X-ray Fluorescence imaging simulation

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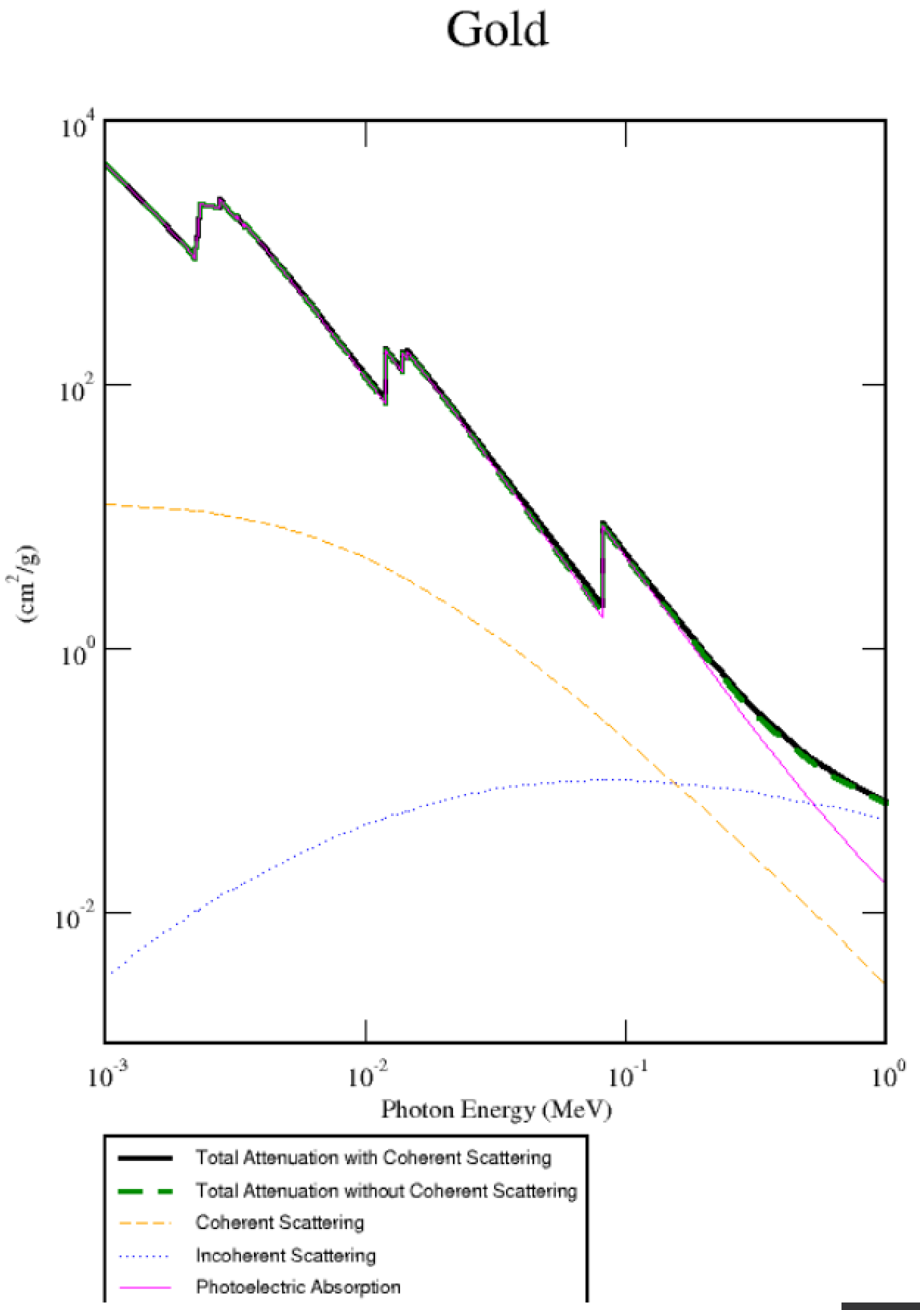
XRF as imaging technique

- fluorecsence source: non-toxic molecules with heavy element – eg. gold – GNP (Golden Nano-Particles)
- irradiating body part with diagnostic photons
  - rtg beam
  - laser beam
  - synchrotron (not useful in cliniclal environment)
- ***signal***: fluorescence photon yield as consequence of photoeffect on target – Au atoms
- ***noise/background:*** mostly Compton photons from scattering in tissue
- ***reducting noise/SNR:*** angle of detection relative to the rtg beam direction, enabling energy measurement with good energy resolution

Gold as fluorescence source

- 79-Au
- GNP – Golden Nano-Particles
- **high attenuation coefficient for photoeffect**, which is dominant over Compton scattering up to ~500 keV
- **high fluorescence yield** after photoeffect (over 90%)
- **K-emmision lines energies**
  - K-alfa: 67 and 69 keV; edge at 70
  - K-beta: 77. and 78; edge at 80 keV
  - → sets minimal source photon energy
- tissue – low Z numbers – Compton much more probale that photoeffect → source of imaging noise/background + dose on patient



Simulation methods

- **Geant4 toolkit** (C++, using standard classes for simulations)
- **simulation code** on GitLab: https://repo.ijs.si/studen/xrf
  - master branch – original code by Kunal Kumar
  - xrf branch – adjusted and developing code; joint work by Andrej Studen and Matevž Hudovernik
- **beam source and geometry setup**
  - GPS – monochromatic/rtg spectrum photons and pencil beam
    - circle area with radius 0.16 mm
    - divergence 1°
  - breast tissue (half cylinder/cone) – diameter 10cm and thickness of 2cm
  - „target with Au" in the „center" of tissue - sphere with radius 5 mm; wt of 2% gold absorbers
- **detector** – plane-shaped, 100% silicon
    - ***thickness***: 2 mm
    - 120 mm x 80 mm x 2 mm (could be reduced to Volume Of Interest, especially directly under the target, eg. 20 mm x 20 mm x 2 mm)
    - 0.1mm air gap between tissue and detector (target isocenter to detector – 1 cm)
    - **position**: under the tissue – perpendicular to source beam – minimum of Compton differential cross-section at energies around 100 keV - fluorescence yield is isotropic [IMAGE]
    - voxels/pixels: 36x36 μm^2 (x 0.5 mm in z axis)

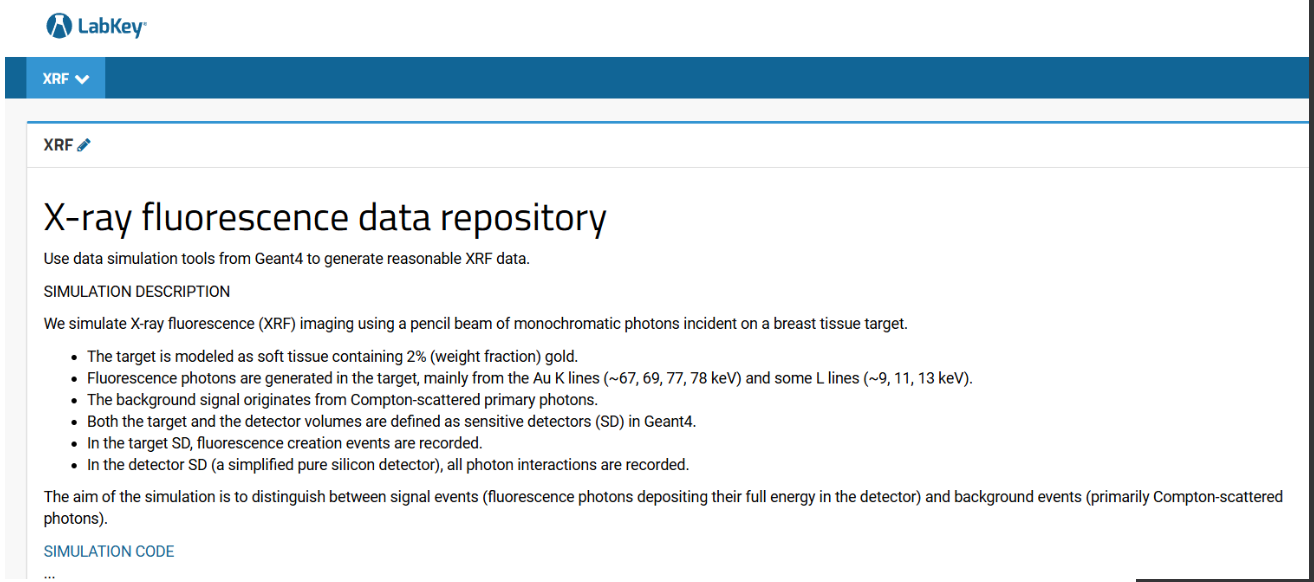
Simulation outputs

- **tracking interactions**
  - a) ***in target***: photoeffect on 79Au, followed by fluorescence photon radiation in target
  - b**) *in detector***: energy deposition in voxels
    - <u>fluorescence photons </u>– contribute to signal, but only K-lines with total energy deposition
    - <u>Compton photons </u>– scattered off tissue –noise – need of precise energy meausremets of detected photons

- data saved as text files
  - one line = one interaction step with energy deposition or fluorescence photon creation
  - **tallies**: eid (event identity), tid (track id), pid (parent id), interaction type, interaction location, energy deposited, particle type (photon or electron), …

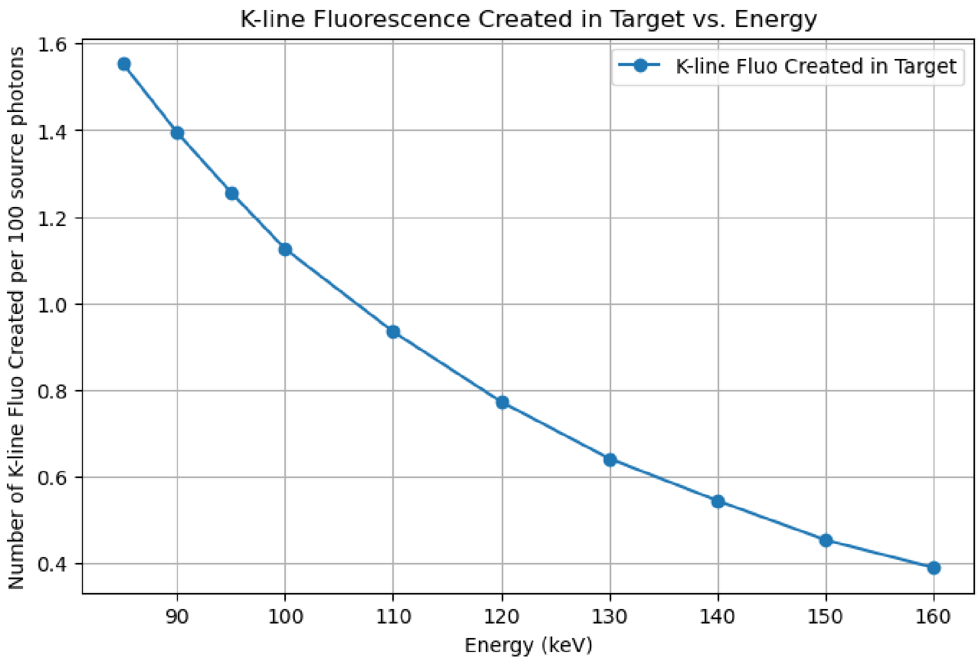
Data processing and storing

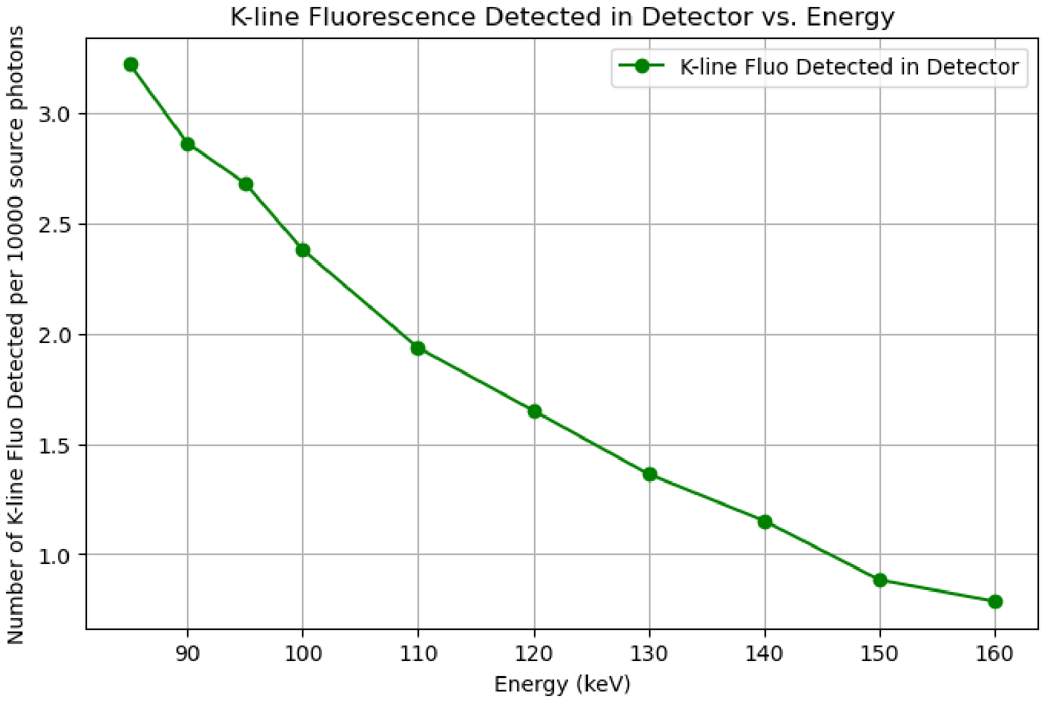
- LabKey website:
  - →https://labkey-klimt.fmf.uni-lj.si/labkey/XRF/project-begin.view [access with account?]
- stores semi-processed simulation data
- description of simulation setup/geometry
- links to GitHub data processing repository



XRF simulation statistics

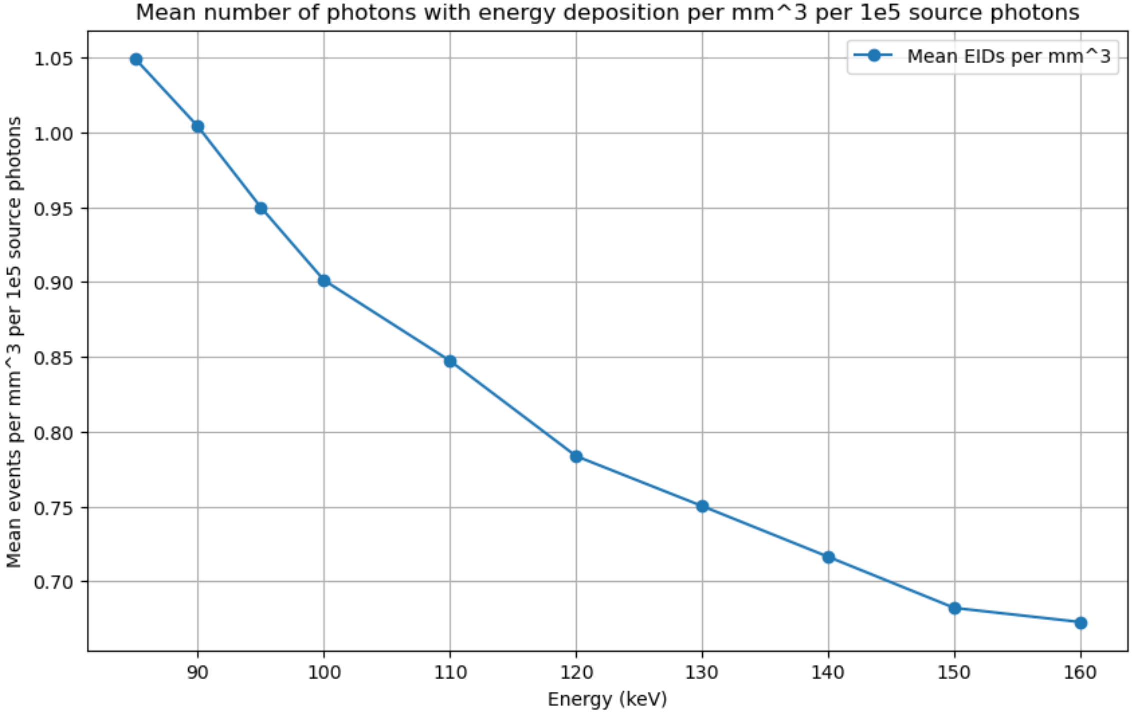
- How many K-line photons do we get?
- How many of those are detected with full energy deposition (signal contribution)?
- How many total photons do we detect?

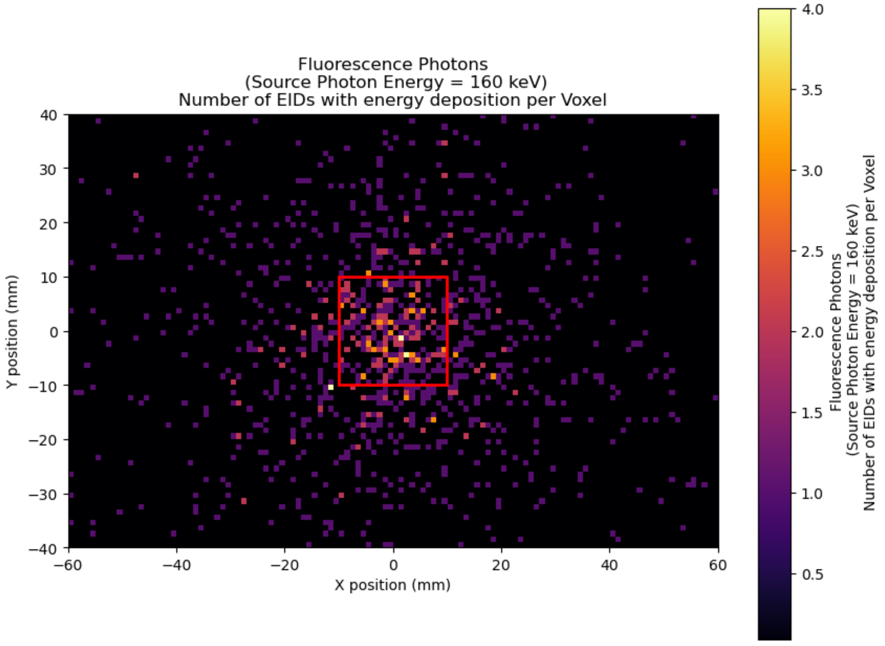


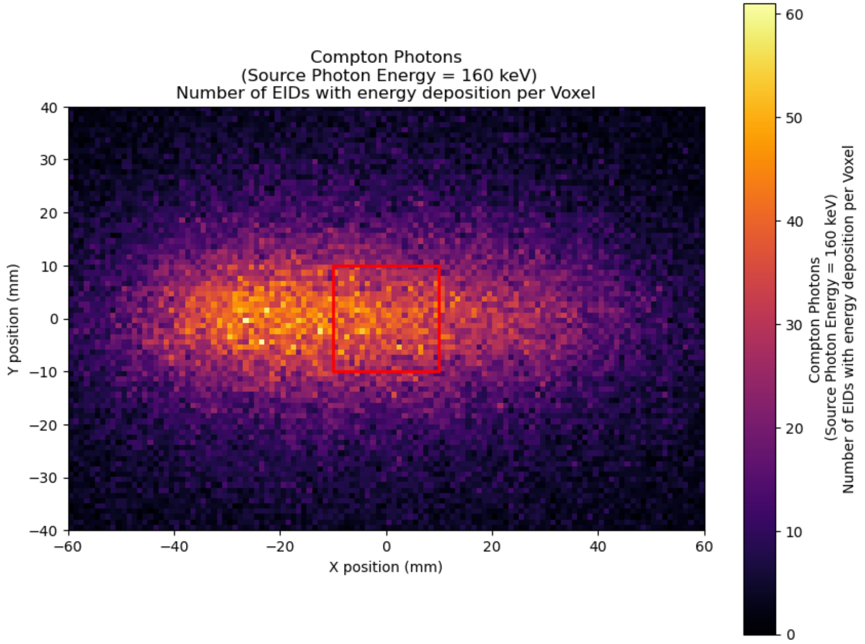


Interaction Rates and Detector Occupancy

- How many photons hit detector per detector volume?
- reminder – in simulation, detector is pure and continous silicon layer
- region of interest: 20x20 mm^2 area around center directly below target (red square on right graphs)

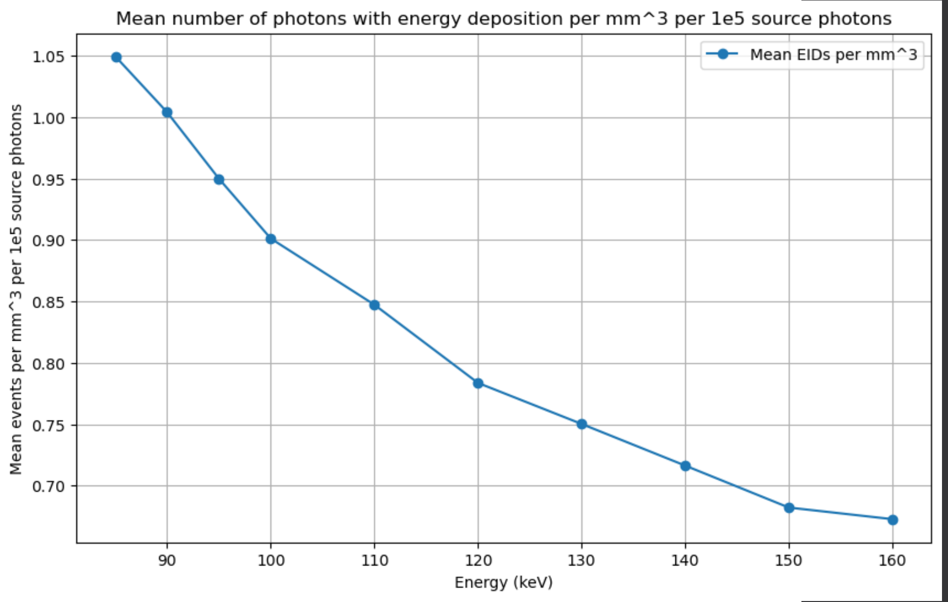




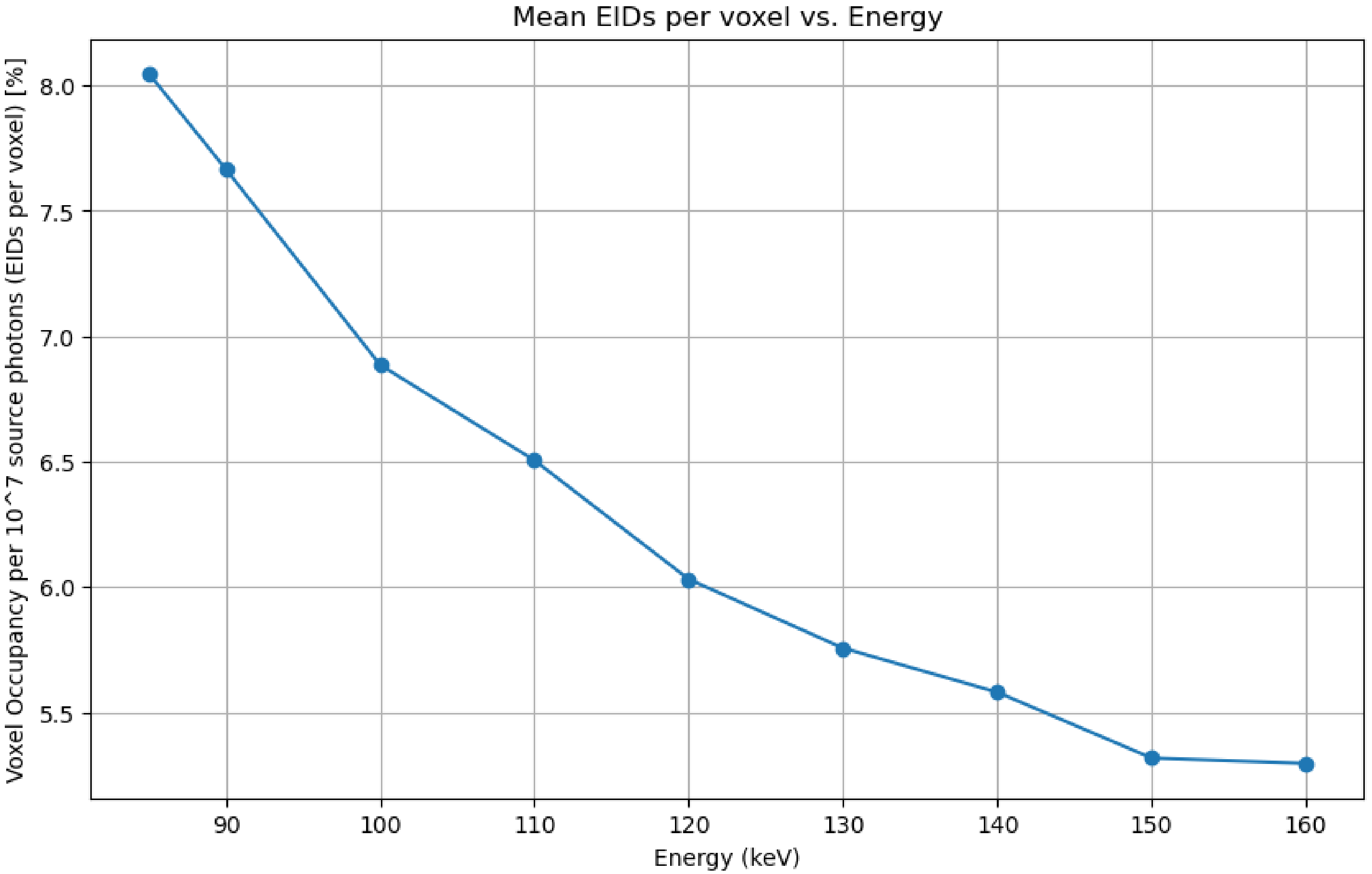


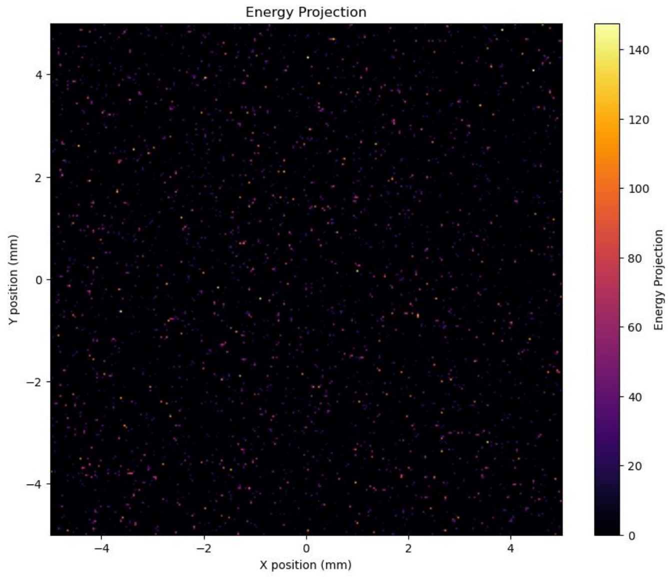
Interaction Rates and Detector Occupancy

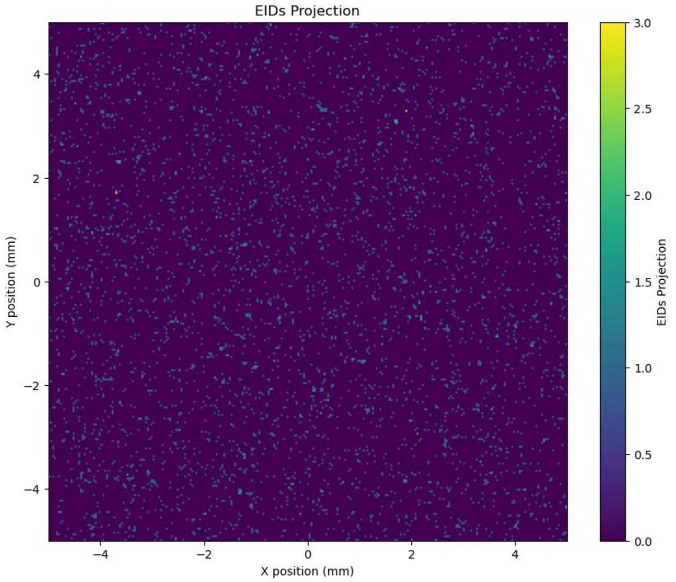
- idea/demand – avoiding pile-ups (occupany 10-20% ?)
- ***PO = dNevts/dV * V_de * SPF * t***
- PO = pixel occupancy (relative number of pixels with a hit)
- dNevts/dV – number of events (source photons that cause energy detection) per volume in detector – „detection/hits density“
- V_de – volume of one detector element
- SPF – source photons (rtg) flux [number of source photons per time unit]
- t – time (***SPF*t gives total number of source photons during imaging***)
- ***simulation results*** – approximately **dNevts/dV ~ 1 /mm^3/10^5** (one hit per 1mm^3 of detector per 10^5 source photons) – look at the graph. Things to consider:
  - descenting trend of Nevts with rising energy
  - this number is strictly related to simulation parameters (like target size, setup geometry, Au concentration of 2% in target ect…)



Interaction Rates and Detector Occupancy

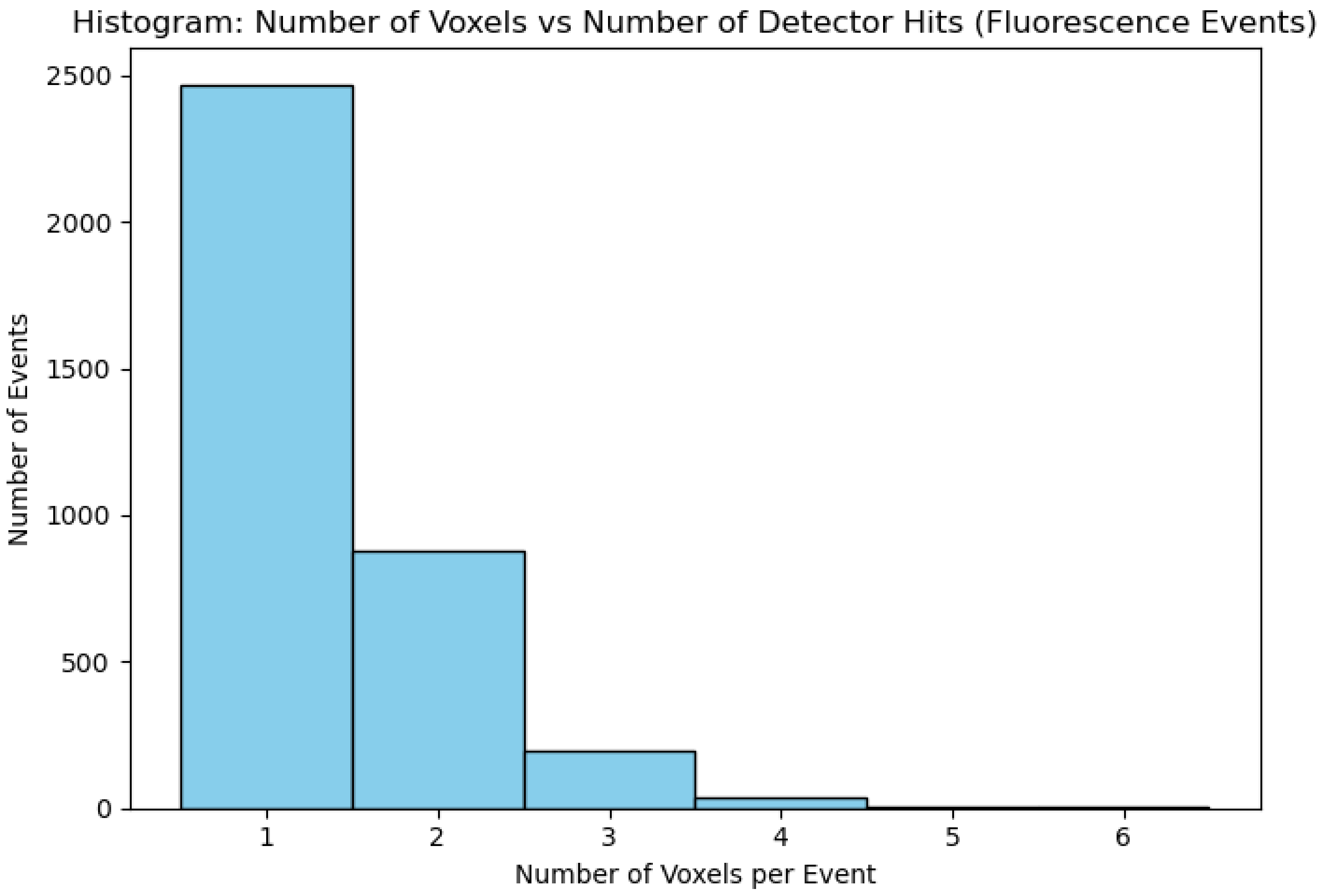






Signal Clustering

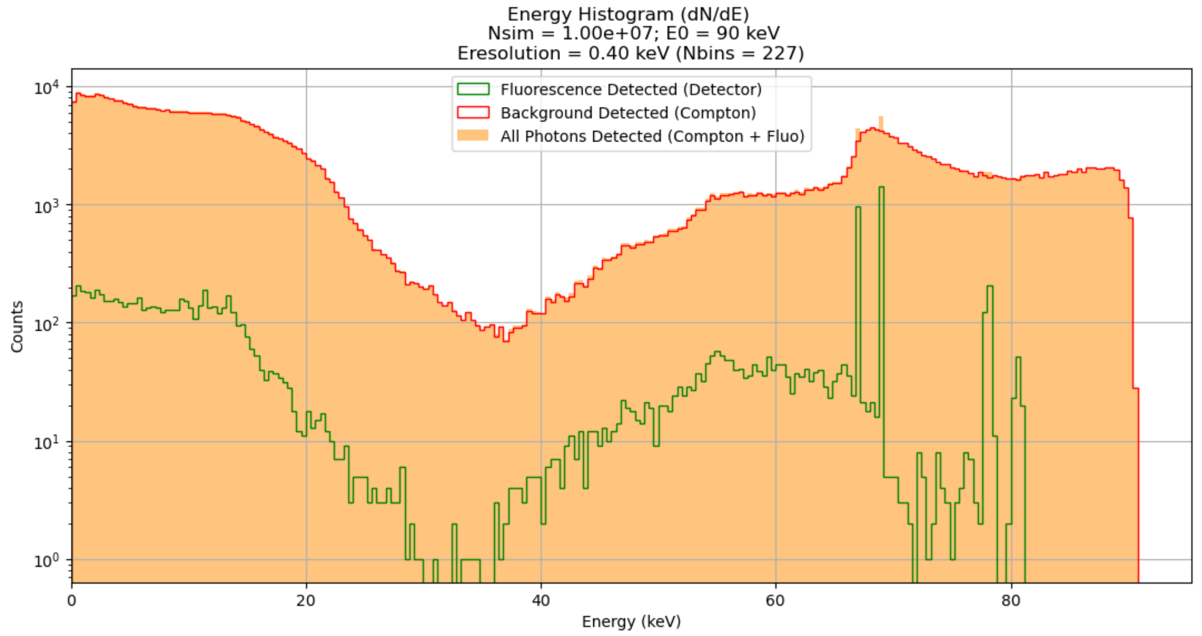
- E_gps = 150 keV

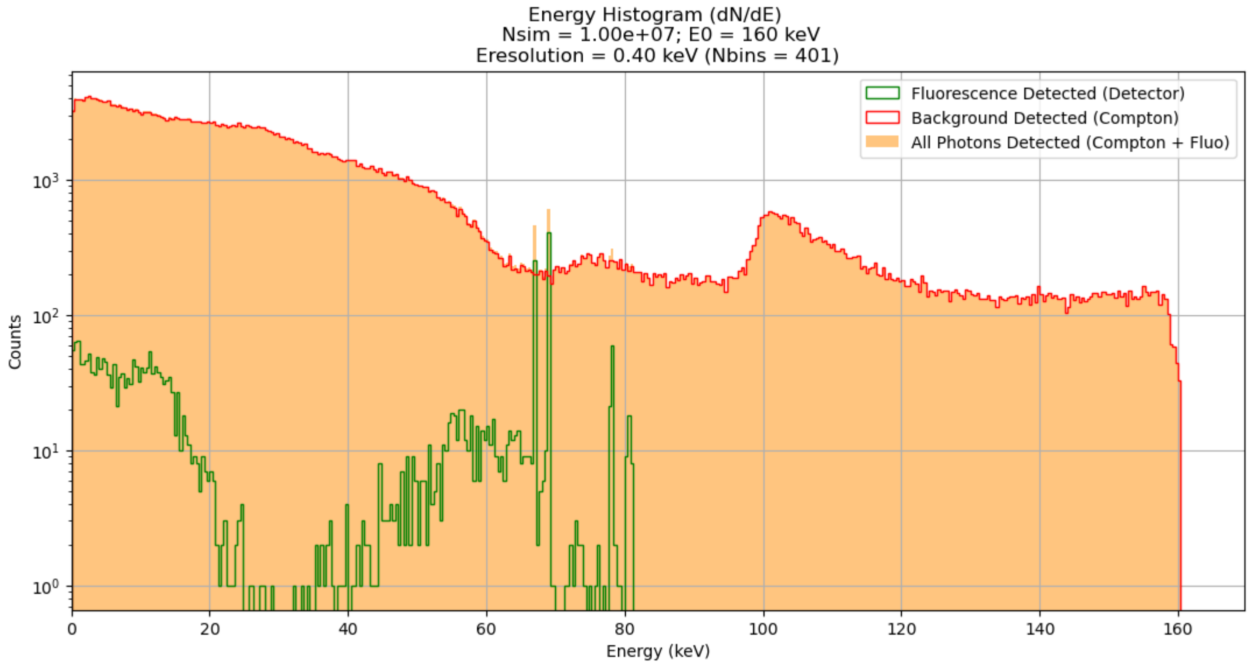


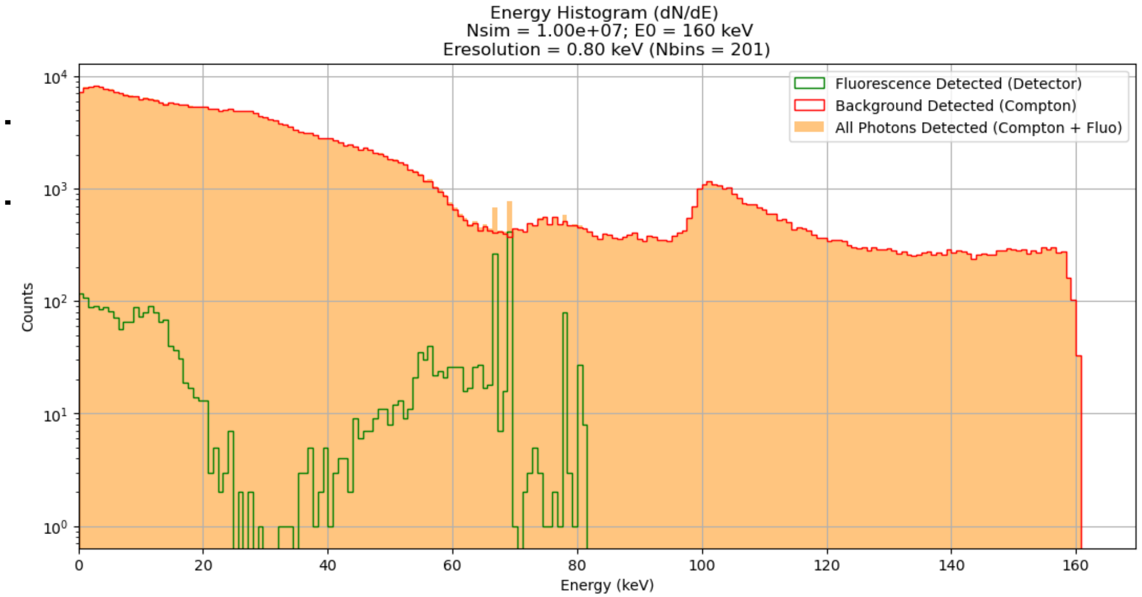
Energies of Detected Photons and Energy Resolution of Detector

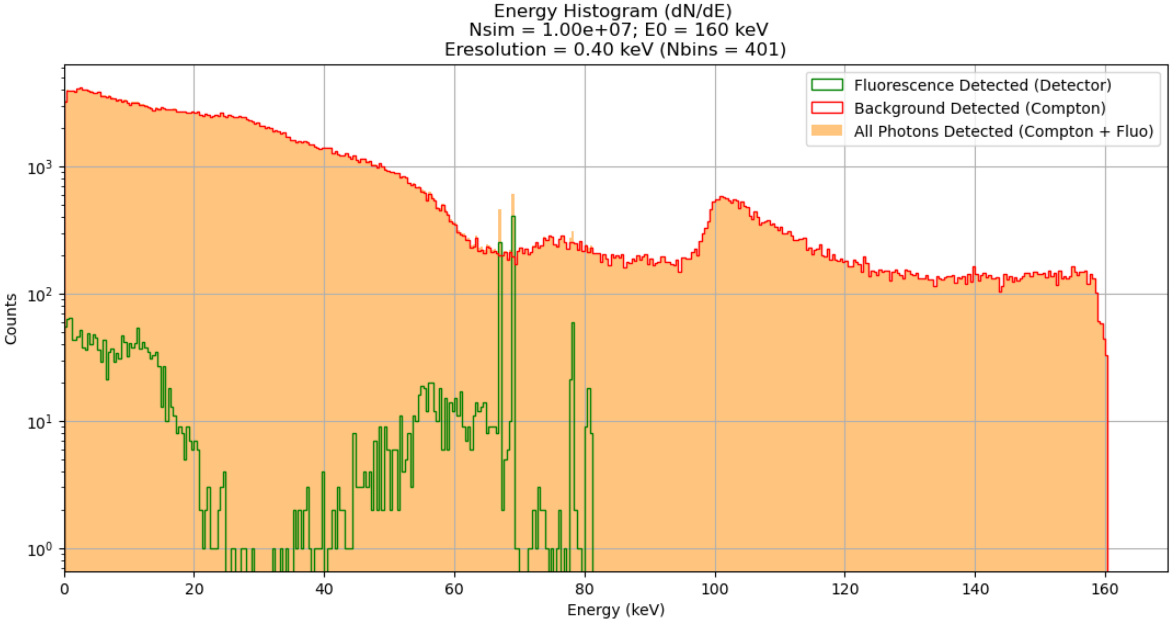
- standard deviation of energy detection = 100 eV ?
- energy resolution ~ 0.4 keV ?
- optimal source photon energy ? (vs. real rtg energy spectrum)

Energy (keV)	Created	Detected	Full Energy Detected
67.184	11453	924	263
69.038	19315	1529	410
77.8157	2035	157	18
78.226	4191	287	59
78.6593	46	3	1
78.7478	62	6	0
80.3237	531	33	9
80.4226	976	70	18
80.6065	12	3	0
80.6249	13	2	0
80.8814	138	12	2
80.8986	221	14	6
80.9495	1	0	0
Total	38994	3040	786






Energy Histogram (dN/dE)
Nsim = 1.00e+07; E0 = 160 keV
Eresolution = 0.80 keV (Nbins = 201)
Fluorescence Detected (Detector)
Background Detected (Compton)
All Photons Detected (Compton + Fluo)
Counts
Energy (keV)


Energy Histogram (dN/dE)
Nsim = 1.00e+07; E0 = 160 keV
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Fluorescence Detected (Detector)
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Counts
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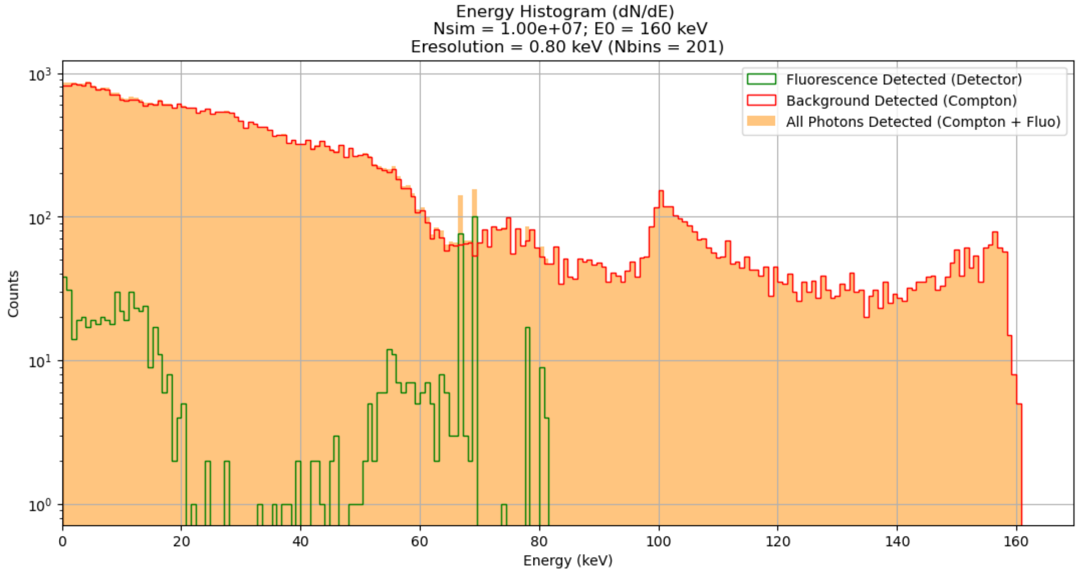
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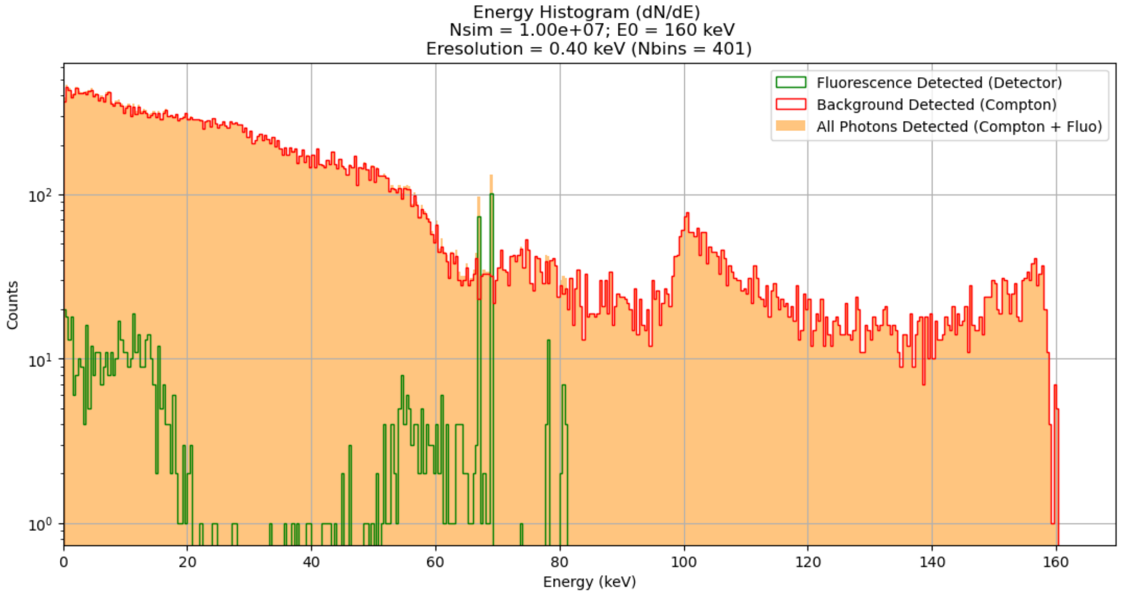
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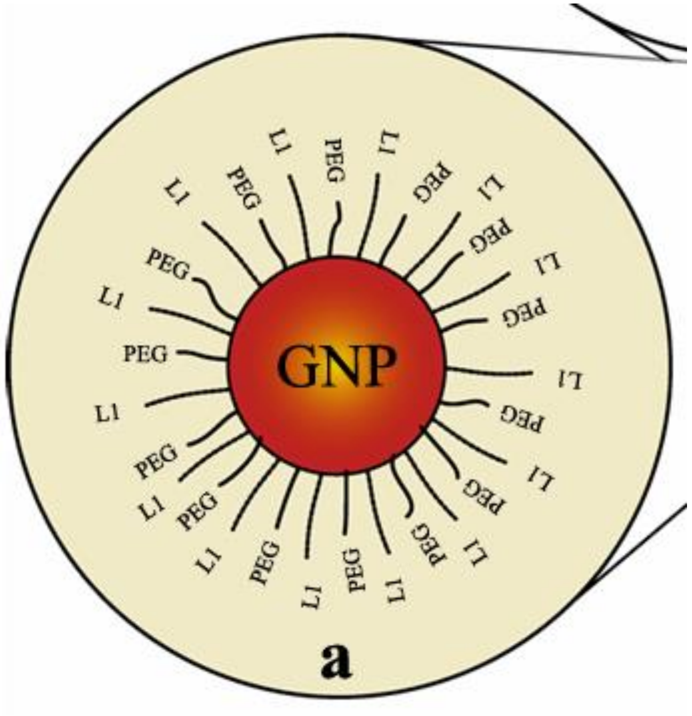
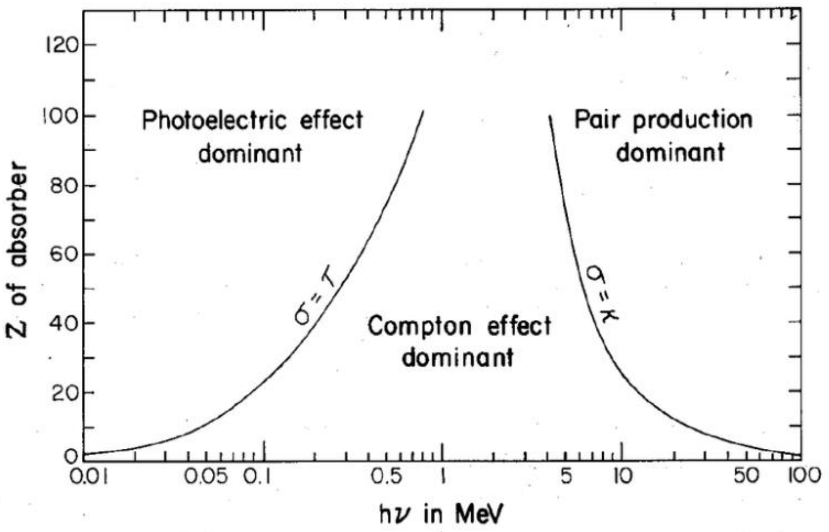
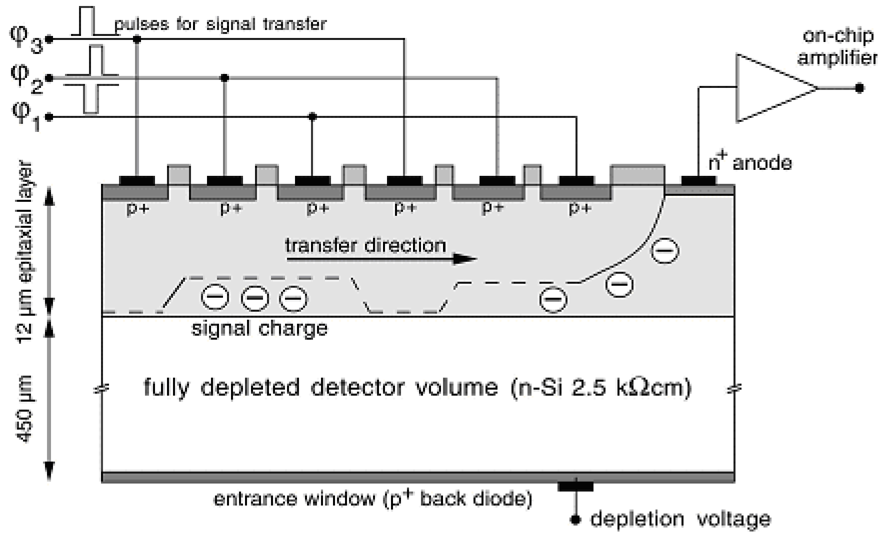
SNR – Singal-To-Noise Ratio

- SNR as function of energy resolution
- …

Thank you!


GNP
PEG
L1
a


Photoelectric effect dominant
Pair production dominant
Compton effect dominant
$\sigma = \tau$
$\sigma = \kappa$
Z of absorber
$h\nu$ in MeV
0
20
40
60
80
100
120
0.01
0.05
0.1
0.5
1
5
10
50
100


pulses for signal transfer
φ_3
φ_2
φ_1
on-chip amplifier
n^+ anode
p+
transfer direction
signal charge
12 µm epitaxial layer
450 µm
fully depleted detector volume (n-Si 2.5 kΩcm)
entrance window (p^+ back diode)
depletion voltage