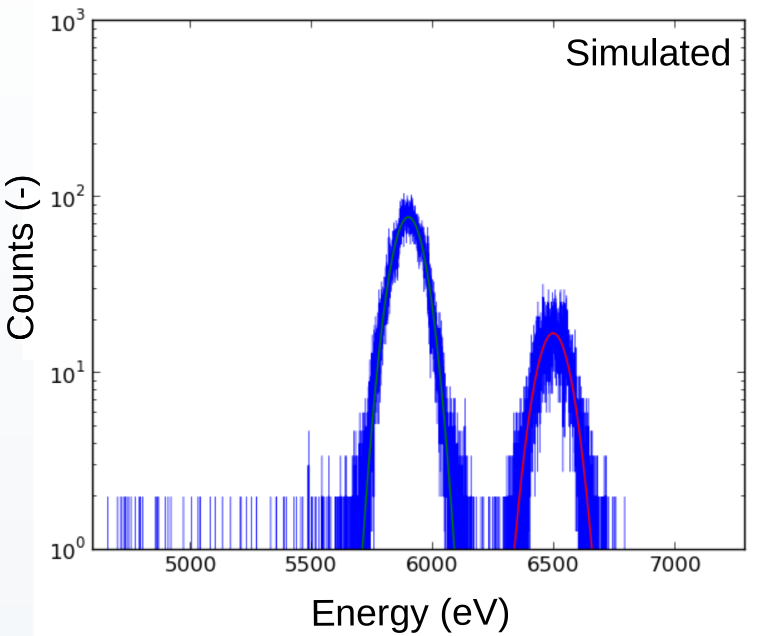


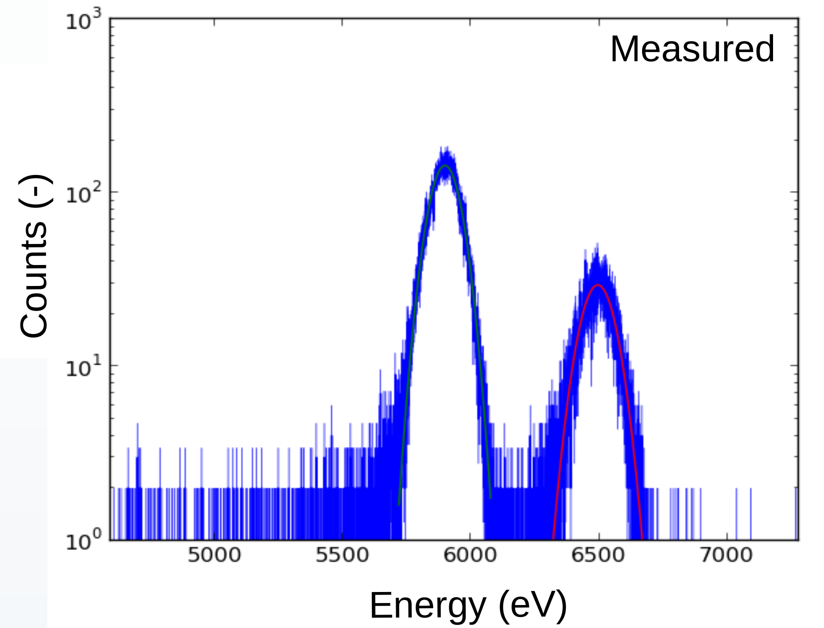
- Absorption spectra by event pattern, offset and common mode corrected
- Simulated and measured data show similar features, although ratios of events patterns differ





Testing - pnCCD





- Charge transfer inefficiency, gain, offset and common mode corrected histograms using only first singles (the first event in a charge transfer column)
- The fit shapes, positions and ratios match closely between simulated and measured data

	Simulated	Measured	Real
Mn Kα	5892.78 (+-2.61) eV	5891.41 (+-2.46) eV	5895.02 eV
FWHM Mn Kα	151.63 (+-0.58) eV	141.20 (+-0.35) eV	
Mn Kβ	6490.19 (+-3.37) eV	6488.13 (+-3.05) eV	6490.45 eV
FWHM Mn Kβ	158.50 (+-1.81) eV	157.67 (+-1.17) eV	

Conclusion and Outlook

- X-CSIT is a toolkit for creating simulations of 2D semiconductor pixel detectors
  - This includes photon interaction, charge sharing between pixels and electronic readout
- An early version of X-CSIT has been used to simulate a prototype of pnCCD
  - Early comparisons indicate good agreement between measurements and simulation, within 3σ on the raw spectrum
- X-CSIT will be used to simulate the pixel detectors at European XFEL and be made available for users through integration into Karabo
- All of the simulations and components of X-CSIT will be validated using detectors and sources available at XFEL
- After work on X-CSIT has been finished and the software has been validated, X-CSIT will be made available as open source for other users or groups

CAD to Geant4 Tool

- To aid with creating set up geometries for X-CSIT, a tool was written to convert CAD step files to GDML for Geant4
- Was built with Qt4 and based on pythonOCC[1], a python wrapper of the openCascade[2]

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

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