Characterising spectral response of the CZT detectors

Cadmium Zinc Telluride ($Cd_{0.9}Zn_{0.1}Te$) detectors are one of the most common X/gamma-ray detectors. They have a good detection efficiency between the energy range ~15 keV to ~300 keV. CZT detectors have been successfully used in many space missions such as Swift/BAT, NuStar, AstroSat/CZTI. One other advantage of these detectors is that they are position sensitive detectors and can be easily pixelated (either physical pixels or electronic pixels) making them a good candidate for doing X/gamma-ray imaging.

In this tutorial we will learn how to model a typical CZT detector in GEANT4, find out its X-ray absorption properties, and study the spectral response. The tutorial will also cover how to use a spectral response matrix, typically used in spectroscopy of astrophysical sources and also how CZT detectors can be used in coded mask imaging.

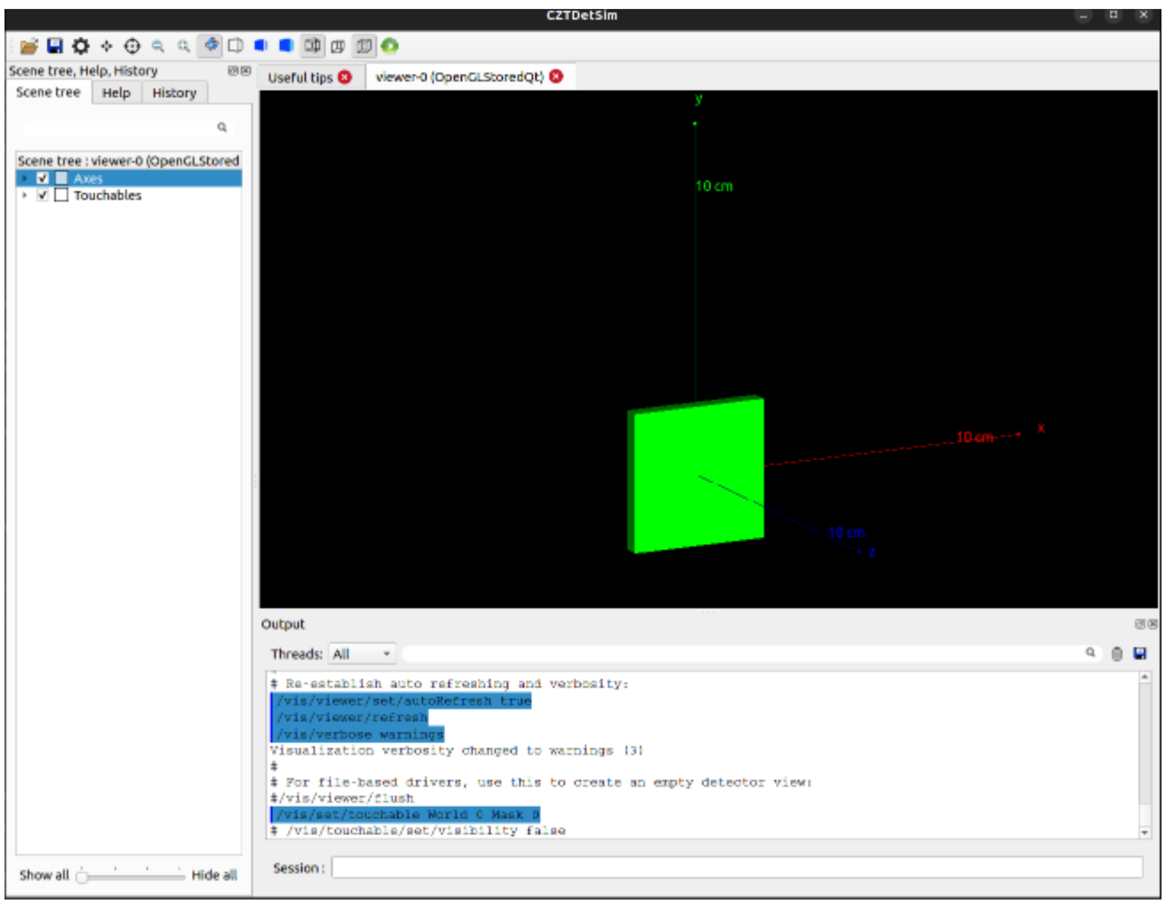
To help in building the GEANT4 application, a template for all the classes necessary to create this application is given in the ***CZT_tutorial_template.tar.gz*** file. The file also contains all the auxiliary information (e.g. absorption coefficients, mask pattern, response matrices) need for this tutorial

1) Set-up the geometry and physics:

a) Build a simple CZT crystal box using the detector construction. The dimension of the wafer and material fractional composition should be:
   - Dimension: 39.36 m x 39.36 mm x 5 mm
   - Composition: Cd = 0.430016; Zn = 0.027790; Te = 0.542194

b) Use the *G4EmLivermorePolarizedPhysics* list and also activate atomic de-excitation.

The crystal should look like:



2) Testing the absorption efficiency:

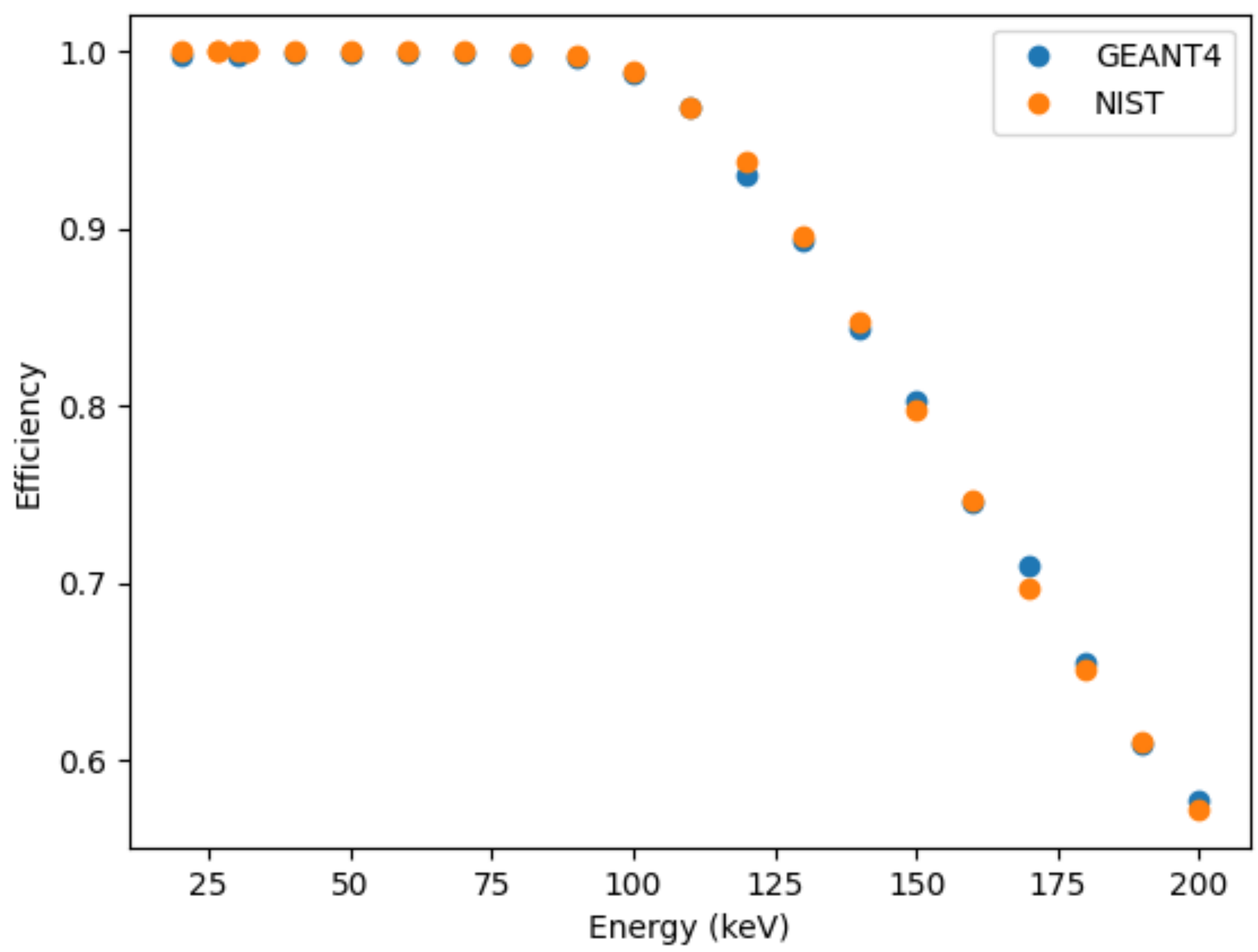
a) Make the CZT volume a sensitive detector and define a Hits class to record total energy deposition in the volume.

- **Hint**: Lectures by Sunanda Banerjee and Raman Sehgal. You can also refer to B02 and B05 examples from GEANT4 to see how SD and hits are defined.
- The energy deposition for each run should be stored in an output file as an ascii file or as a root file.
- **Hint**: You can use the analysis manager class to record energy depositions as root ntuples.

b) Once you are able to record energy depositions, shine mono-energy photons from 20 keV to 200 keV in steps of 10 keV and find out the total detection efficiency of the detectors for each energy. Compare this efficiency with the analytical estimate obtained from the NIST interaction cross-sections (Details of the formula to compute efficiency in Sujay Mate's talk).

- The NIST cross-section values as a function of energy are provided in the file ***czt.dat***.
- For these simulations, 10k photons per energy should be good enough to have acceptable statistics.
- Post-processing of the simulation data can be done in python or c++ or any other analysis tools you are most familiar wiht

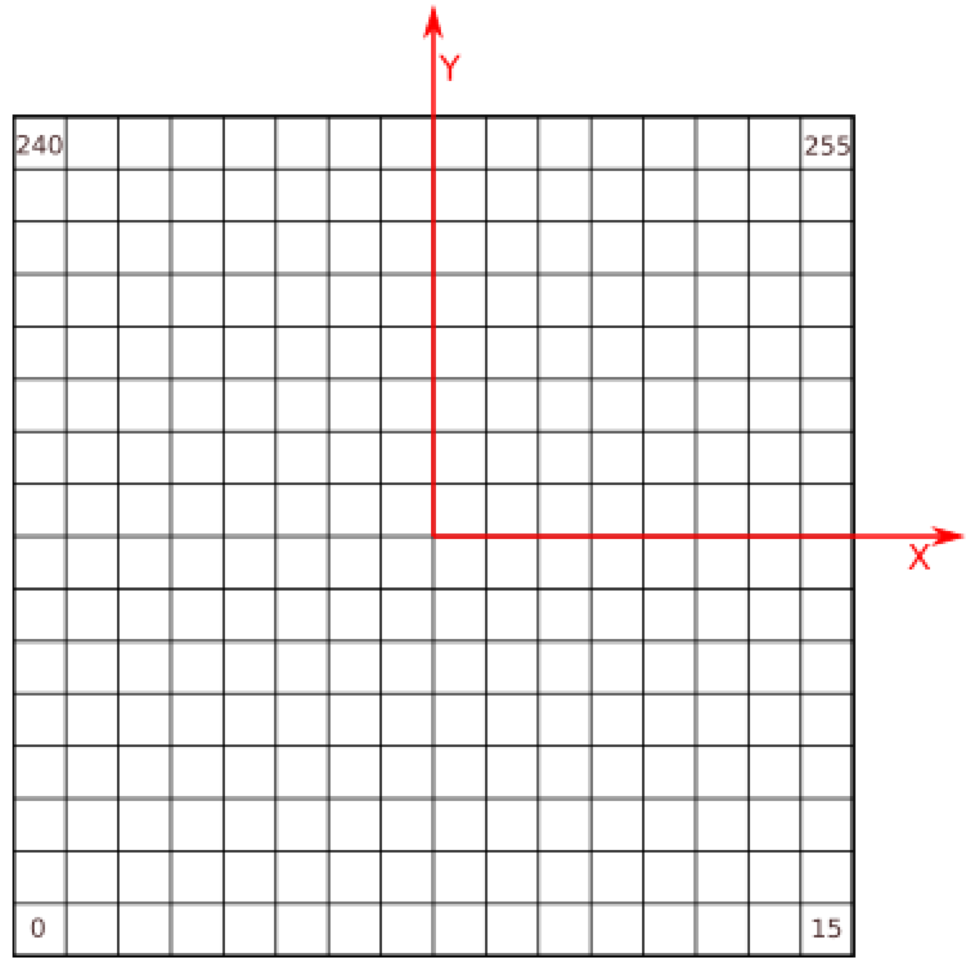
The comparison of efficiency from simulations and analytical estimate should look like the plot below:



3) Pixelating the detector and understanding the detected spectra:

a) Divide the entire crystal into a 16 x 16 pixel grid and record the energy deposition for each pixel separately. The pixel size should be 2.46 mm.

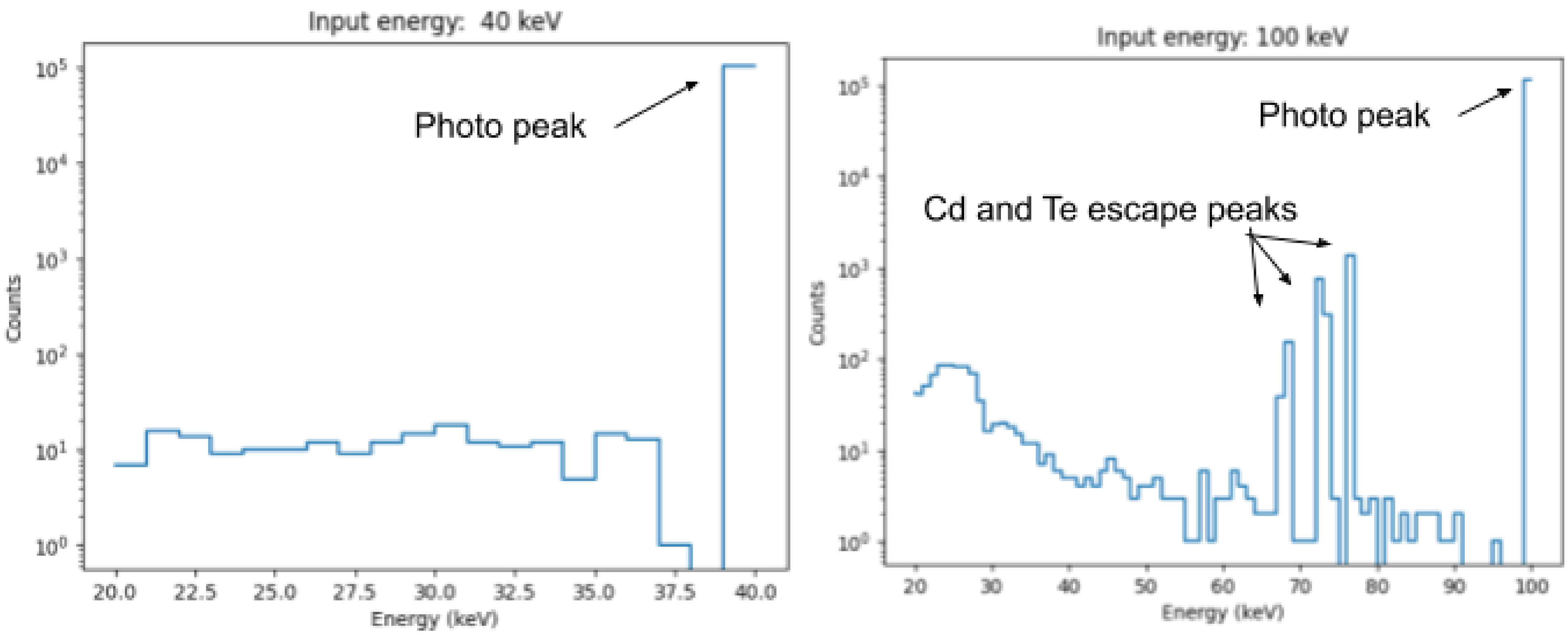
- **Hint 1:** In SD, one can access energy deposition positions with G4Step and G4PreStepPoint classes.
- **Hint 2:** Create separate hits (total 256) to store energy deposition of each pixel.
- The pixel orientation should look like the figure below:



b) Modify the SD, EventAction and RunAction such that the code stores the output as an "event" in a root or txt file. The output file should have following information for each event:

- eventID, pixID, total energy deposition (totalEdep)

c) Run a few simulations for different input energies (e.g. 40 keV, 100 keV, 150 keV) and study the detected spectra. To plot the detected spectra, only use the events where energy deposition has happened in one pixel. These are called "single events" and are most commonly used for X-ray spectroscopy. Detected spectra for two energies is shown below:



4) Verifying spectra response of the CZT detectors:

a) Simulate a power-law spectrum in GEANT4 with the following parameters:

- power-law norm = 2 ph/cm2/keV/s
- photon index (alpha) = -1
- Incident area = 3.9392 cm2 (crystal area)
- Duration = 1000 s

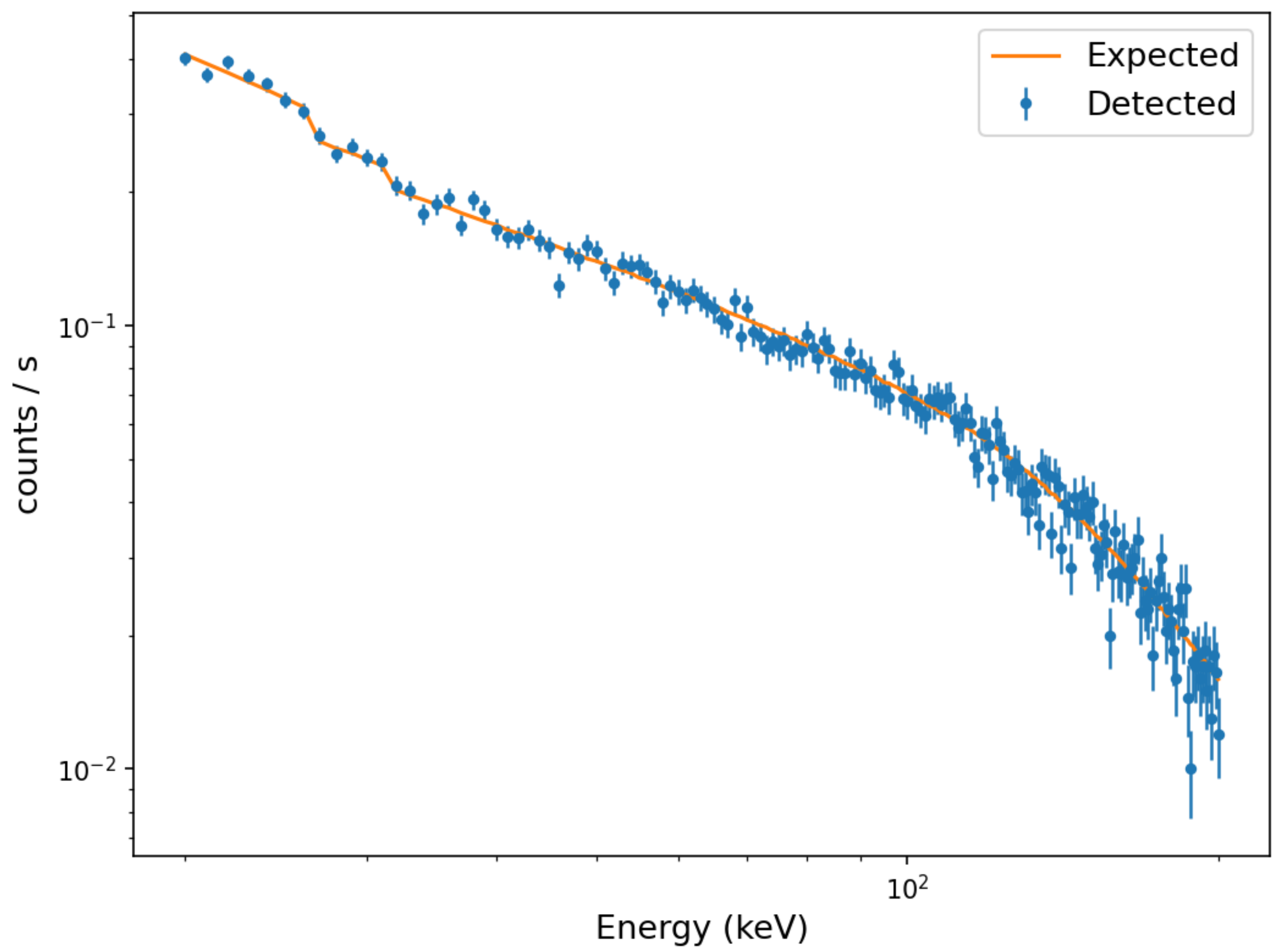
A power-law spectrum can be directly simulated using the GeneralParticleSource, refer to the GPS documentation to know how to simulate power-law. Use emin and emax to be 10 and 210, the total number of photons to simulate corresponding to above parameters are 94332.

b) From this simulation, find out the detected spectra in 1 keV bins.

c) Compare the detected spectra (for single pixel events) with the expected spectra obtained from the pre-computed response matrix (***rsp/rsp_mat_no_mask.npz***)

- **Hint**: You will need to load the matrix into a python code and convolve it with a power-law input spectra with parameters given above (for more info refer to Gulab Dewangan's talk).
- The **.npz** file has three arrays with keywords **ebins_in** (input energy bins), **ebins_out** (output energy bins) and **matrix** (the 2D response matrix)

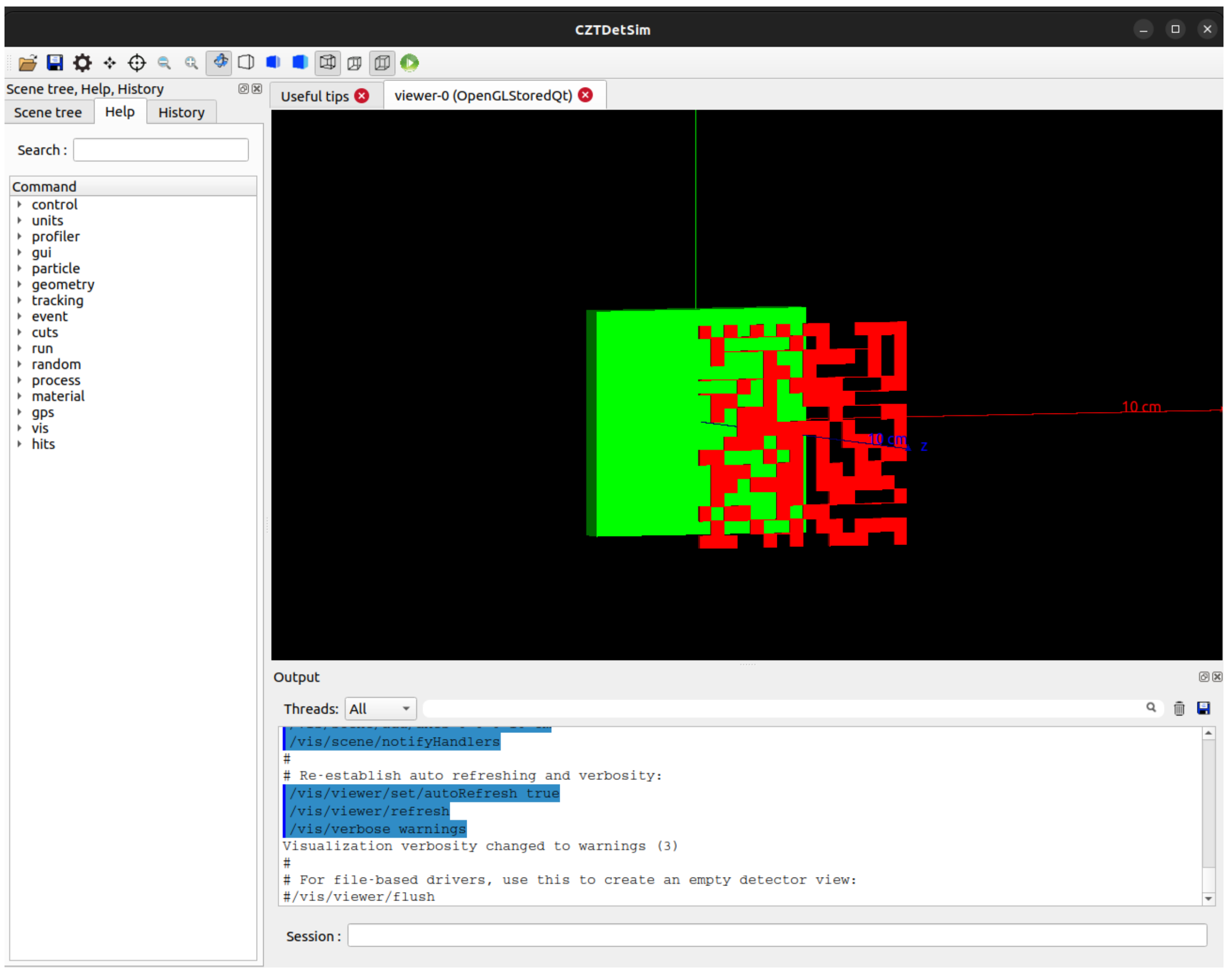
d) The detected and expected spectra should look like the plot below:



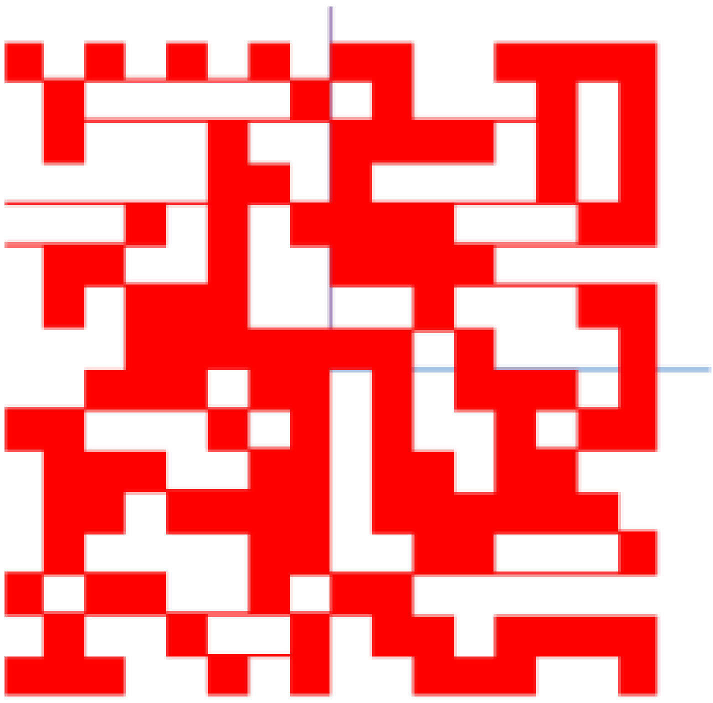
5) Importing complex geometry:

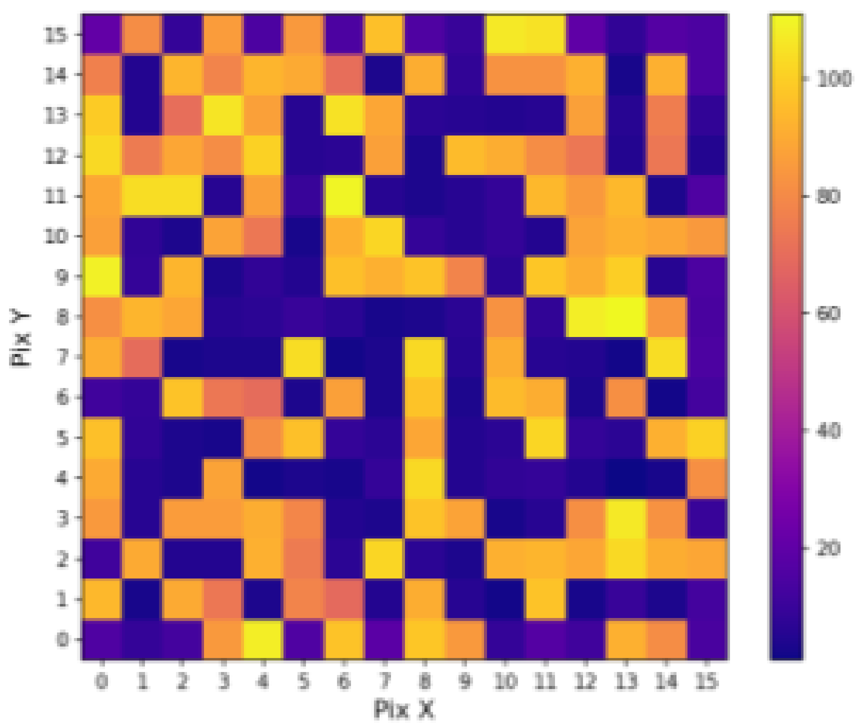
As mentioned before, pixelated CZT detectors can be used for hard X-ray imaging. Often such imaging is done by putting a coded aperture mask in-from the pixelated detector. The mask has a unique pattern of opaque and transparent elements. These elements cast a unique shadow onto the detector plane for different directions in the sky. Knowing the pattern the shadows can be back projected to find the position of the source. Since the mask pattern is often complicated, it is easier to import it using GDML or CAD format file instead of coding it in detector construction. Here we will learn how to import complex geometry using GDML, how the mask casts shadow onto the detector plane and replicates the complement of the pattern and also how mask response changes with energy.

a) Import the coded mask using GDML import or CADmesh library and place it 5 cm above the origin.
b) The resulting geometries should look like the figure below:



c) Simulate mono-energy photons at energies 40, 60, 100, 140 and 180 keV and plot the detector plane histogram (DPH), i.e. total counts in each pixel, by selecting only single pixel events. The mask pattern (as seen from top) and DPH for 60 keV should look as shown below:





d) **Optional 1:** Plot the detected spectra and see if Tantalum fluorescence lines can be seen.
e) **Optional 2**: Repeat the power-law simulation with photons incident through the mask and compare the detected spectra with response matrix generated using the mask (***rsp/rsp_mat_mask.npz***)

6) Response of CZT detectors for charged particles:

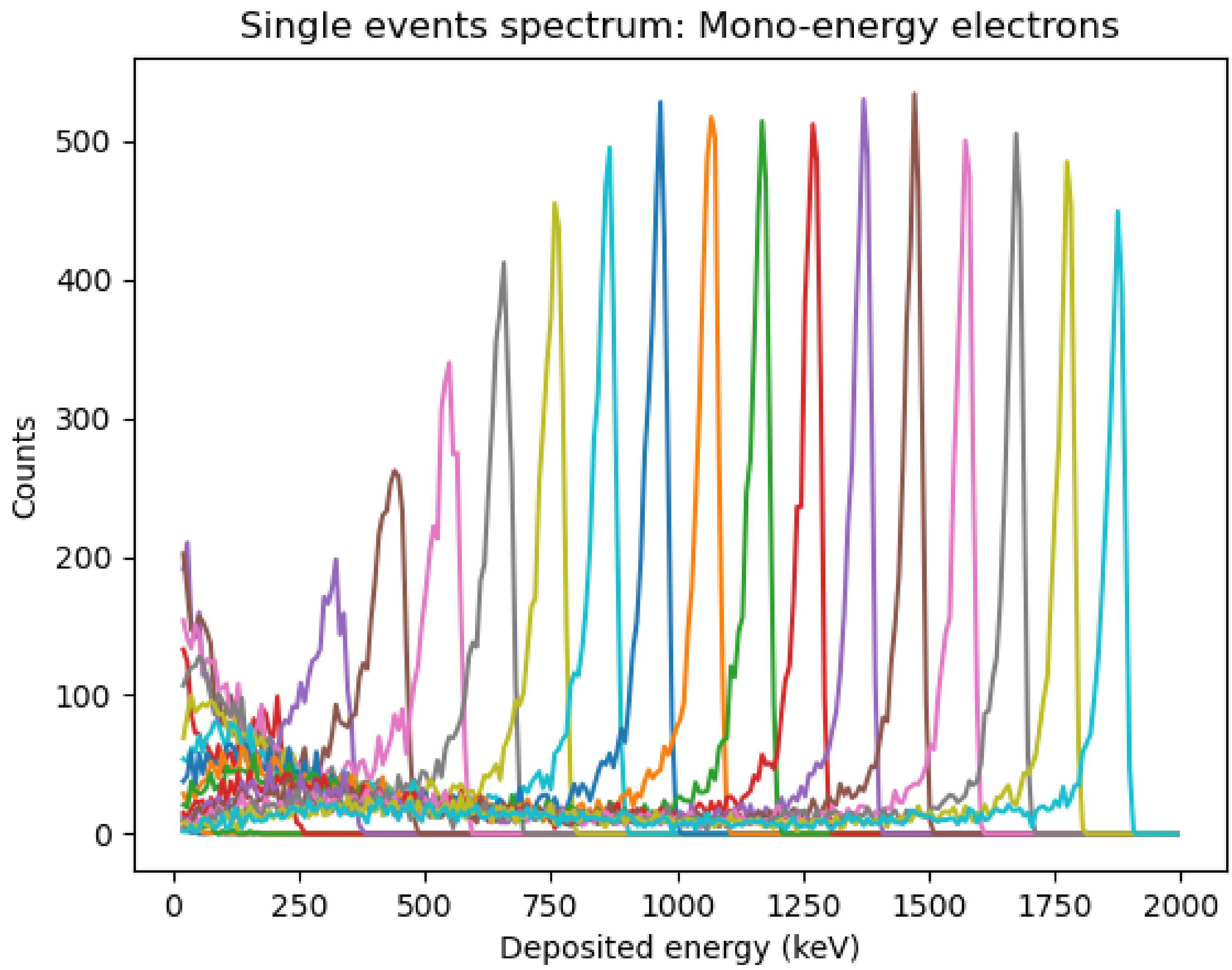
a) Repeat exercise 2 (e), 3 (c), and 4 for electrons and compare the spectra with the ones obtained for photons

Charged particles in space are another type of ionising radiation that can be detected in the detectors. These often tend to form the background counts in the observed spectrum. Thus, understanding their efficiency and spectral distribution is relevant for background modelling for X-ray spectrometers/polarimeters.

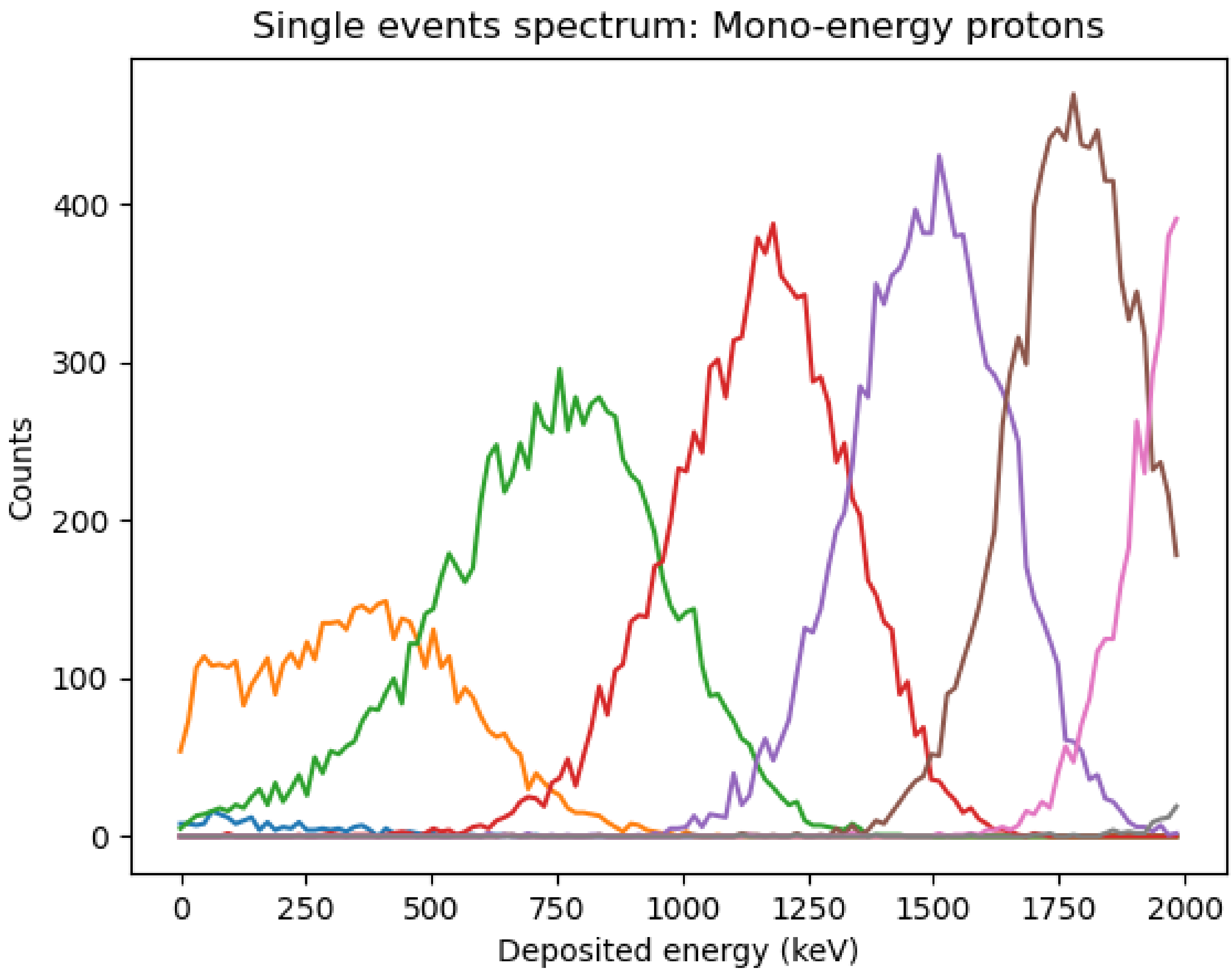
a) If the energy range of interest for an instrument with CZT detectors is X-rays in 20 – 500 keV(say), then find out:
   i) The energy range of charged particles that can be detected in the CZT. Consider electrons and protons with normal incidence.

      Hint : Start with the low limit end of the energy and increase the incident energy, to check if there are any events detected in the CZT. If dead-layers of the CZT are added, then the sensitive energy range of particles gets pushed to higher energies.

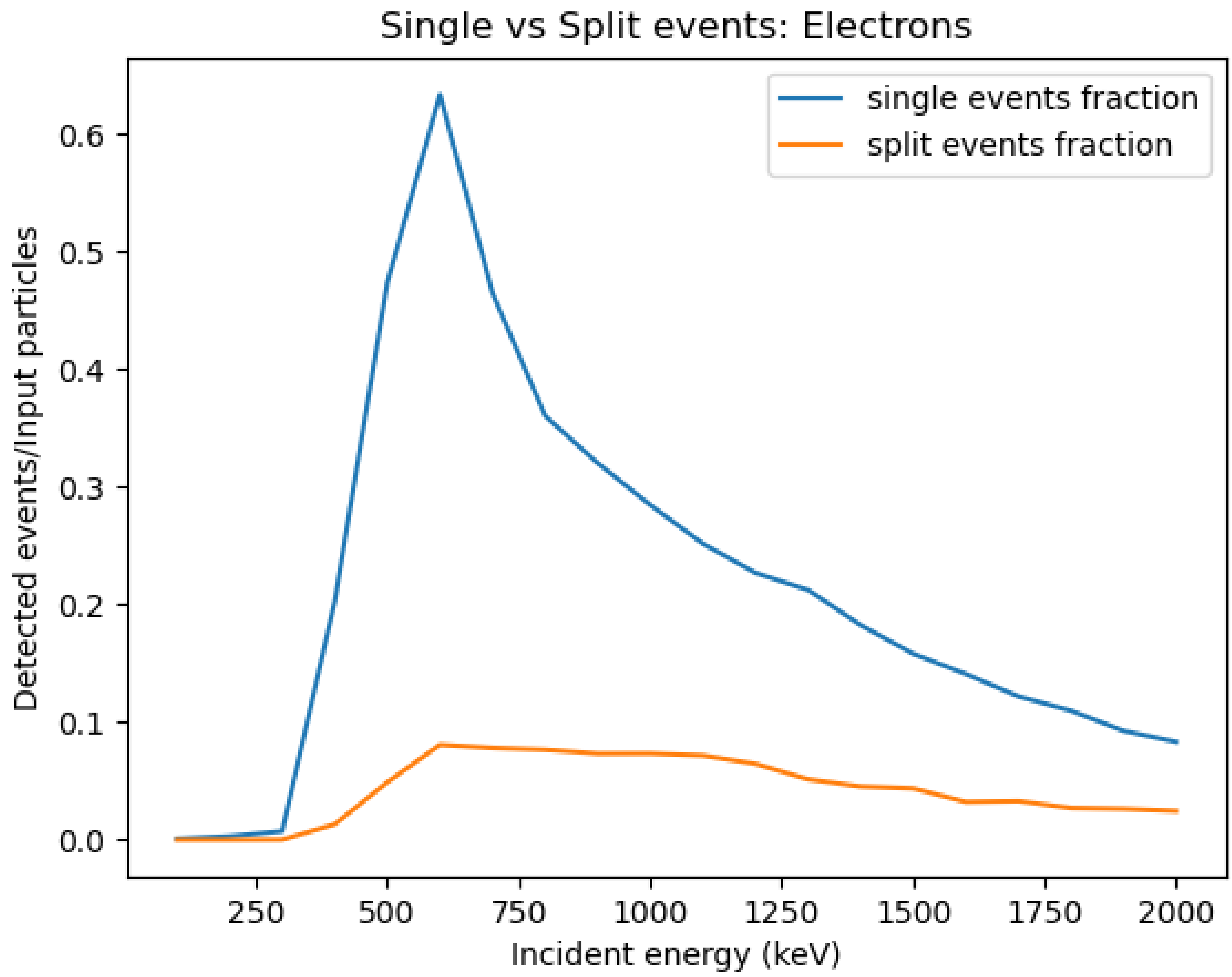
   ii) How does their interaction efficiency compare with the QE of X-rays in CZT.
      Note: In-situ particle flux in space can be many orders higher than an astronomical source flux. So, even particle energies with low detection efficiency can affect the observed spectrum.
   iii) Find out the ratio of single events spectra for particles and compare that with photons.



The above figure shows the energy deposition distribution due to mono-energetic electrons normally incident onto CZT , with energies from 100 to 2000 keV in steps of 100 keV.



The above figure shows the energy deposition distribution due to mono-energetic protons normally incident onto CZT , with energies from 6500 to 7200 keV in steps of 100 keV.



The above figure shows the efficiency fraction of single events vs incident energy for electrons , in the energy band of 20 - 500keV; split events' fraction vs incident energy is also plotted.