Fluorescence & PIXE models in GEANT4

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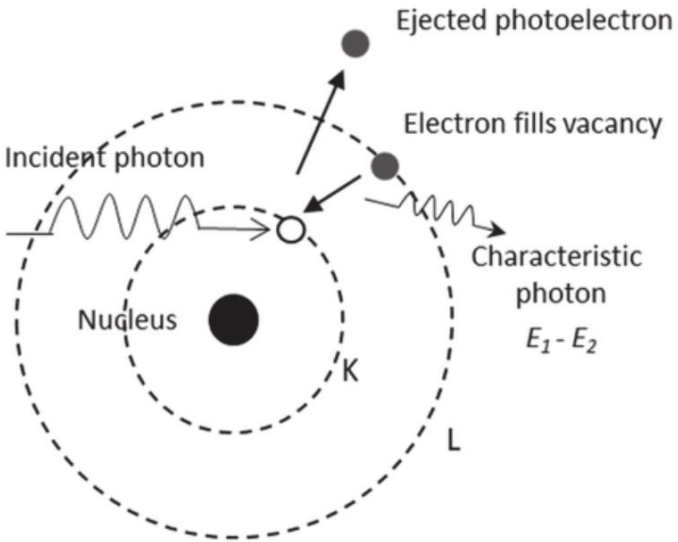
GEANT4 models: Atomic de-excitation

- Activated for process
  - Photoelectric effect
  - Ionization
  - Compton scattering
- Available for some physics packages:
  - Livermore
  - Penelope
  - Standard Electromagnetic
  - GEANT4-DNA

GEANT4 models: Atomic de-excitation

- Simulation of atomic relaxation GEANT4
  - Creation of a vacancy by a primary process, handled by any GEANT4 Electromagnetic Physics Package (like Livermore or Penelope)
    - manage the primary interaction, photoelectric, Compton scattering and ionization
  - Generation of the relaxation cascade, handled by the Atomic Relaxation Package
    - secondaries are then passed to GEANT4 tracking and manage as any other particle in the simulation



Atomic Relaxation Options in GEANT4:

- Fluorescence
    - Activated by default in G4EmLivermore, G4EmLivermorePolarized and G4EmPenelope
- PIXE
- Auger
- The library used in GEANT4 to provide the binding energy and the radiative (fluorescence) and non-radiative (Auger and Coster-Kronig electrons) transition probabilities is Evaluated Atom Data Library, EADL (https://www.iaea.org/resources/databases/evaluated-nuclear-data-file)

Fluorescence

- Lines data set
  - Default
    - binding energies & radiative transitions probabilities from EADL
  - Bearden data
    - binding energy from EADL, radiative transitions probabilities from Bearden (1967)
  - XDB (X-ray Data Booklet) (https://xdb.lbl.gov/)
    - XDB & EADL for binding energies, EADL for radiative transitions probabilities
  - ANSTO
    - binding energies from EADL, radiative transitions probabilities from library developed by the Australian Nuclear Science and Technology Organisation (ANSTO)

PIXE

- Cross section model
  - Shell ionization
    - Empirical, empirical and semi-empirical compilations from Paul et al (K-shell) and Orlic et al (L-shell)
    - ECPSSR_Analytical, ECPSSR theory for K-shell and L-shell
    - ECPSSR_FormFactor, an empirical polynomial approximation
      - Taborda et al, X-ray Spectrometry 40, 3, 2011 (https://doi.org/10.1002/xrs.1305)
      - Taborda et al, X-ray Spectrometry 42, 4, 2013 (https://doi.org/10.1002/xrs.2483)
    - ECPSSR_ANSTO, theoretical work from Brandt and Lapicki (ECPSSR)
  - For electrons (needed only for simulations that use continuous ionization process)
    - Livermore
    - Penelope

GEANT4 PIXE Empirical and Analytical cross section sets only generate K and L vacancies

PIXE ANSTO

- ANSTO uses Hartree-Fock while EADL uses Hartree-Slater
  - HF better PIXE experimental values than HS
- ANSTO and EADL equivalent results for the K and L shells, but there are differences at M shell

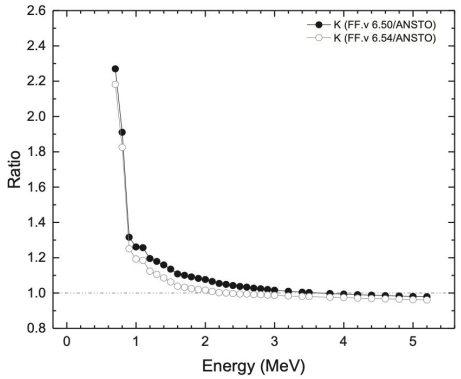


Fig. 6a. K shell ionisation cross section ratios for protons incident on a gold target.

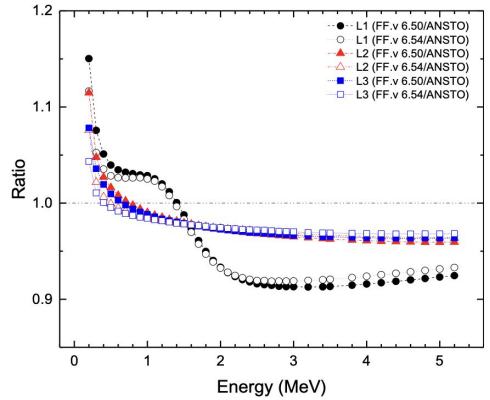


Fig. 6b. L subshells ionisation cross section ratios for protons incident on a gold target.

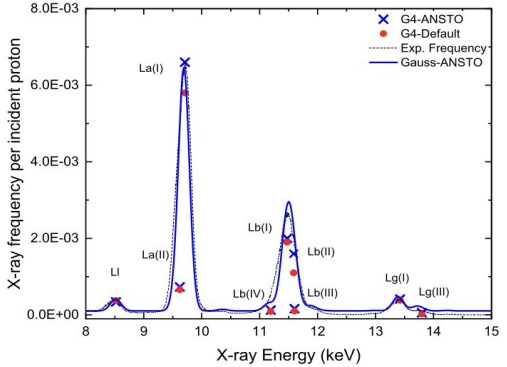


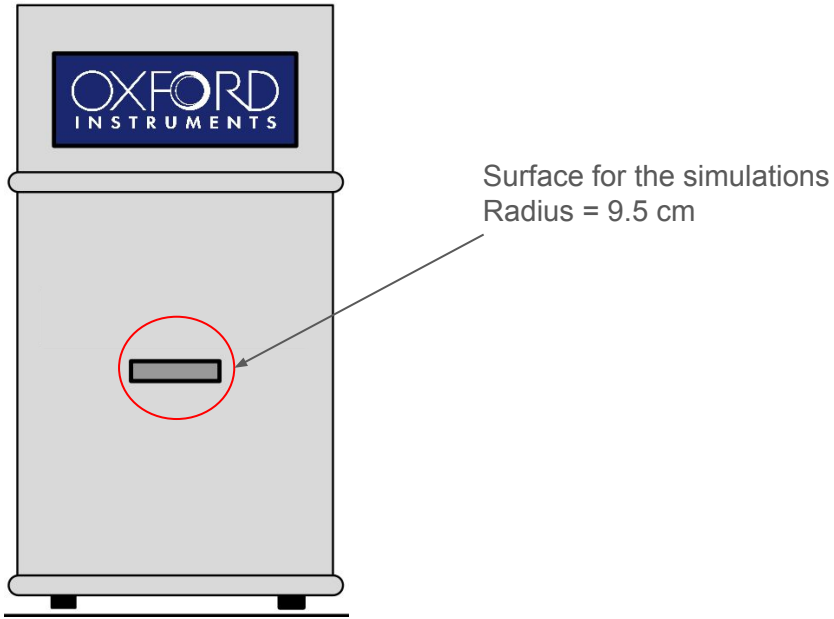
Fig. 7c. X-ray emission generated by 3 MeV incident protons on a gold target, Z = 79.

EMLOW 6.50 en Geant4 10.3
EMLOW 6.54 en Genat4 10.4 beta

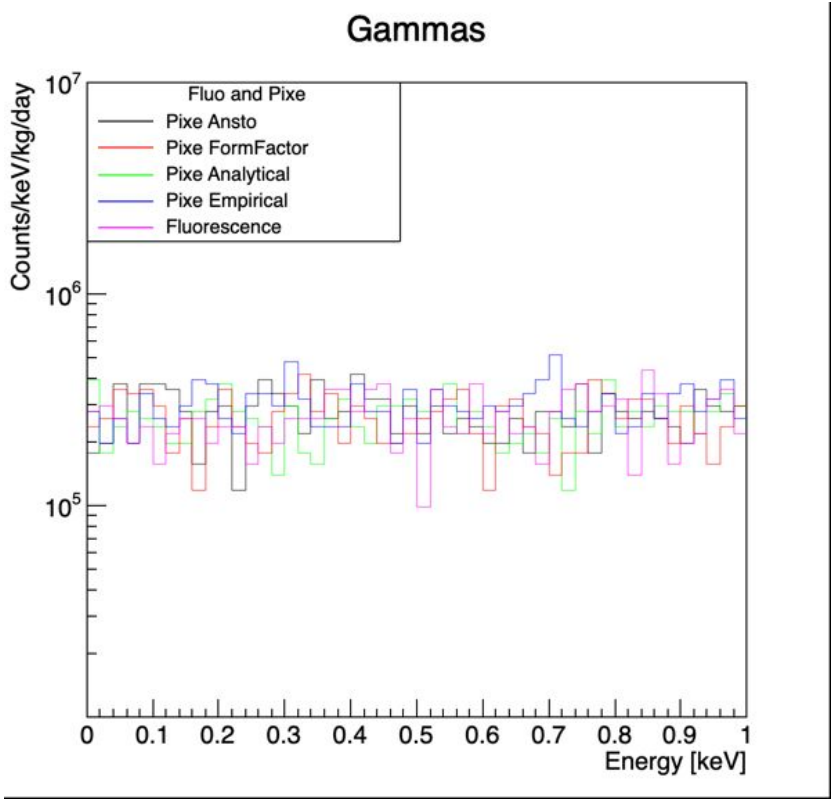
Bakr S., et al NIM-B, 507 2021 (https://doi.org/10.1016/j.nimb.2021.09.009)
Bakr S., et al NIM-B, 532 2022 (https://doi.org/10.1016/j.nimb.2022.10.010)

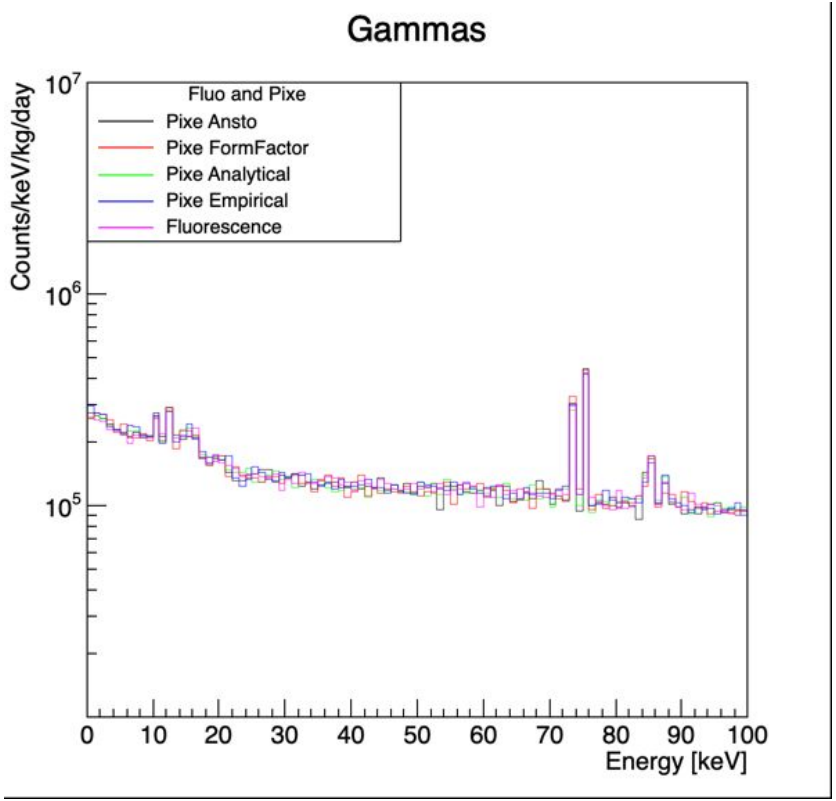
Simulations for BULLKID (Sapienza)

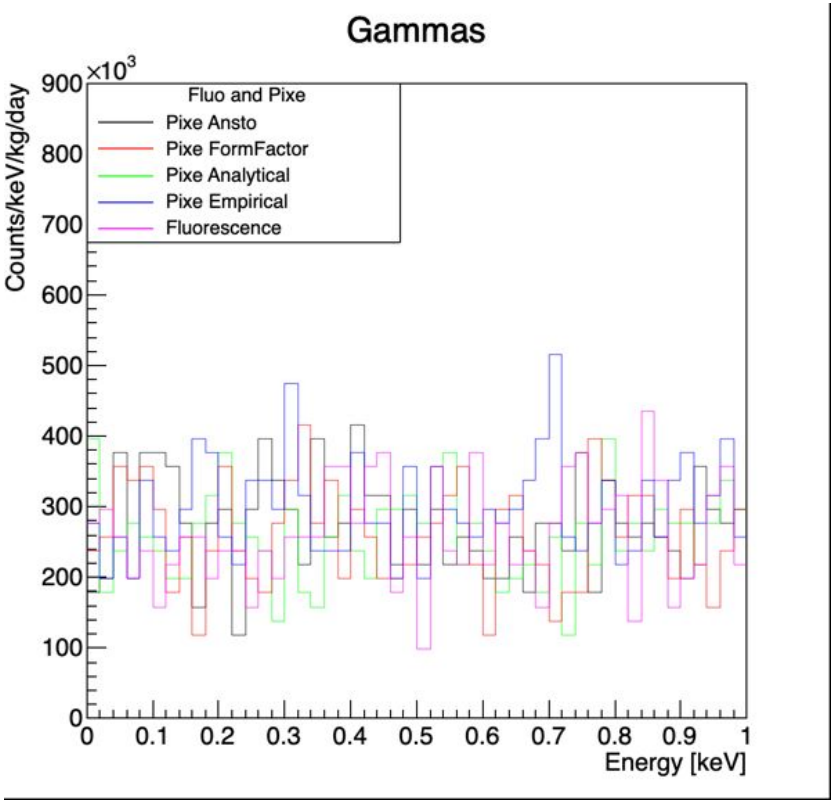
- To analyze the different PIXE models and the Fluorescence model for BULLKID at Sapienza
  - Gamma spectrum simulated inside the cryostat for each model
  - Considered gamma flux at Sapienza 13.47 $\gamma cm^{-2}s^{-1}$

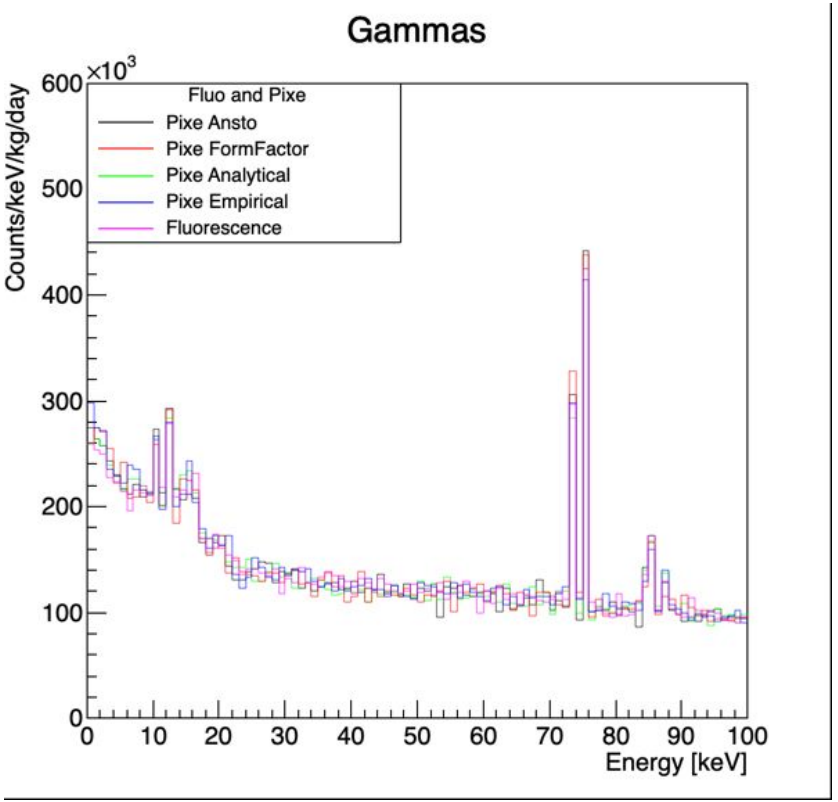


Simulations for BULLKID, G4EMLOW8.2 GEANT4 version 11.1.3





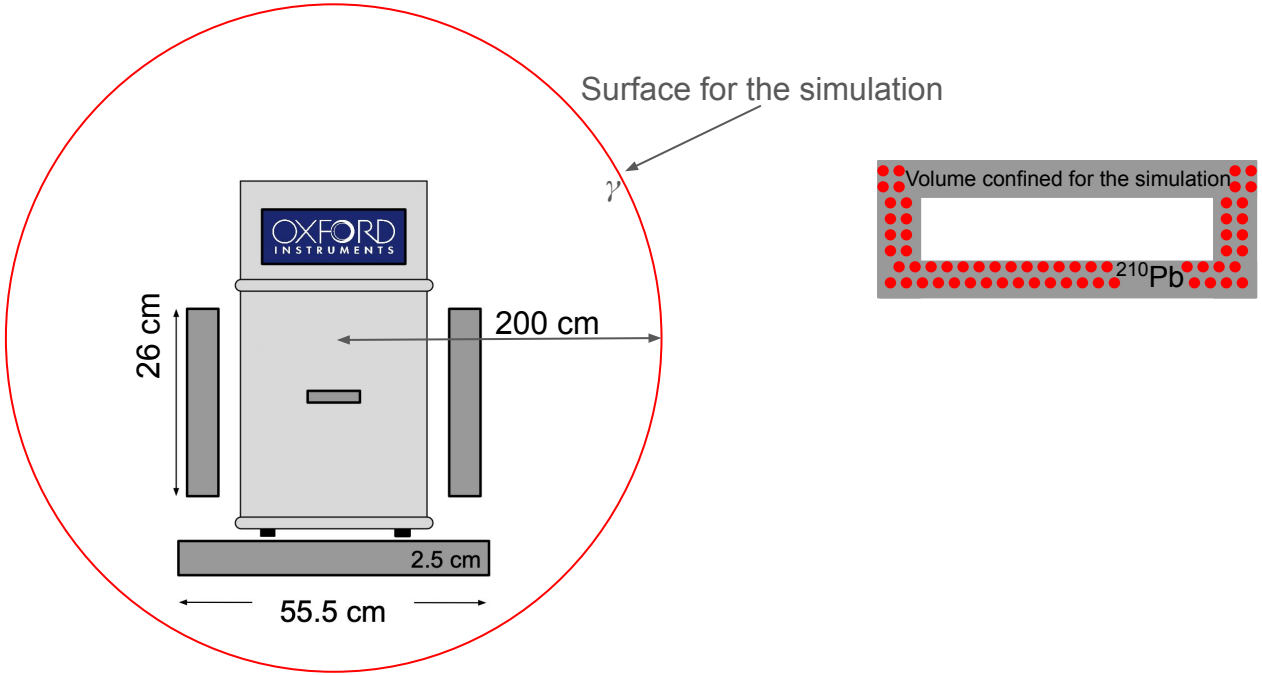




- Not significant difference found for this case (same behavior)

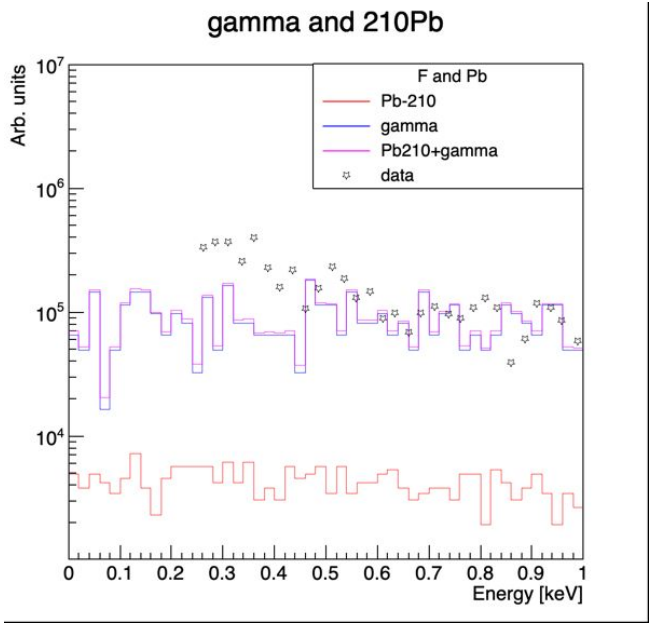
Simulations for BULLKID (Sapienza): ^{210}Pb contribution in holder

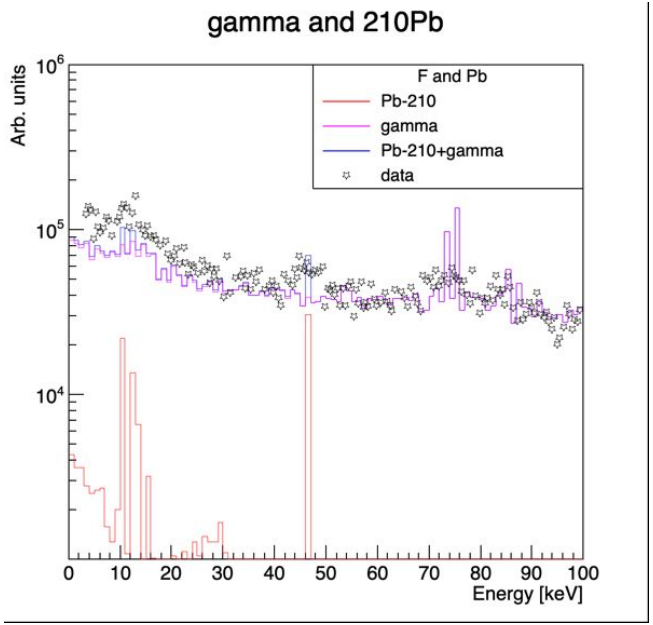
- Considering experimental set up:
  - gamma spectrum simulated outside the cryostat
  - Simulation of ^{210}Pb for the holder
- From the last slide, it seems we can use any model. Fluorescence model used



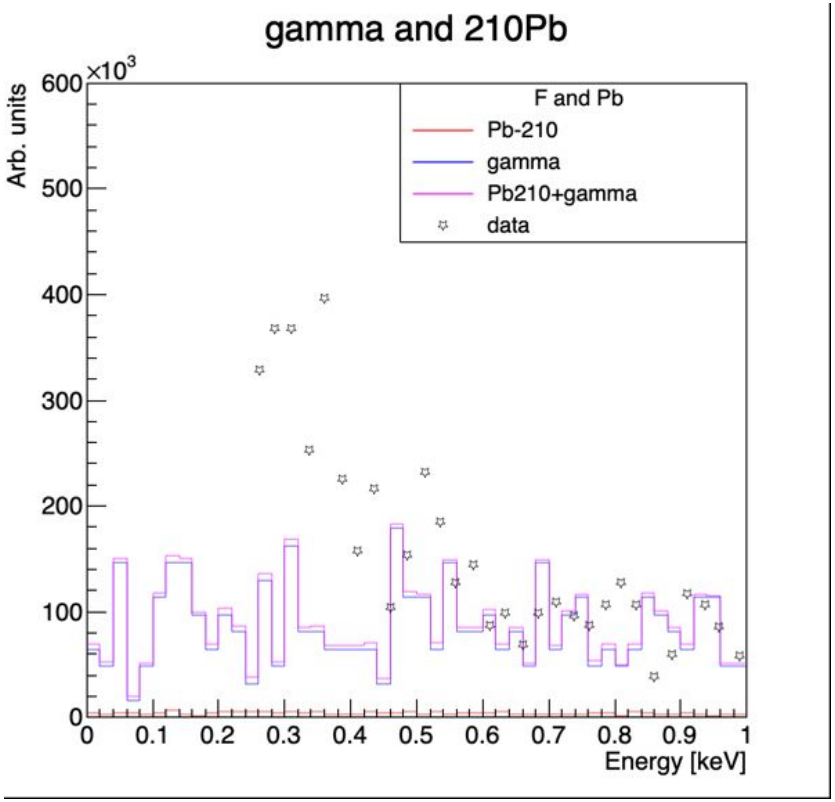
Simulations for BULLKID

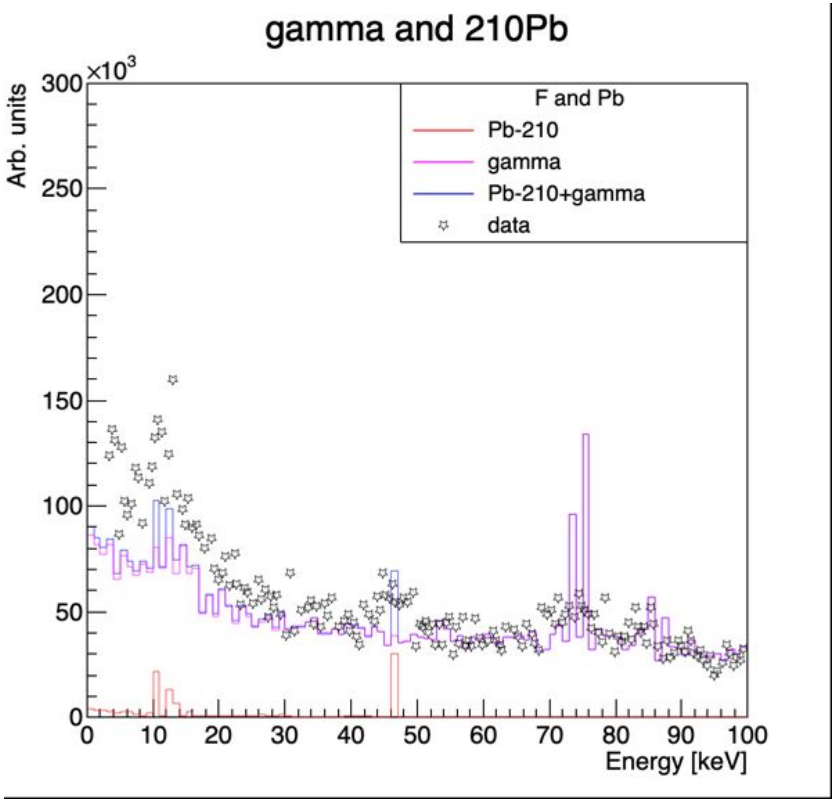
- Data points from Daniele (0.2-1 keV) and Matteo (3-100 keV) [digest may 14th]
- Units:
  - gamma simulations dru
  - Data dru for 0.2-1 keV, re-scaled (arbitrary units) for 3-100 keV
  - ^{210}Pb re-scaled (arbitrary units)





Simulations for BULLKID (Sapienza)

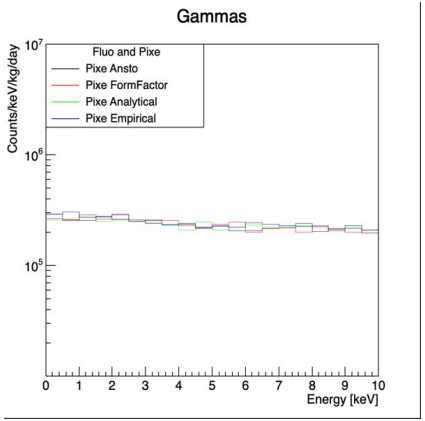


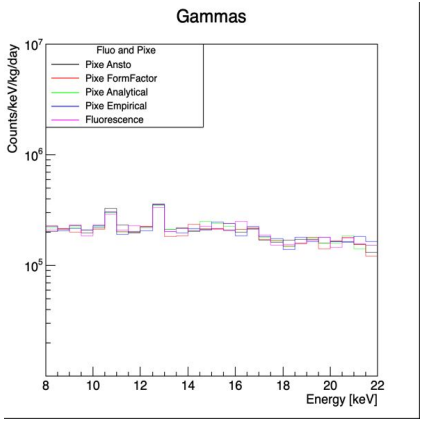


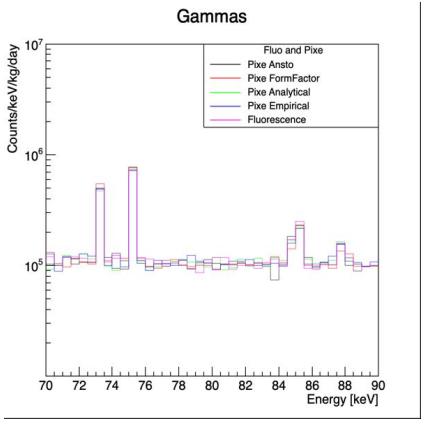
Summary

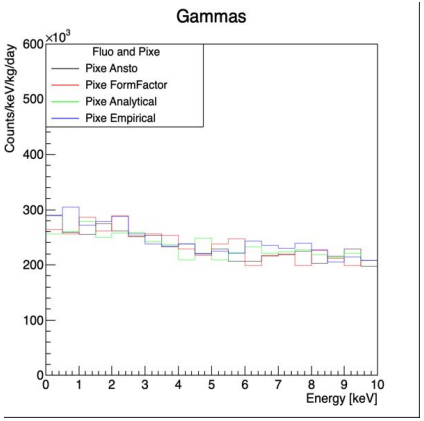
- All models for the atomic de-excitation show the x-ray characteristics of Lead from K and L shell
  - Only ANSTO and FromFactor include x-ray characteristics from M shell
- In the GEANT4 version used for the simulations, it seems that there is no considerable difference between the four PIXE models and the Fluorescence model
- Simulation for gammas and ^{210}Pb does not fit the rise observed at Sapienza independent of the model considered for PIXE
- Keep search and continue study/understanding models

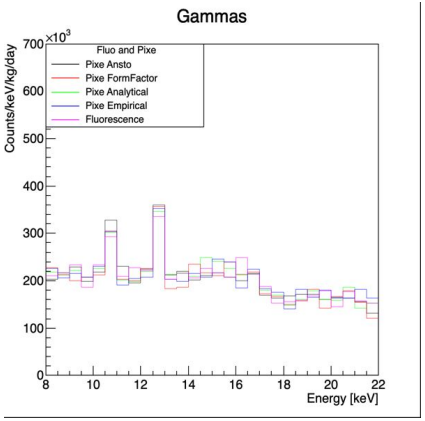
Auxiliary histograms

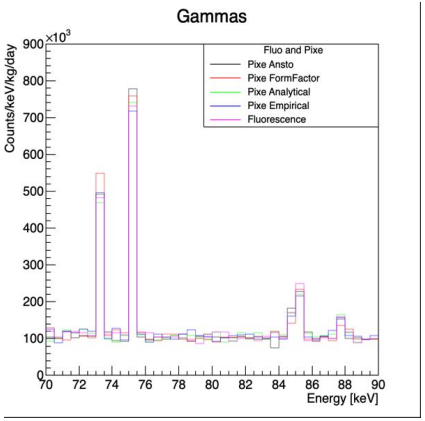


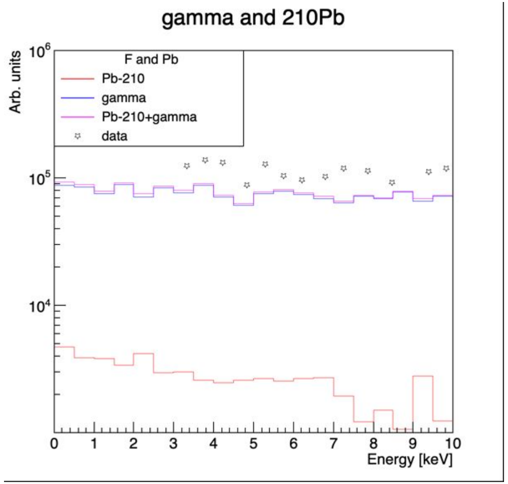


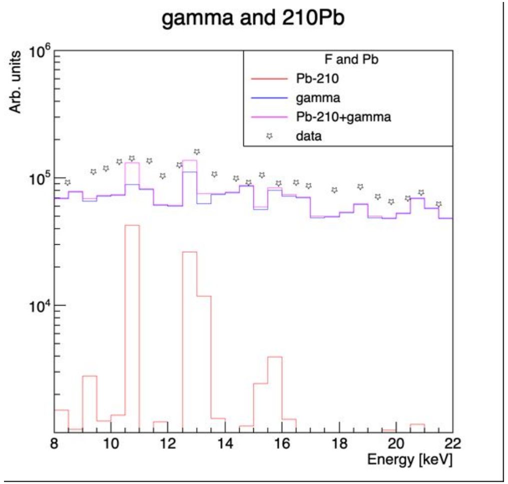









gamma and 210Pb
F and Pb
Pb-210
gamma
Pb-210+gamma
data
Arb. units
Energy [keV]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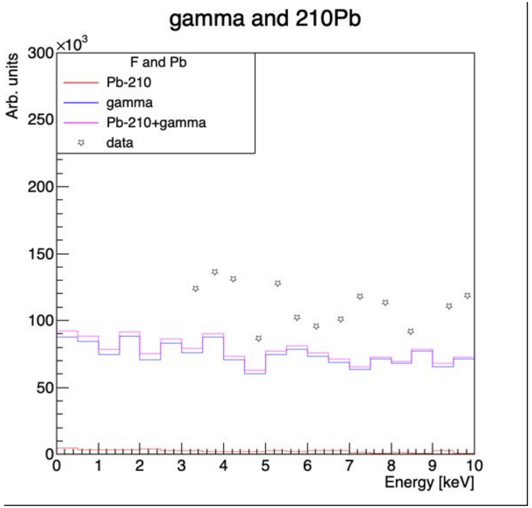
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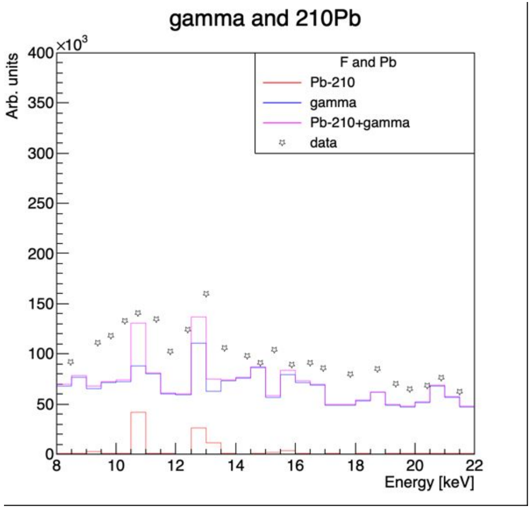
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