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

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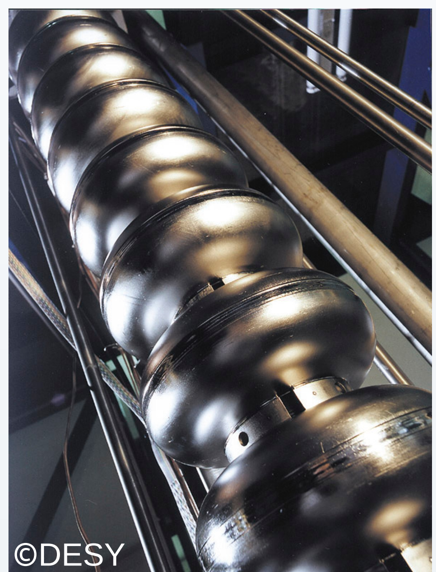
European XFEL

- X-ray Free Electron Laser starting at DESY in Hamburg, ending 3.4 km later, just over the state border in Schleswig-Holstein
- Electrons are accelerated over 1.7 km up to 17.5 GeV by superconducting linear accelerator
- Electrons then pass through a set of undulators, undergoing Self Amplified Stimulated Emission (SASE)

European XFEL [Aerial views: FHH, Landesbetrieb Geoinf. Und Vermessung]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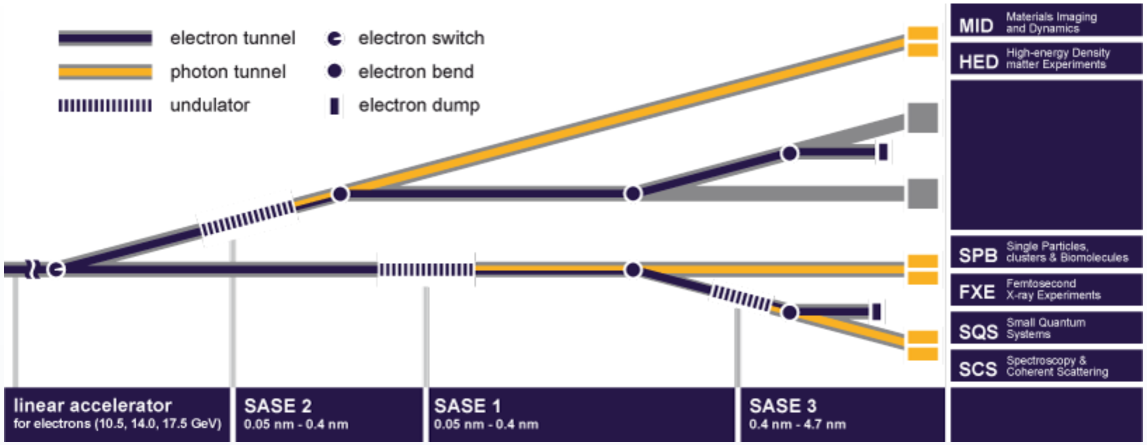
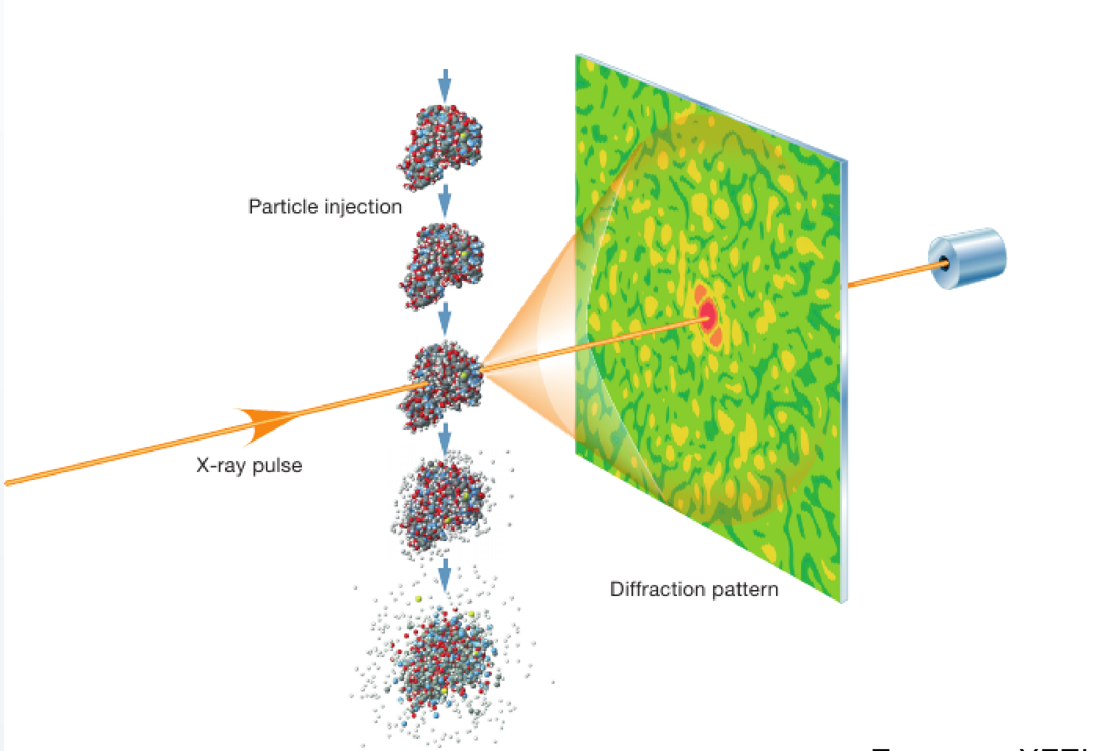
European XFEL

European XFEL

- The facility can provide up to 27 000 flashes of light per second, to three beamlines and seven instruments
- SASE 1 & 2 will provide hard X-rays in the 3-24 keV range with SASE 3 providing softer X-rays down to 250 eV
- This light is then used for experiments, including creating diffraction images of targets seen by a pixel detector

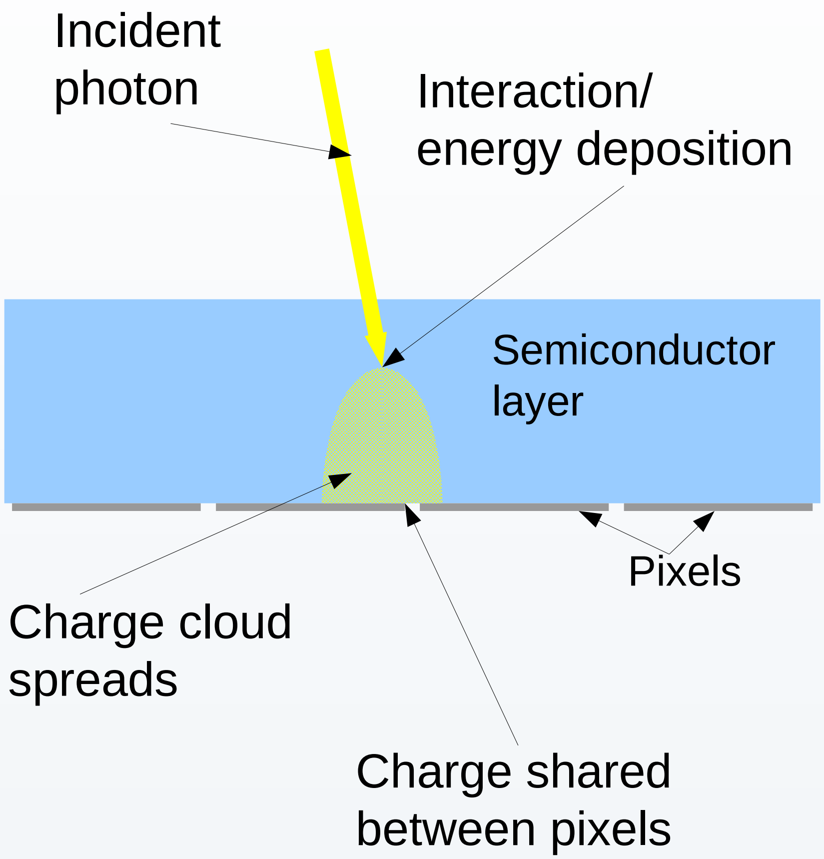




European XFEL

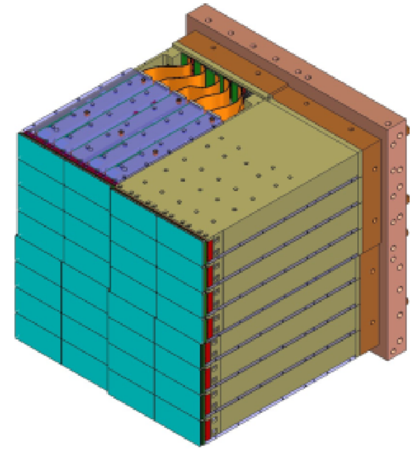
2D Pixel Detectors

- Semiconductor X-ray pixel detectors consist of a sensitive semiconductor sensor layer that absorbs scattered X-ray light
- Photon energy frees electron-hole pairs which, in the potential created by the reverse bias voltage, move towards the pixels, which in the case of active pixel sensors are collection bump bonds
- The electrons are collected and moved as charge to an electronic circuit where they are stored, amplified and digitized



Detectors at XFEL

- XFEL will use a range of 2D pixel detectors for imaging, including three built specially for the project: DSSC, LPD and AGIPD
- These three detectors will all feature
  - 1024x1024 pixels (1 MPixel)
  - 4.5 MHz capture for XFEL repetition rate
  - Dynamic energy range and single photon sensitivity
- Sensitive area on DSSC and AGIPD is approximately 20cmx20cm, 50cmx50cm for LPD

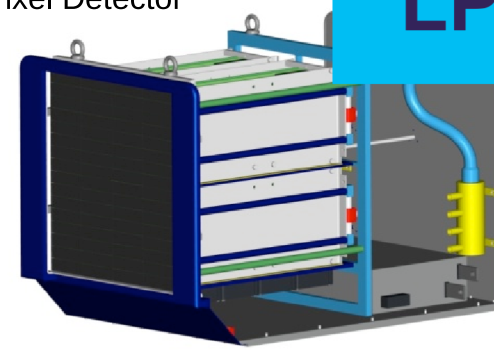


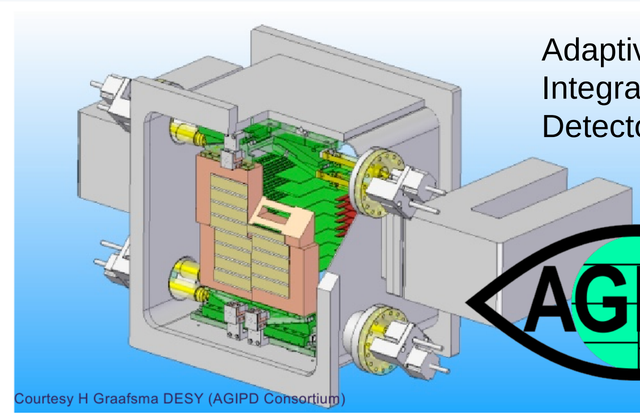
DSSC

DEPFET Sensor with Signal Compression

Large Pixel Detector

LPD





Adaptive Gain Integrating Pixel Detector

AGIPD

Detectors at XFEL

- Despite their similar design goals, the three bespoke XFEL detectors still differ from each other

	LPD	AGIPD	DSSC
Pixels	1Mpixel	1Mpixel	1Mpixel
Pixel size	500µm square	200µm square	204µm hexagonal
Dynamic range	1×10^5 at 12 keV	1×10^4 at 12 keV	6000 at 1 keV
Dynamic range profile	Triple gain profile, most accurate chosen in readout	3 gain profiles, chosen by pre-amplifier	DEPFET non-linear gain
ASIC size	32x16 pixels	64x64 pixels	256x128
Sensor size	32x128 pixels	512x128 pixels	256x128 pixels
Energy range	1-24 keV, 12 keV optimal	3-13 keV	0.5-24 keV, 0.5-6 keV optimal

Objectives of X-CSIT

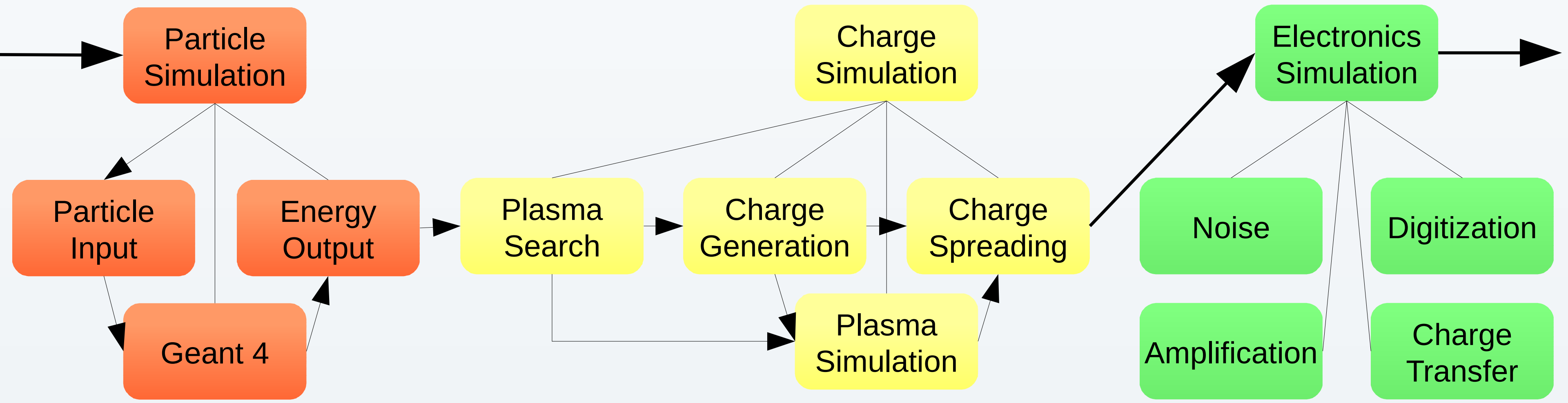
- X-CSIT (X-ray Camera Simulation Toolkit) is designed to provide a single common simulation framework for the pixel detectors to be used at XFEL, including LPD, AGIPD, DSSC and pnCCDs
- These simulations will be important for understanding detector characteristics and helping XFEL users plan and analyse experiments
- Several detector aspects require simulation
  - Photon interaction in the semiconductor layer
  - Charge spreading between pixels
  - Electronic noise and gain profile
- To provide a common simulation while accounting for the differences in the initial three detectors, as well as future detectors, X-CSIT needs to be very adaptable
- To provide an estimate of the simulation accuracy, X-CSIT also requires validation of all components of its simulations

Objectives of X-CSIT

- X-CSIT must reconcile a desire for a common simulation with detectors that can differ substantially
- Attempting to characterise all possible ways detectors vary will result in failure
  - The code will become bloated, tangled and difficult to test
  - Any characteristic not considered in the design of X-CSIT will be very difficult to add later on
- The solution is to create a modular tool kit for creating simulations
  - This tool kit will provide validated physics simulations dependent on user provided detector definitions
  - If X-CSIT does not simulate a predetermined detector configuration or layout, it is modular enough for code to be added or replaced

Design - Physics

- X-CSIT splits the simulation of semiconductor detectors into three stages
  - A particle simulation of incoming photons and any scattered particles
  - A charge simulation of the electron-hole clouds in the semiconductor
  - An electronics simulation of the ASIC circuit and front end electronics

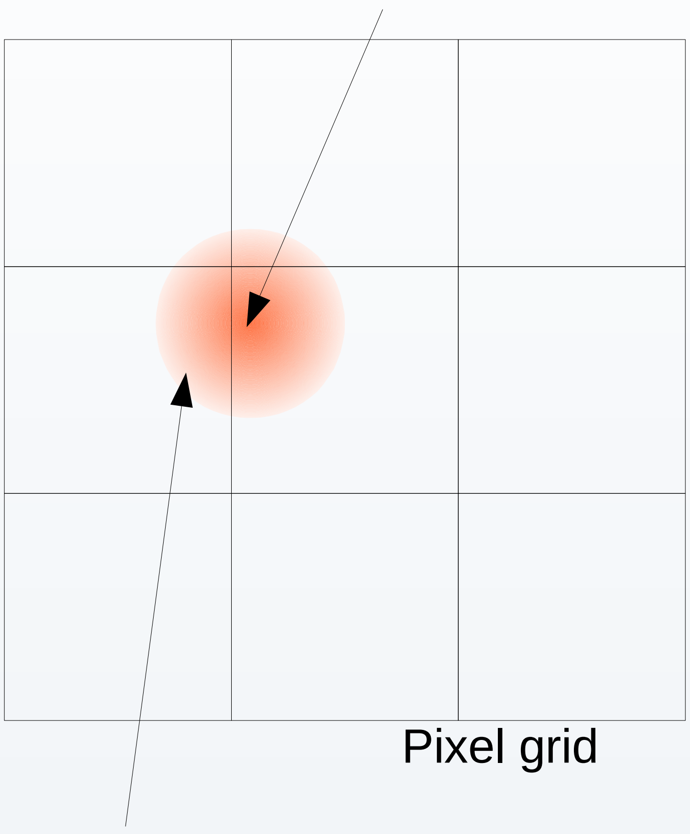


Particle Simulation

- This module simulates incident photons on the detector and calculates where they deposit energy in the semiconductor
- Uses Geant4, fully packaged inside the particle simulation
  - Incident photons are generated in Geant4 from an input list provided by X-CSIT
  - Energy deposited in the sensitive volumes is recorded and output from the particle simulation
- Geant4 can simulate photo electric effects, Compton and Rayleigh scattering as well as fluorescence and auger emissions down to 250 eV using the livermore physics list
- Geant4 has previously been validated for low energy EM processes and additional validation will be carried out in-house

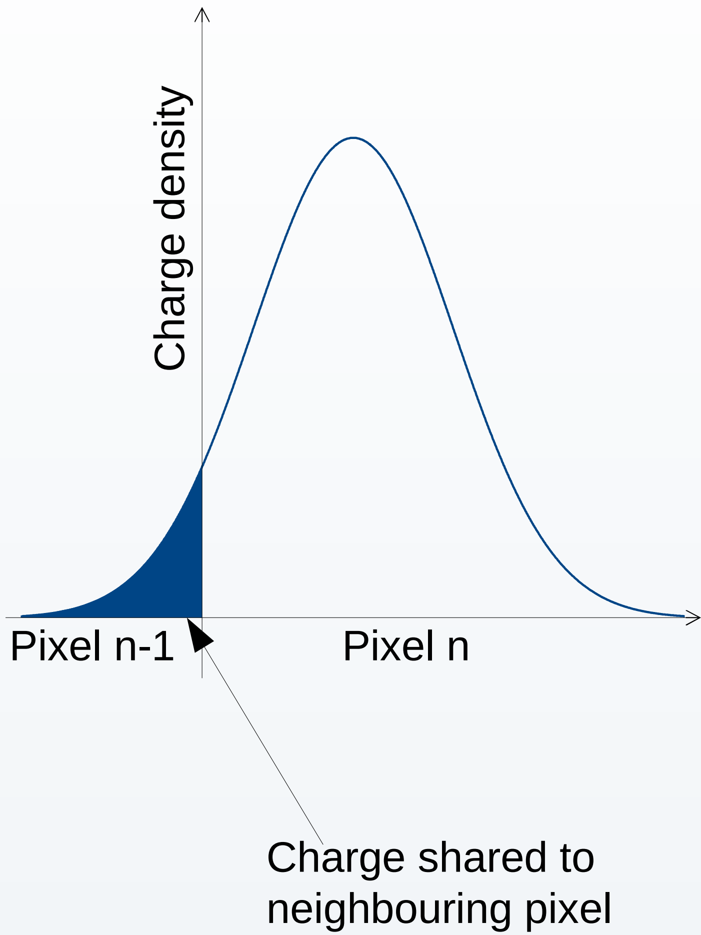
Charge Simulation

- The charge simulation has been built to simulate how energy deposited in the semiconductor layer is moved onto the readout pixels, including charge sharing between neighbouring pixels
- Because of the large number of electron-holes present, the charge simulation uses a statistical simulation
- The simulation is split into two regimes
  - In most cases, electron-holes act independently of each other and only diffusion needs be considered
  - At very high electron-hole densities, electron-hole plasmas can form



Charge Diffusion Simulation

- The charge diffusion simulation assumes a statistical distribution of collected electrons due to large number produced (~300 electrons per keV)
- Diffusion is calculated as a Gaussian distribution, with a standard deviation proportional to the root of the distance to the collection plates
  - This two dimensional Gaussian is approximated as a Gaussian distribution in both X and Y
  - The proportion of charge crossing a pixel boundary in either X or Y can then be calculated inexpensively with the cumulative distribution function



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

Charge Plasma Simulation

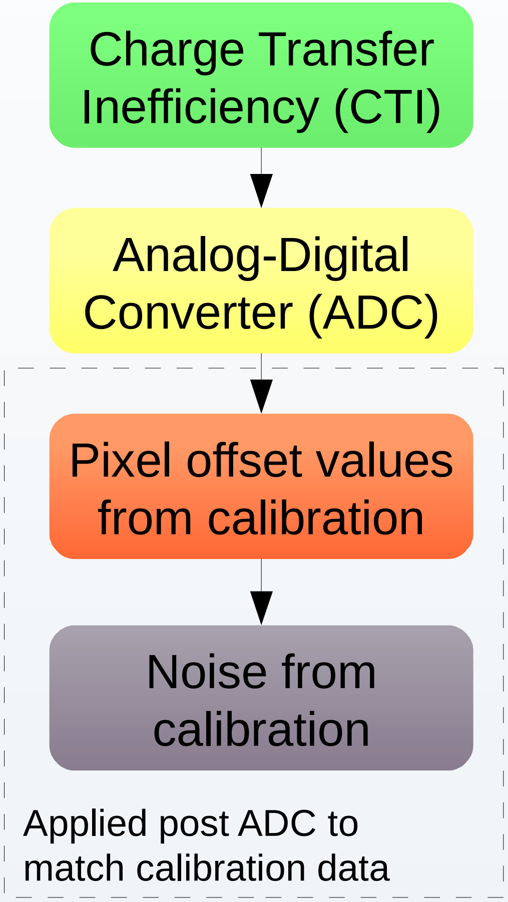
- When enough charge is deposited in a small enough location, the charge can screen itself from the electric field of the sensor, creating a pocket of plasma
- This pocket of plasma releases charge slowly, increasing the range over which charge is spread and the time it takes for collection
- The plasma effect is well studied in the field of heavy ion detectors, but not in the field of X-Ray science, which before XFELs did not reach the charge densities required
  - In particular the boundary where plasma effects begin to occur is not well understood
  - Later this year sources will become available at XFEL that will allow better investigation of this effect so a simulation can be written and validated

J. Becker et al. Nucl. Instr. And meth. A 615 (2010) 230

Electronics Simulation

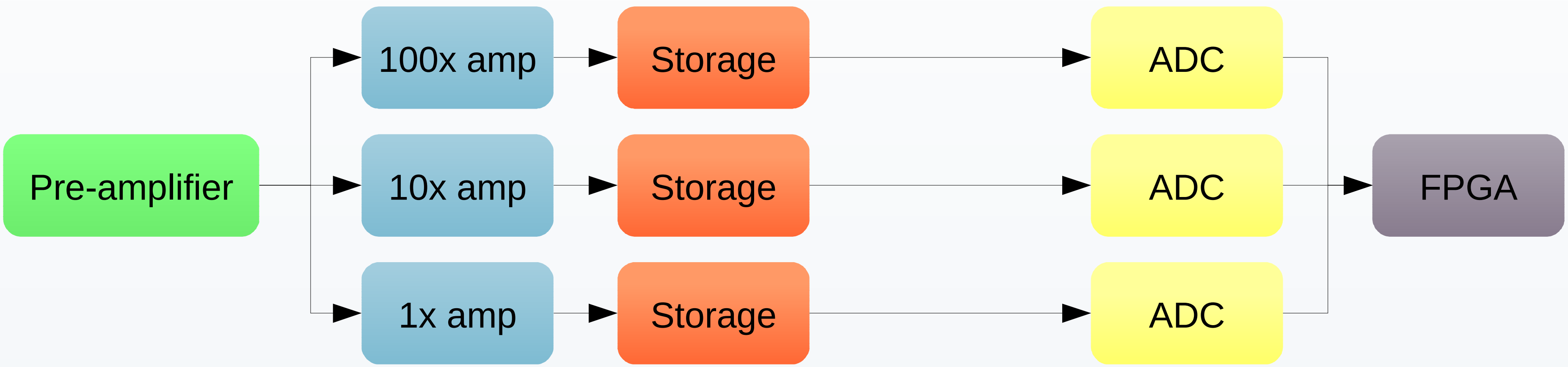
- The electronics simulation consists of a set of modular devices to simulate common electronic components
- Although most detector electronics are uniquely constructed, they perform similar functions such as storage, charge transfer, amplification and digitization, even if the order of these varies
- A simulation of the electronics of a detector is then created by chaining together these functions to create a functional representation of a real circuit
- The Karabo integrated version of X-CSIT (more later) will also include GUI tools to lay out this chain visually

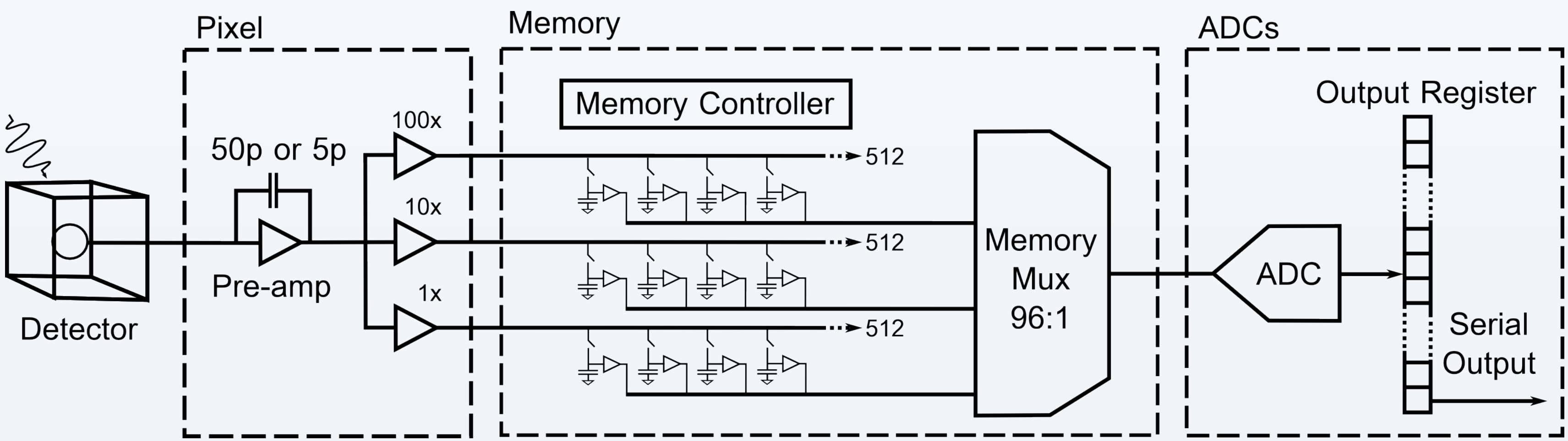
Electronics diagram for a pnCCD simulation



Electronics Simulation

- Comparison of the LPD ASIC and an example of the simulation layout in X-CSIT





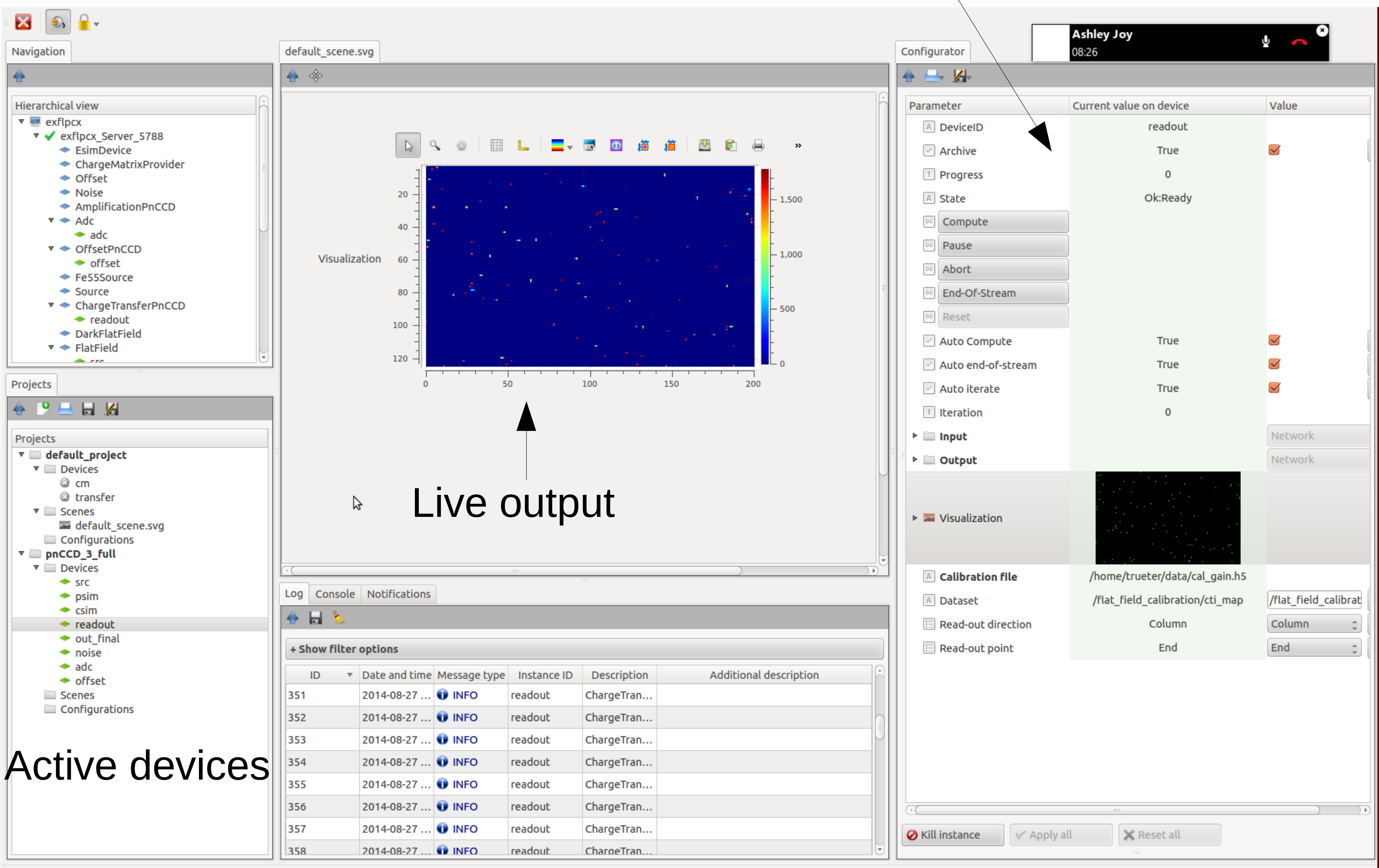
Use at European XFEL

- X-CSIT will be used to simulate the detectors used at XFEL, including LPD, AGIPD, DSSC and pnCCDs
- X-CSIT and these simulations are being integrated into Karabo, the control, DAQ and processing framework at XFEL, where they will be available to users on XFELs computer network.
- Integration into Karabo will include dependency on calibration data taken from the real detectors and output in the same format, allowing X-CSIT simulations to be slot into an analysis chain in place of a real detector
  - This will enable users at XFEL to test analysis pipelines with respect to detector performance before arriving to perform their experiments
  - After conducting experiments, X-CSIT simulations will help understanding measurements and detector uncertainties
- Additionally, X-CSIT is planned to form a part of an end-to-end simulation for the SPB (Single Particles, clusters and Biomolecules) instrument on SASE 1

Use at European XFEL

- Karabo in use

Device settings panel

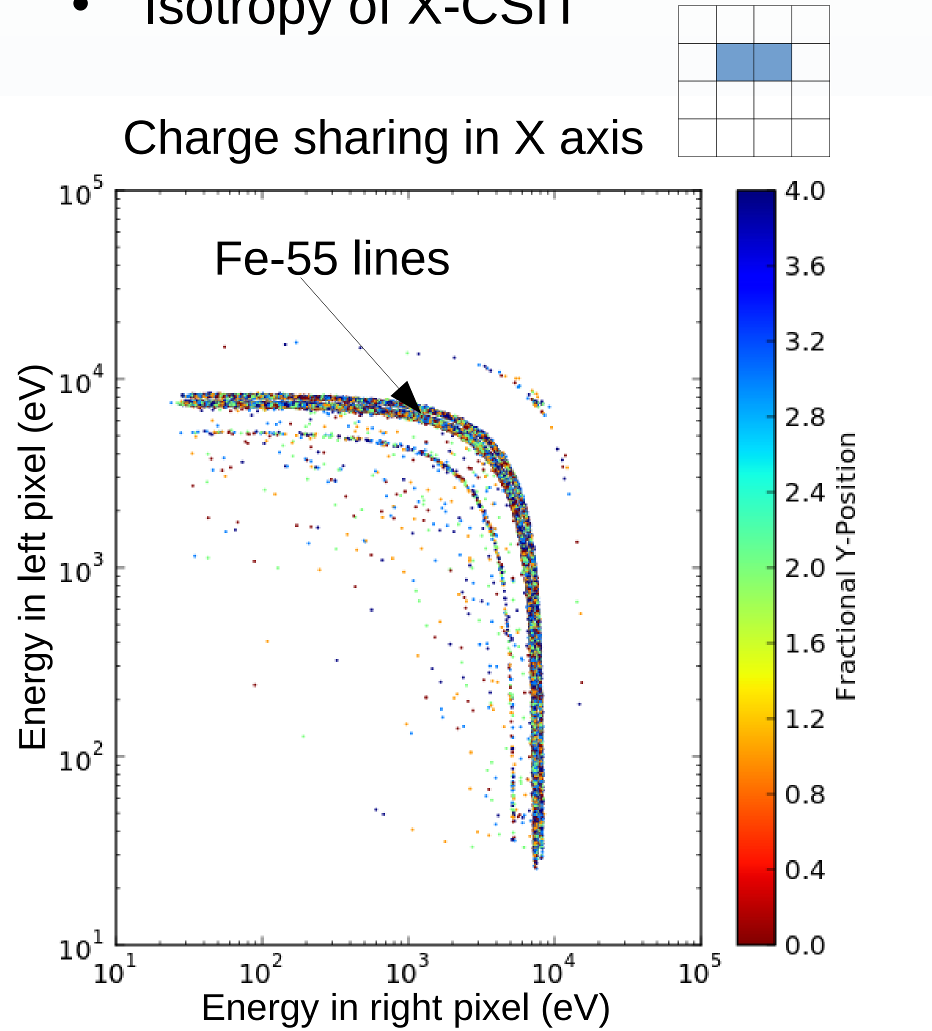


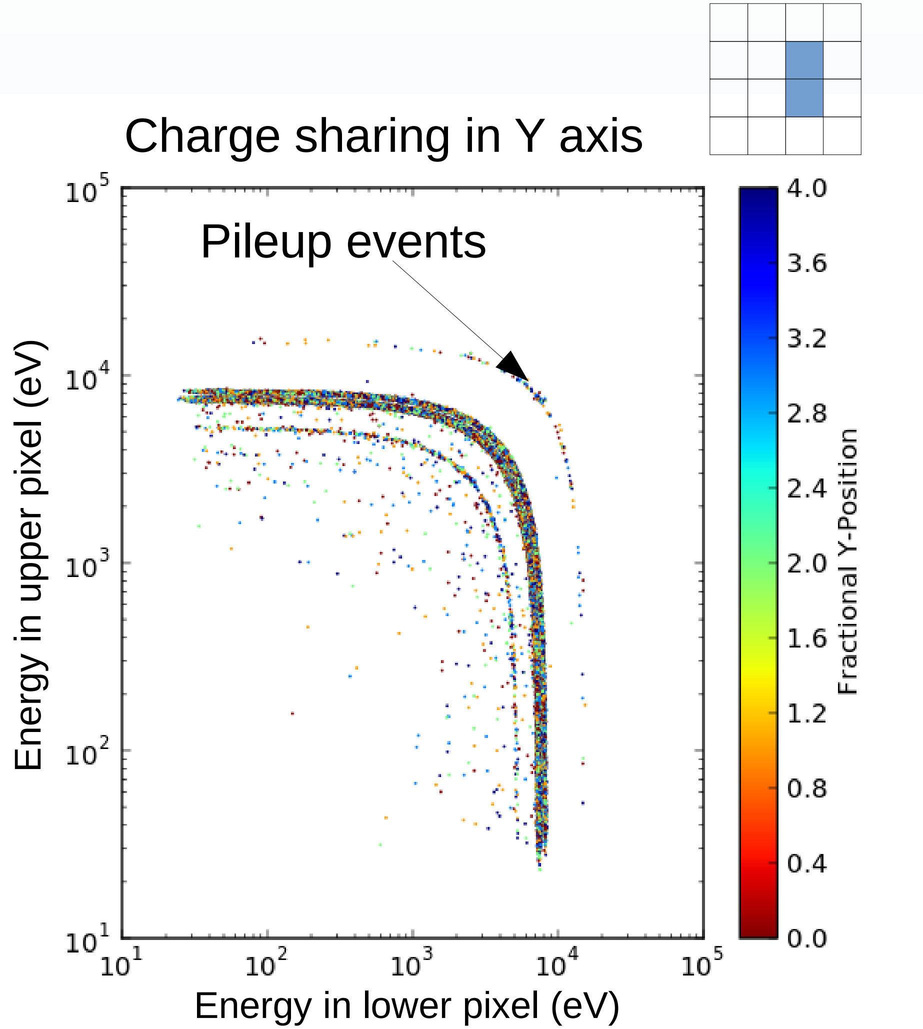
Testing

- 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 different group 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 in Karabo and compared

Testing - pnCCD

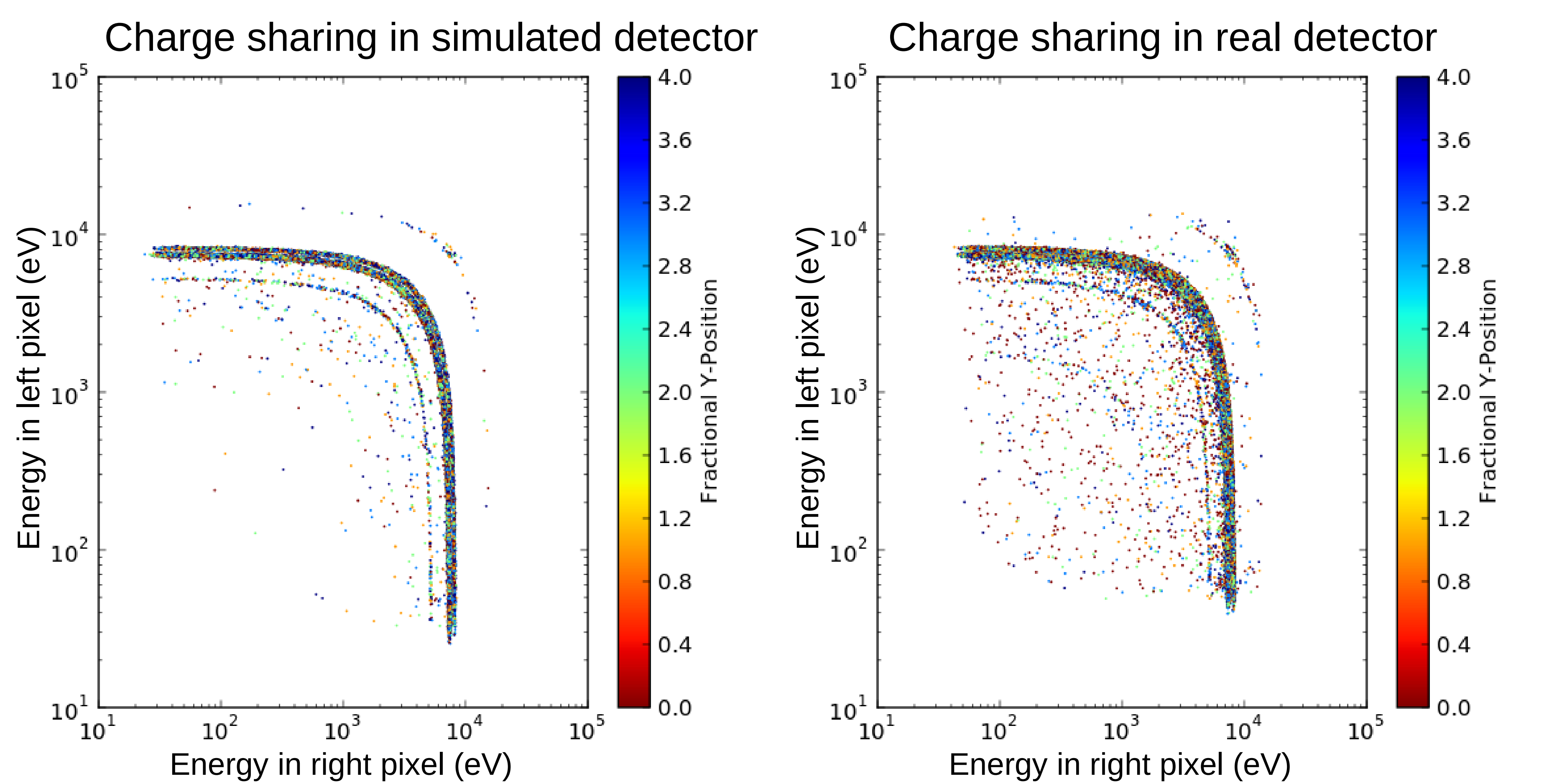
- Isotropy of X-CSIT





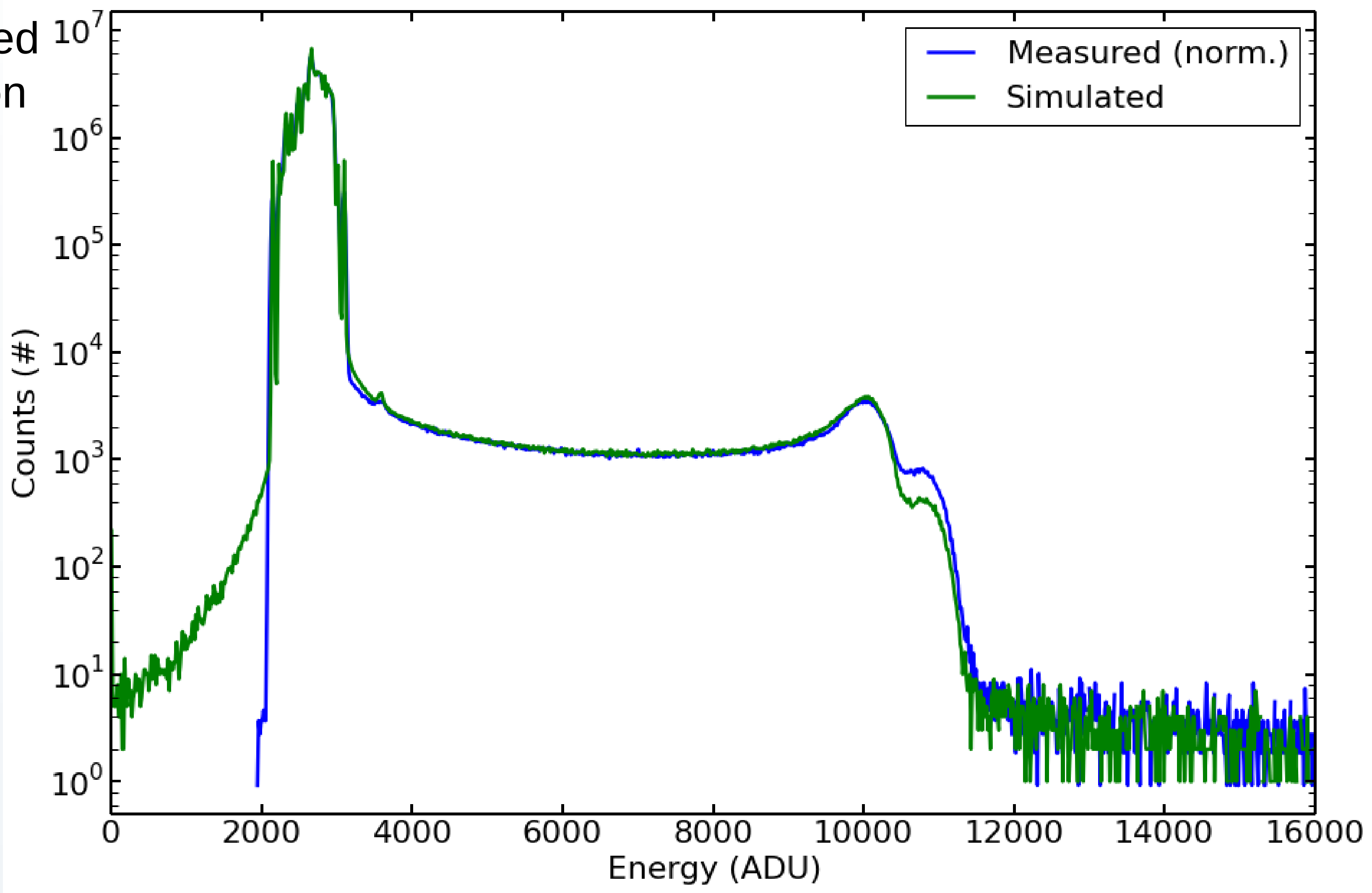
Testing - pnCCD

- Comparison of measured to simulated events



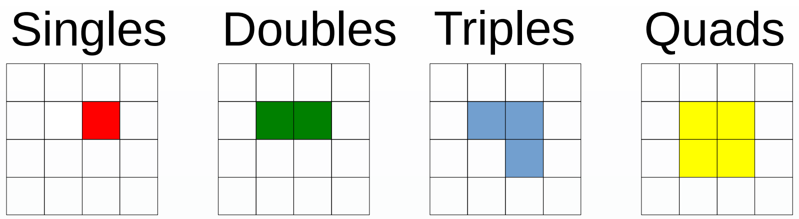
Testing - pnCCD

Normalised Absorption Spectra

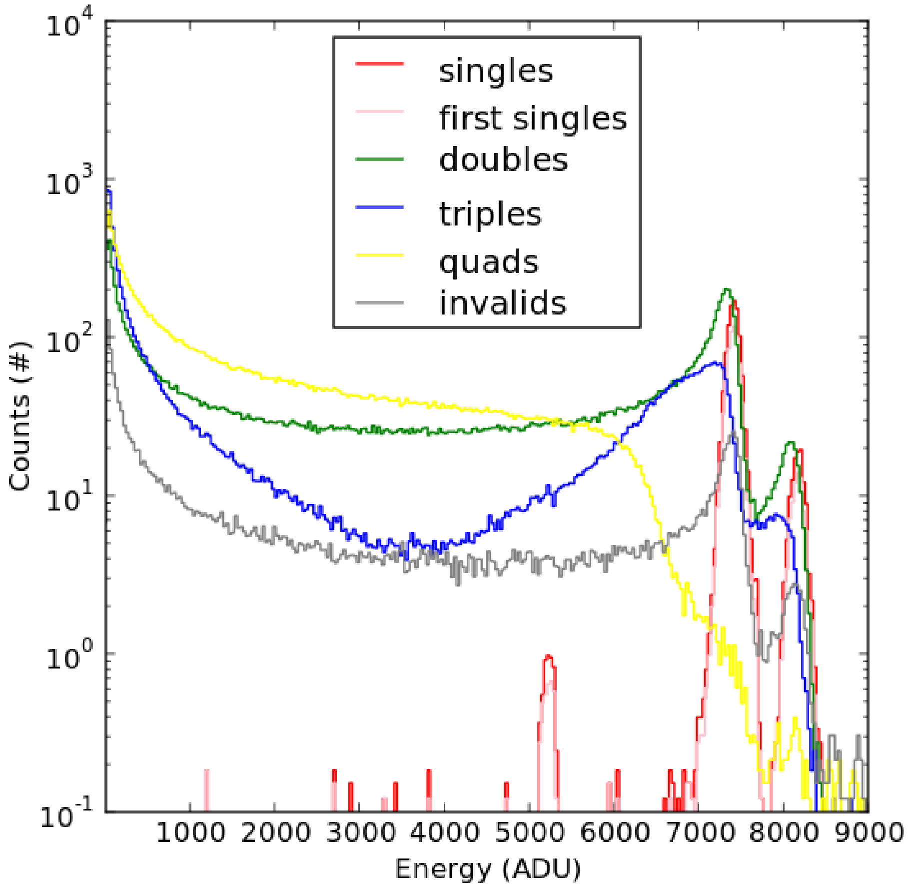


Testing - pnCCD

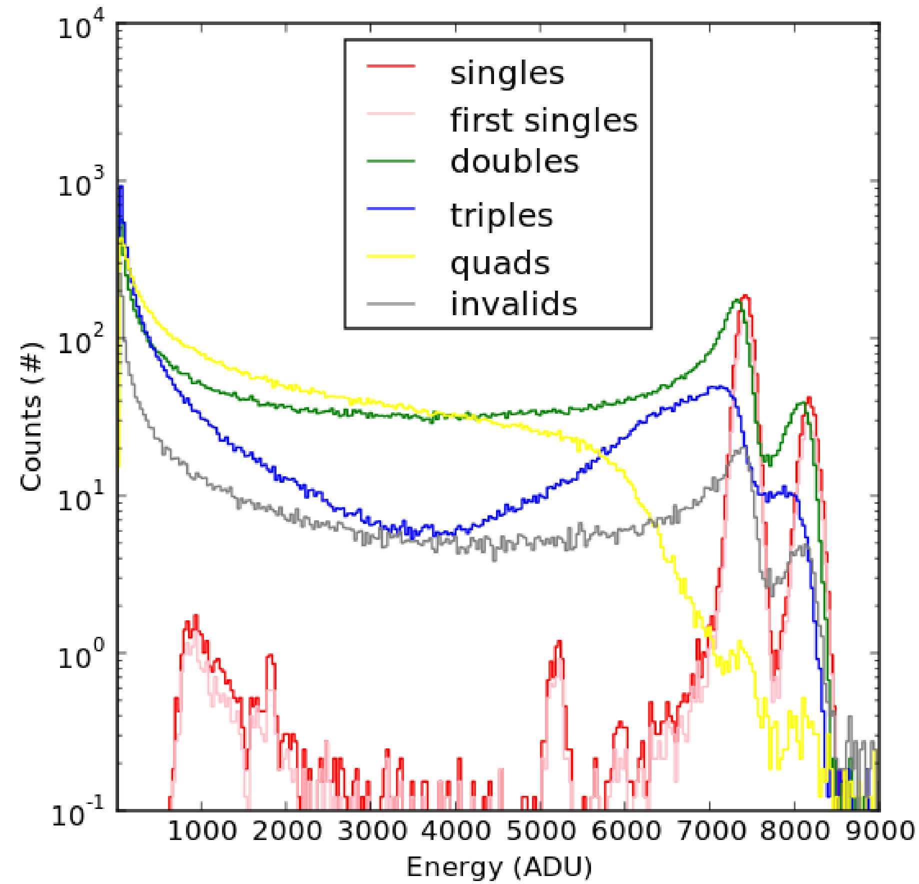
- Pattern absorption spectra



Simulated detector



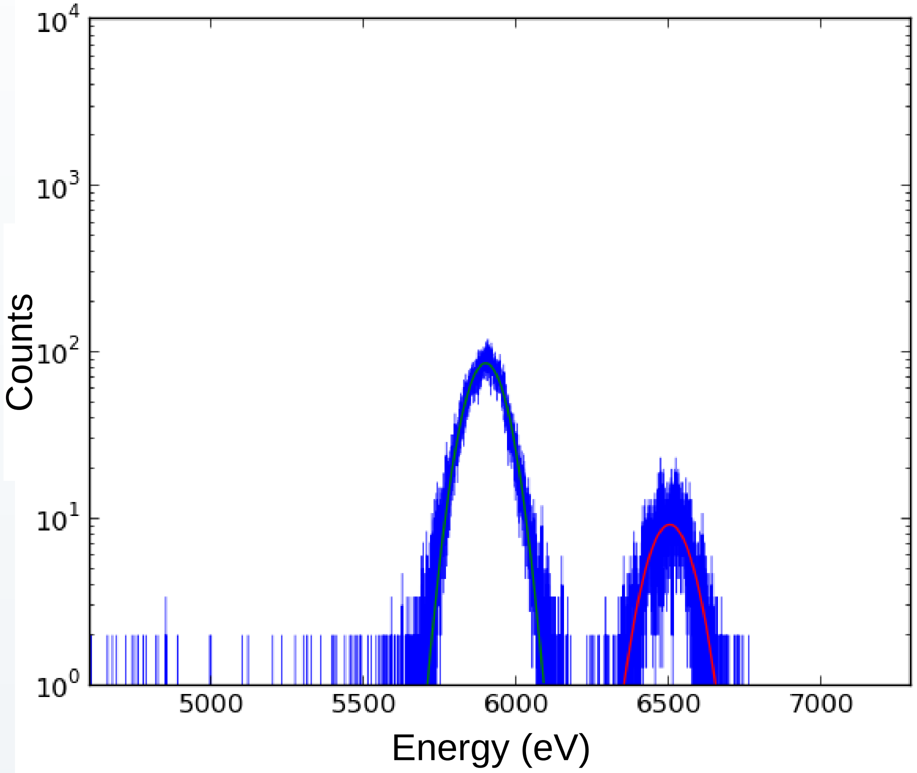
Real detector



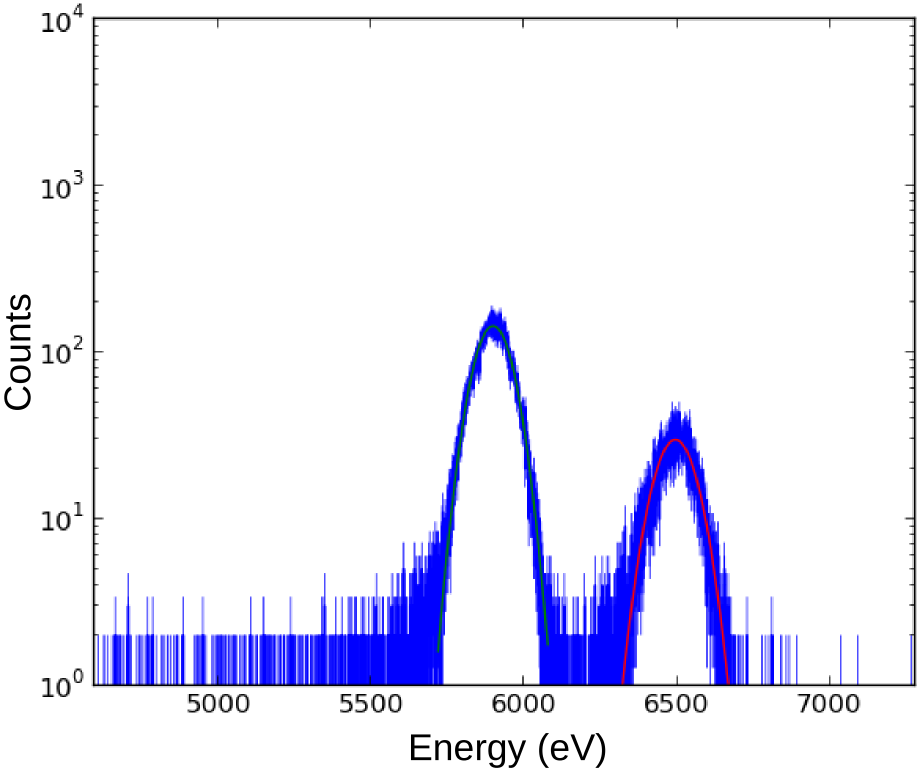
Testing - pnCCD

- Comparison of emission spectra

Emission in simulated detector



Charge sharing in real detector



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 LPD and a pnCCD
- 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 for free for other users or groups