Livermore photoelectric model data discrepancy in Geant4 v10.7+

Alberto Manfreda, Simone Castellano

alberto.manfreda@pi.infn.it

INFN–Pisa

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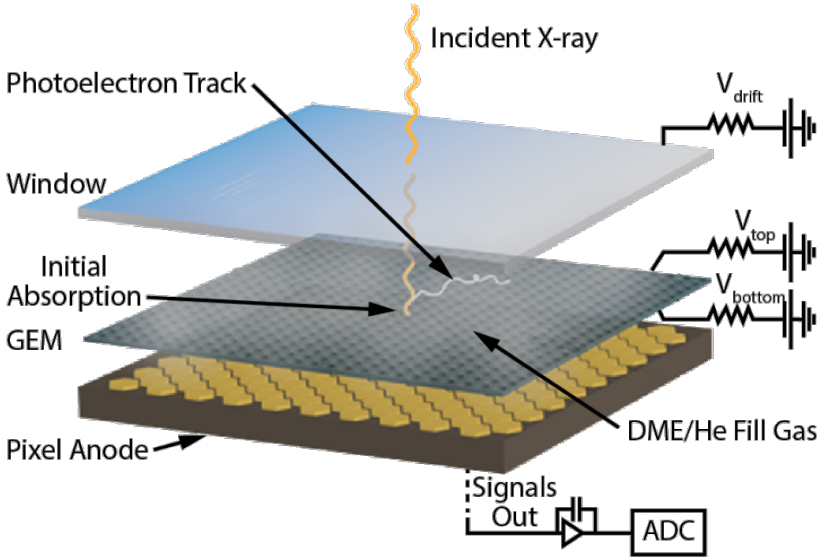
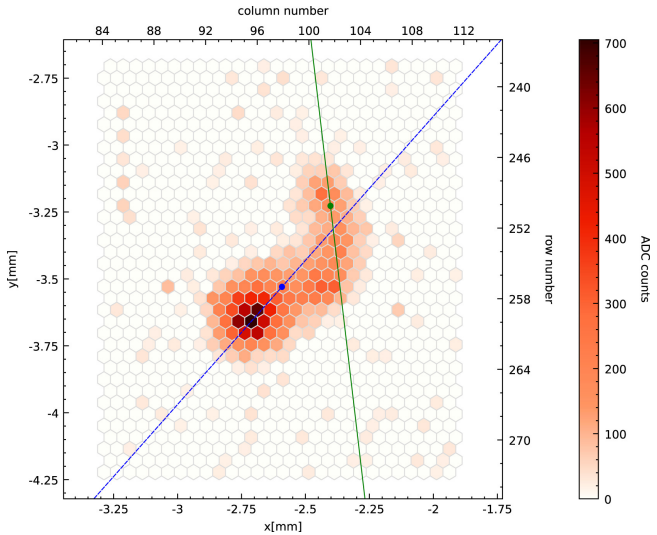
Summary

- Reporting a data - MonteCarlo discrepancy observed when simulating X-ray interactions in a photoelectric based gas detectors in the 2-8 keV energy range
- More specifically, the shape of simulated output spectra from monochromatic x-ray input beams show a prominent difference with experimental data in its left tail
- The discrepancy is specific of the Livermore Pysics lists and has been observed with versions 10.7 and 11.0 of Geant4, while it was not present with version 10.3, which has a very good agreement with our data
- We tracked down this discrepancy to a variation in the fluorescence emission from copper around $\sim$1 keV, which seems to be much larger in version 10.7 and 11.0 compared to version 10.3

Detector description





- A Gas Pixel Detector (GPD) is a photoelectric based polarimeter for soft X-rays (< 10 keV), employed by the IXPE mission
- Photons are absorbed in the gas cell, where photoelectron tracks are drifted towards a segmented anode (a custom ASIC)
- A GEM guarantees the required signal amplification
- The output is a 2D image of the photoelectron track, from which the initial emission direction can be reconstructed

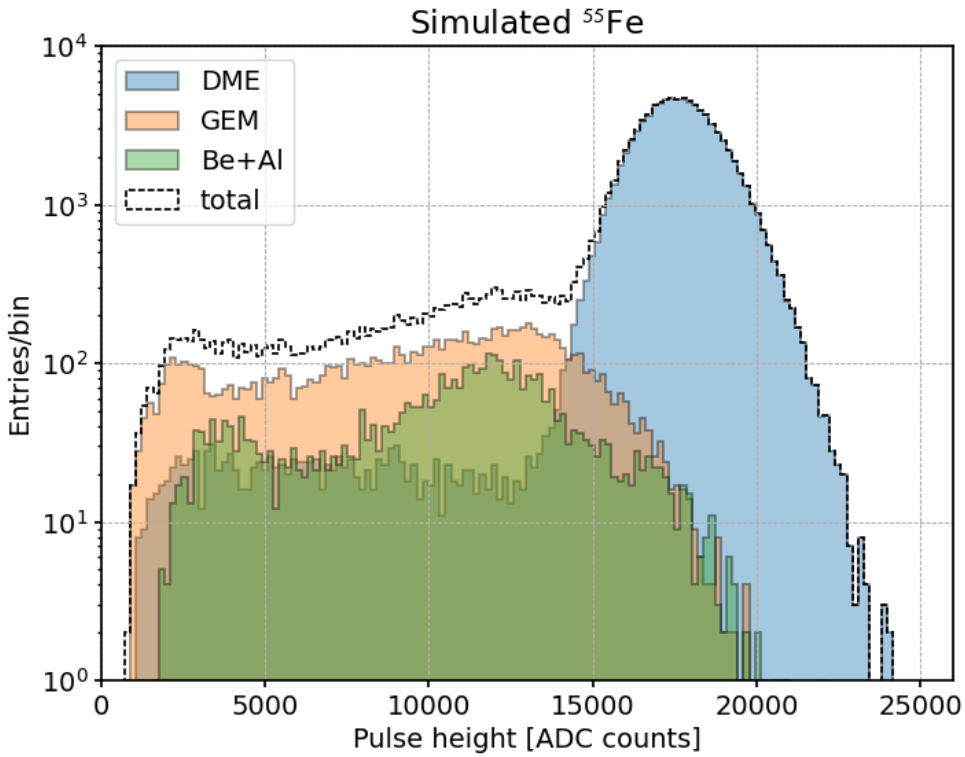
Simulation workflow

- Our simulation of the GPD uses a mix of Geant4 and empirical parametrizations
- We use Geant4 to:
  - Simulate the primary interaction (typically photoelectric absorbtion, very seldomly Compton scatter)
  - Follow the photo-electron track (and all its secondaries) in the gas until it stops or leave the detector
  - Simulate de-excitation / Auger emission
- The energy deposited at each step in the gas is used to generate an appropriate number of ionization pairs at the step position
- The rest of the simulation (drift, diffusion, multiplication, readout) is based on our own parametrizations
  - It is essentially independent from Geant4

Geant4 setup in ixpesim

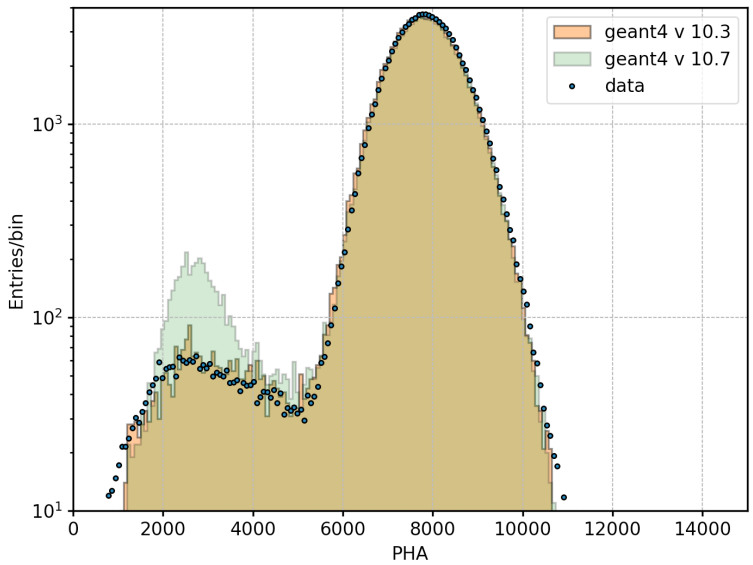
- We use a slightly customized version of the Livermore Polarized physics list (as we need polarization-aware photoelectric cross section)
- Using 'out-of-the-box' Livermore physics list (Polarized or not) gives exactly the same results, for what concern the issue discussed here. The only settings required to reproduce the problem are:
  - **SetAuger**: True
  - **SetDeexcitationIgnoreCut**: True
- Our reference Geant4 version is **10.3**

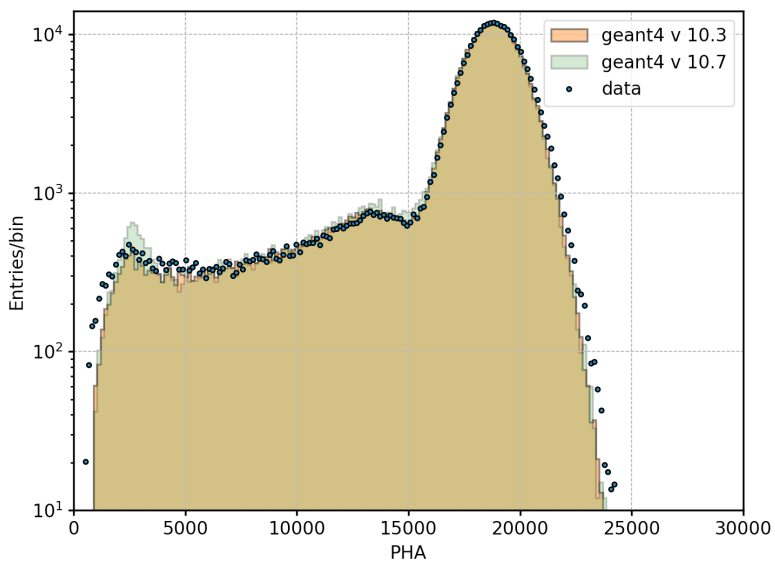
Spectral tail



- Spectral tail components:
  1. Incomplete charge collection in the DME-filled gas cell
  2. Photoeletric absorption in the entrance window (Al + Be) or on the copper surface of the GEM. The signal is given either by the photoelectron escaping from the solid into the gas cell or by fluorescence photons

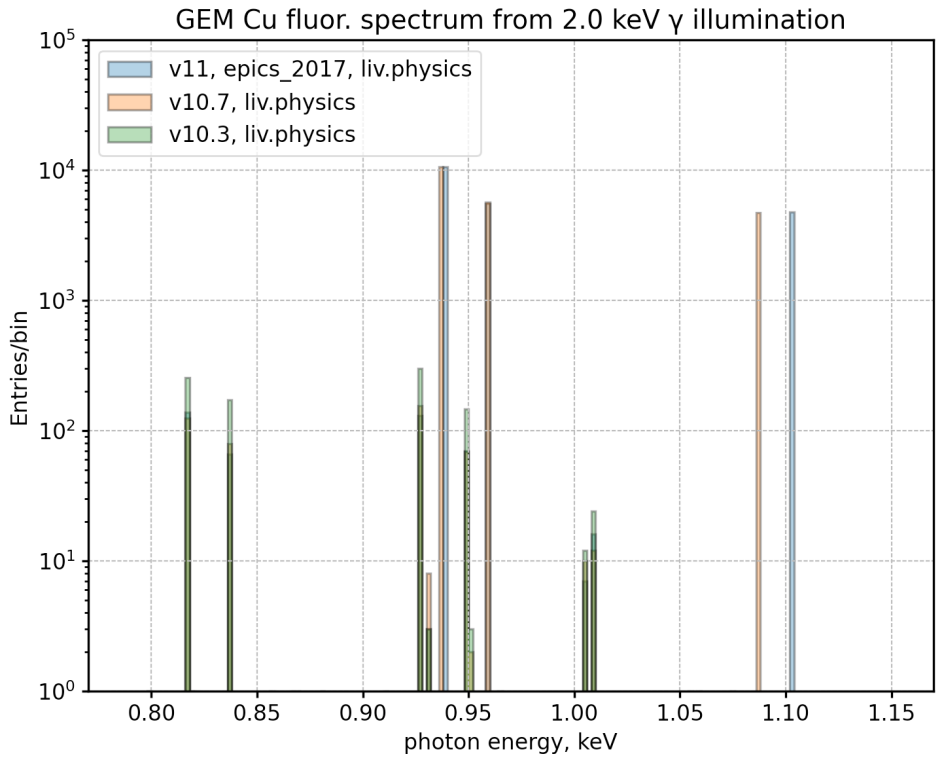
Geant4 10.3 vs 10.7





- Moving from Geant4 10.3 to 10.7 we noticed that a bump appears in the spectral tail, roughly at $\sim$ 1 keV
- The bump is visible simulating photons of all energies in our range of interest (2-8 keV), but more prominent at low energy
- Left: data - MonteCarlo comparison for 2.7 keV photons with versions 10.3 and 10.7; right: same at 6.4 keV
- Further investigation showed that these excess events are fluorescence photons originating in the GEM copper layer

Cu spectrum from StackingAction



- Taking the spectrum of fluorescence photons produced in copper directly from StackingAction (and thus before transport) a few things are noticeable:
  - There are $\sim$ 20 times more of such photons around 1 keV in version 10.7 and 11.0 compared to 10.3
  - The position of the lines does not match
- Such bright emission does not show in our data

Additional checks

- We have checked that this difference is robust against any change in our simulation settings (including production cuts)
- We have checked that a different physics list (Penelope) does not show such change when comparing the two Geant4 versions
- However, using Penelope but with the Livermore photoelectric model the difference is back there
- Apparently a change in the Livermore photoelectric model is the most likely origin for this difference

Conclusions

- The spectral response to 2-8 keV photons of our detector simulated with Geant4 10.7 an 11.0, shows a discrepancy with data that was not present in version 10.3 (we did not test intermediate versions)
- The discrepancy is due to an excess of fluorescence emission from copper, peaking slightly below 1 keV
- Our tests point to a change of the Livermore photoelectric model as the origin of the discrepancy
- Is there a way to fix this in the Livermore Polarized without manually suppressing the extra line(s)? We really need the polarization-aware photoelectric cross section, so switching physics list just won't do.