Simulation Tools for Detector Performance and Calibration Sources at European XFEL

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Abstract

The detectors to be used at the European XFEL have to deal with the unique time structure of the machine, delivering up to 2700 pulses, with a repetition rate of 4.5 Mhz, ten times per second, the very high photon flux of up to 10^{12} photons/pulse and the need to combine single-photon sensitivity and a large dynamic range. These machine properties present a challenge for the large-area 2D imaging detectors to be used at European XFEL.

In order to thoroughly characterize the detectors, optimize their performance and the required calibration concepts, as well as give estimates of the expected scientific performance in a wide range of experimental scenarios, we are currently pursuing different simulation projects.

Initially, small self-contained simulation tools were developed e.g. for estimating the performance of calibration sources or for estimates on the performance of the large 2D-pixel detectors, results of which are presented here.

Additionally, we are currently developing a large scale simulation toolkit, which will be tightly integrated into the European XFEL software framework, Karabo [1]. It is envisaged that this framework will be available to XFEL facility users and allow the simulation of the 2D-pixel detectors used at European XFEL – starting from the photons incident on the detector down to the level of the read-out electronics.

Self-contained Simulation Tools – X-ray Source Sim.

Calibration of the 1 Mega-pixel 2D detectors with 4.5 Mhz readout will pose unique challenges for the laboratory infrastructure at European XFEL. In order to allow for a realistic representation of XFEL operating conditions, calibration measurements must be performed with a time structure and dynamic ranges similar to the FEL. In consequence, the laboratory calibration sources must provide pulses of up to 10^3 photons per pixel and pulse. As part of a continuous optimization strategy for this infrastructure a Geant4-based Monte-Carlo simulation [2,3] (Geant4 0.4.p03) has been created. It currently allows for performance estimates of different source geometries using Penelope physics, which were found to be better suited for this specific simulation task than the Livermore-based physics simulations are [4].

Estimates of the achievable X-ray fluxes for different target materials are presented on poster NP02-108.

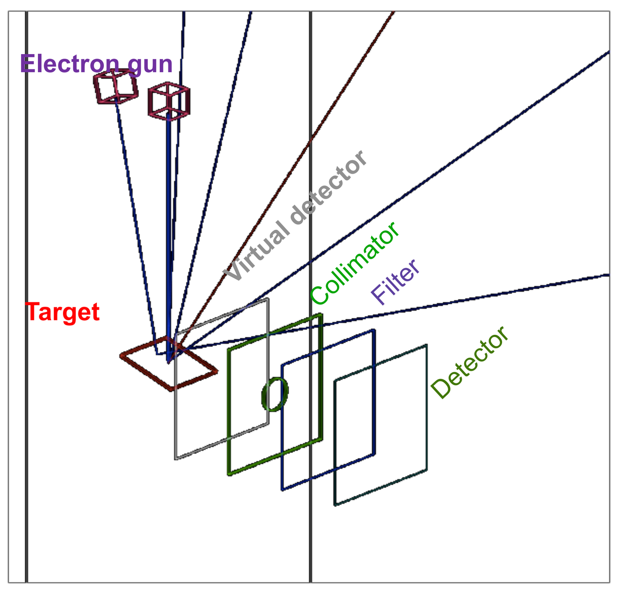

Figure 1: The Geant4 detector geometry for the X-ray source simulation. Electron gun and target position/angle are fully parameterized and accessible through macro functions as is target material selection.

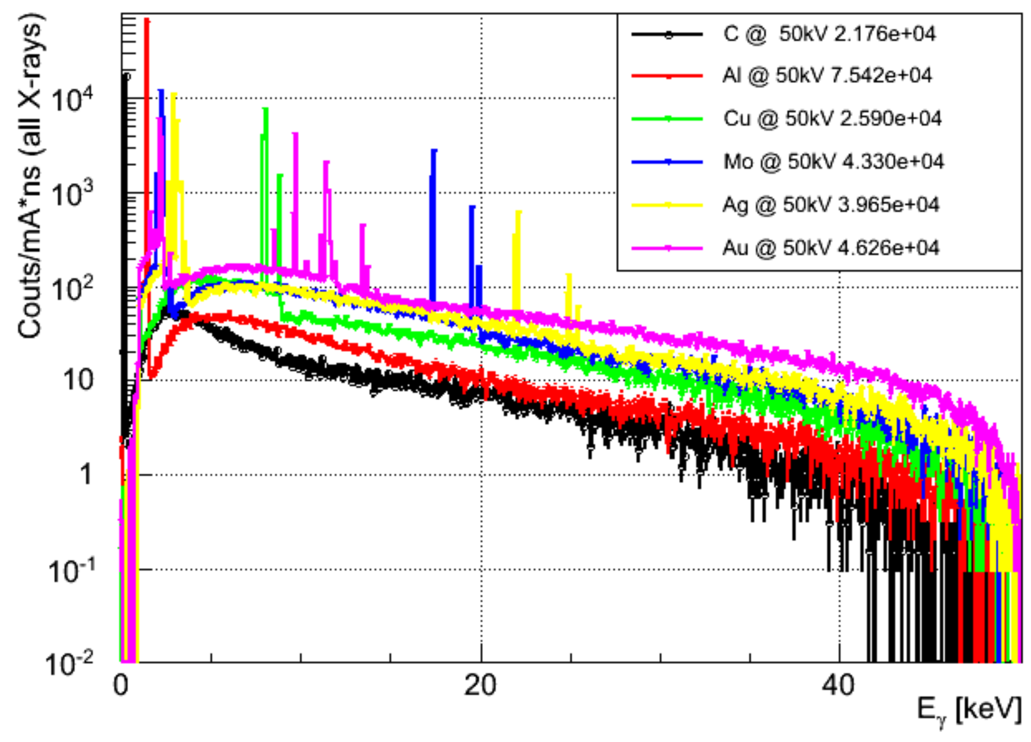

Figure 2: Geant4 simulation of the X-ray source setup for target materials **C**, **Al**, **Cu**, **Mo**, **Ag** and **Au** consisting of 20 million primary electrons at 50kV. The target angle was set to 18°. Counts are given for a plane detector of infinite size. The simulation correctly reproduces the fluorescence lines for each of the simulated target materials.

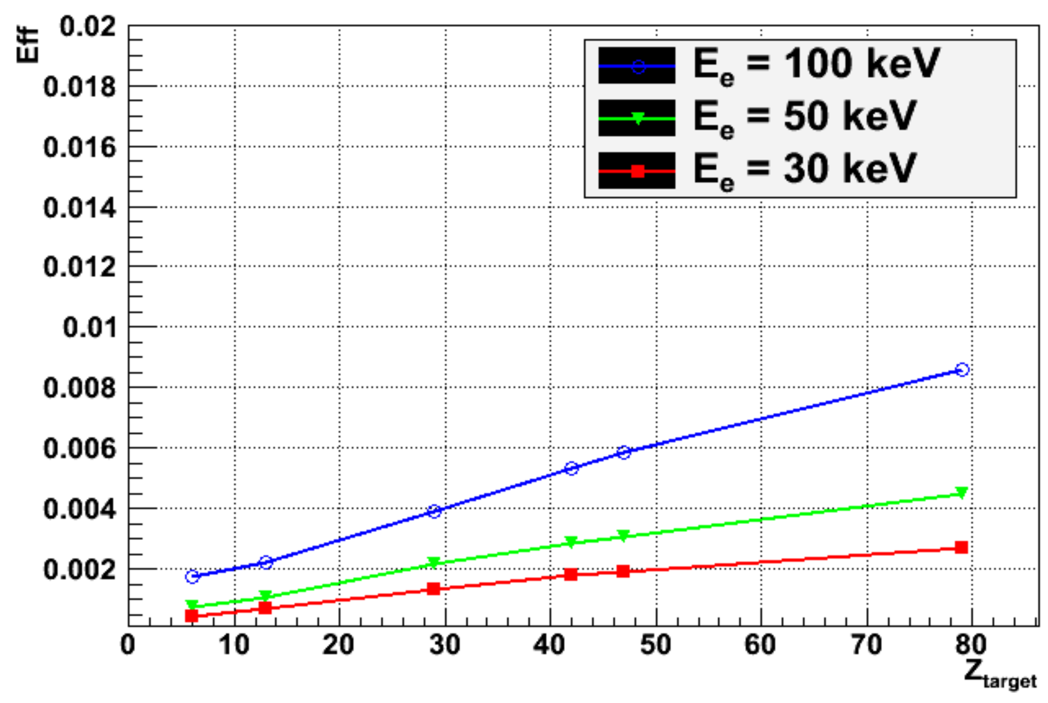

Figure 3: Conversion efficiency of incident primary electrons into Bremsstrahlung X-rays depending on target material.

Estimates for incident electrons at energies of 30 keV, 50 keV and 100 keV and elements C (Z=6), Al (Z=13), Cu (Z=29), Mo (Z=42), Ag (Z=49) and Au (Z=79) are shown.

Each simulation consisted of 40 Million primary electrons. The target angle was set to 18°.

Self-contained Simulation Tools – 2D Pixel Detectors

During the design phase of the large 2D-pixel detectors, which are to be used at European XFEL, simulations for estimating detector performance have been performed by each of the external consortia involved in their development (AGIPD[5,6], LPD[7], DSSC[8,9]).

In order to allow for follow-up in-house performance estimates, optionally including the influence of the diverse environmental conditions of the instrument stations, an evolvable Geant4-based simulation tool (Geant4 9.6) for these detectors has been developed. It uses Livermore-based physics simulation. Building upon the initial proof-of-principle quantum efficiency simulations presented here, it is planned to become a pluggable component for the X-ray source simulation (see above). Additionally, it is currently being used to investigate the influence of beam scattering from residual gas in SPB-instrument chamber and will serve as a reference benchmark for the Karabo-integrated simulation framework presented on the right.

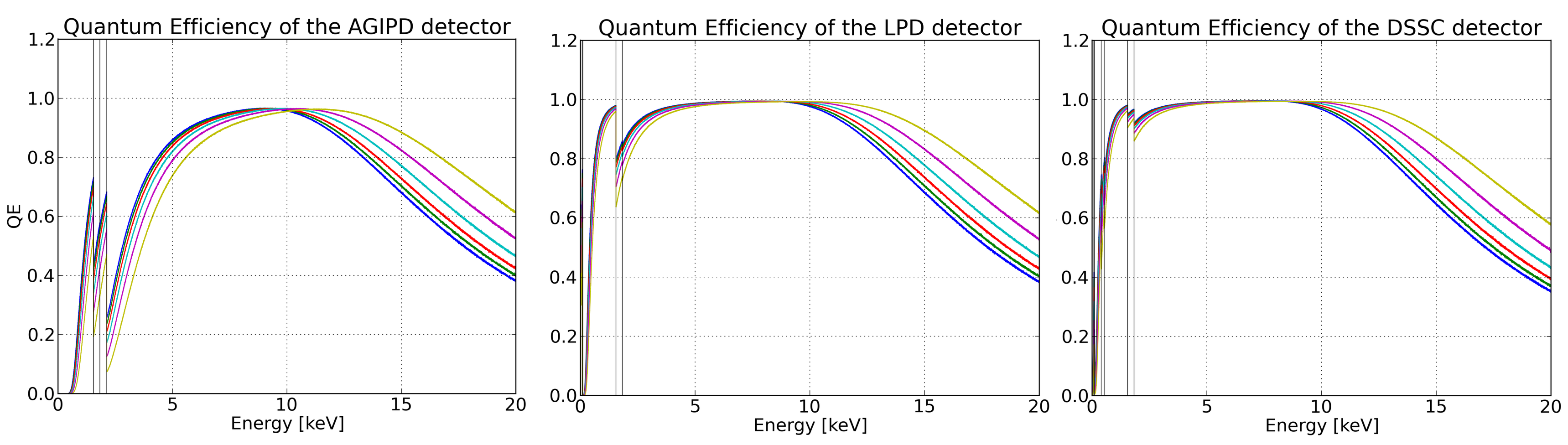

Figure 4: Geant4-based quantum efficiency simulations for the three large 2D-pixel detectors with Mhz readout capability at European XFEL. From left to right the AGIPD, LPD and DSSC are shown. The individual absorption edges, determined by the respective detectors' entrance windows, are visible. For each detector the efficiency was simulated at different incidence angles: 0°, 20°, 30°, 40°, 50° and 60°. Additional simulations were made to verify that the energy-dependent variation of efficiency is due to back scattering (reduction for large angles at small energies) and geometric length' (enhancement for large angles at high energies).

The X-ray Camera Simulation Toolkit: X–CSIT

As a mid-term goal, European XFEL in collaboration with University College London plans to create a simulation toolkit which can simulate a semi-conductor pixel detector from the incident photon down to the characteristics of the read-out electronics. The toolkit will be used to create simulations of the three bespoke detectors being built for XFEL and will be made available to users through integration into Karabo, the data processing and control system at XFEL.

A first prototype of the **X-ray Camera Simulation Toolkit (X-CSIT)** is currently implemented at UCL, using Geant4 integrated into the framework to simulate photon interaction and initial charge carrier creation.

X-CSIT is designed as a modular toolkit, rather than a bespoke simulation, which will allow it to simulate of a wide variety of pixel detectors and swap out modules for improved simulations if they become available.

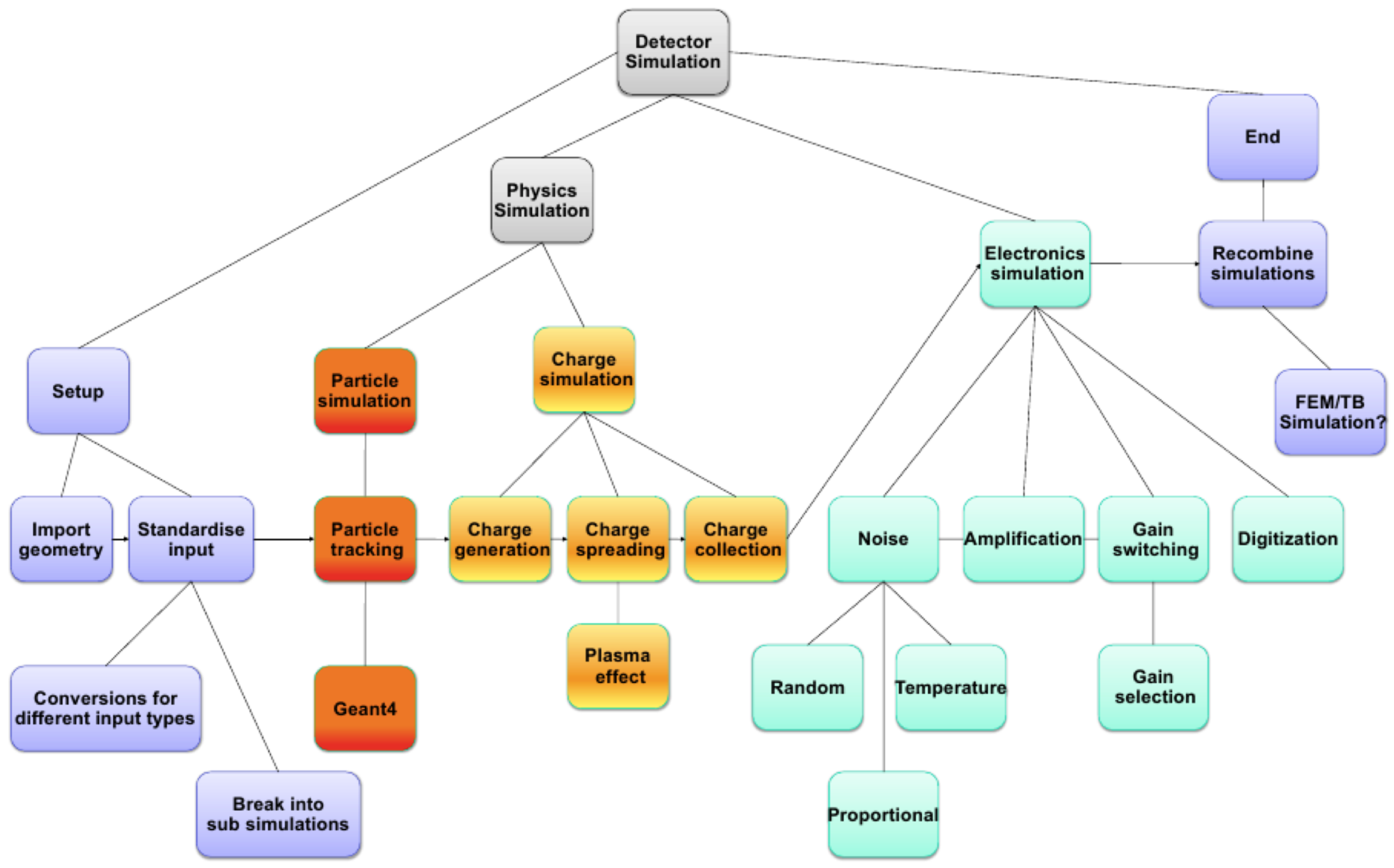

Figure 5: An early diagram giving an overview of the design considerations for X-CSIT, which will be written in C++ including use of the boost library. This roughly shows the class layout of the software and framework. The photon and high energy electron tracking is shown in red, the charge cloud simulation in yellow, the electronics and front-end module simulation in green and auxiliary components in blue.

X–CSIT: Current Status and Preliminary Results

Thus far, the framework for X-CSIT has been written and is undergoing unit testing. In addition Geant4 has been integrated into the particle particle simulation of the framework and is communicating data back and forth.

For testing a Geant4 simulation, currently consisting of a single block of silicon 500um thick with a 1um thick entrance window has been implemented. All photons enter the silicon at the normal and the block is sufficiently large that charge scatter through edges is negligible.

As a further proof of concept the framework has been linked to the python interpreter and can pass data to it. The plots below were made with matplotlib[10], a python plotting library.

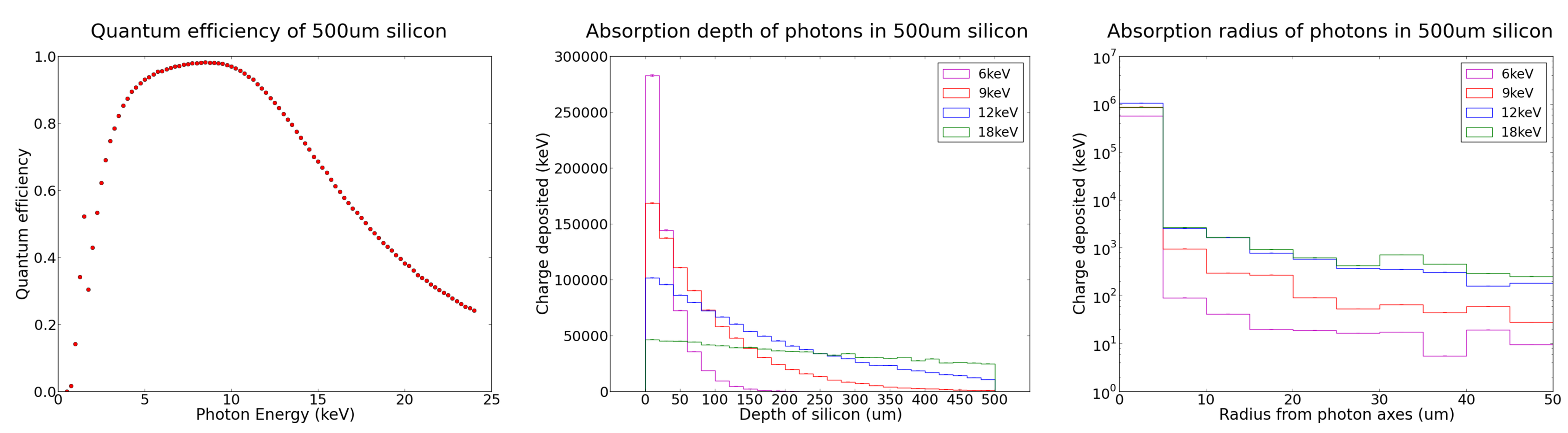

Figure 6: Quantum efficiency and absorption graphs with 100k photons per energy bracket. The positions of charge deposition was extracted from Geant4, passed back to the framework, then on to a python link and displayed using a matplotlib script. The plots are as expected, demonstrating the simulation and data framework is working correctly.

X–CSIT: Outlook

X-CSIT is still in very early development and prototyping. Features still to be added include: a charge carrier simulation including charge spreading and plasma effects, an electronics simulation toolkit, an expanded Geant4 simulation that handles detector modules and better links to plotting libraries for visualisation and analysis.

To account for the wide variety in detector electronics, the electronics simulation toolkit will consist of smaller electronic functions that can be combined together to quickly form a simulation. There are also plans to integrate the electronics toolkit into the Karabo GUI, allowing Karabo users to layout the electronics simulation visually.

As part of its use at XFEL, simulations of LPD, AGIPD and DSSC will be written using X-CSIT and tightly integrated into Karabo. These simulations will be made available to XFEL users and written so that they can replace detectors in the data chain, allowing users to test their analysis before taking data.

Lastly there are plans to validate X-CSIT using data taken by an early prototype of LPD, which took test data at the SLAC and PETRA III facilities early in 2013.

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2013 IEEE NSS/MIC/RTSD Seoul, Korea