Technical note 6: comparative study of simulation results based on EPICS2017 and EPDL97 with XCOM data

The principal goal of this study is to compare the mass attenuation coefficient, obtained from Geant4 simulations, using EPICS2017 database and EPDL97 respectively, with XCOM reference database from National Institute of Standards and Technology (NIST) (*https://www.nist.gov/pml/xcom-photon-cross-sections-database*) [1], for total photon interaction and each process. Simulations were performed on the modified example:
g4tests-verification-master/electromagnetic/attenuation.

1. Details of the *attenuation* example

1.1. Set-up

A monoenergetic photon beam (point source) passes through a sample, with a given thickness, density and composition, made of one of the selected elements or materials: beryllium, carbon, aluminum, silicon, germanium, iron, silver, cesium, gold, lead, uranium, water and ICRU compact bone [2]. 50 energy values varying from 0.001 MeV to 100 000 MeV were tested. In order to reduce the statistical error, a high number of incident photons ($N_0 = 10^6$) was emitted. Moreover, the thickness *d* of the slab was adjusted so as to have a sufficient number *N* of photons that did not interact with the slab. In this way, we could ensure that the corresponding statistical error on the attenuation coefficient was always less than 0.3%. The total mass attenuation coefficient $\frac{\mu}{\rho}$ is calculated as follows:

$$\frac{\mu}{\rho} = -\frac{1}{\rho d}\ln\left(\frac{N}{N_0}\right)$$

where ρ represents the density (g/cm^3) of the sample. The partial interaction coefficient $\left(\frac{\mu}{\rho}\right)_p$ is calculated using the linear attenuation coefficient μ_l, which is available from Geant4 simulation according to the implemented physical model:

$$\left(\frac{\mu}{\rho}\right)_p = \frac{\mu_l}{\rho}$$

The simulations based on EPICS2017 were performed on Geant4 10.07 version with updated models, and on Geant4 10.06 version for simulations based on EPDL97.

The macros for the execution of simulations are placed in the ***Validation_final/Macros*** directory. There is one macro for each element. For instance, for cesium, the macro is named ***total_Cs.mac***.

1.2. Calculation of simulation relative uncertainty

Mass attenuation coefficient μ_m is defined as:

$$\mu_m = -\frac{1}{\rho d}\ln\left(\frac{N}{N_0}\right)$$

The statistical error (stardard deviation) of σ_{μ_m} is calculated as:

$$\sigma_{\mu_m} = \sqrt{\left(\frac{d\mu_m}{dN}\right)^2 {\sigma_N}^2}$$

where σ_N is the stardard deviation of *N*, and:

$$\frac{d\mu_m}{dN} = -\frac{1}{\rho d N}$$

We consider:

$$\sigma_N = \sqrt{N}$$

So,

$$\sigma_{\mu_m} = \sqrt{\left(\frac{1}{\rho d}\right)^2 \left(\frac{{\sigma_N}^2}{N^2}\right)} = \sqrt{\left(\frac{1}{\rho d}\right)^2 \frac{1}{N}}$$

$$\boxed{\frac{\sigma\mu_m}{\mu_m} = \frac{1}{\ln(\frac{N_0}{N})}\sqrt{\frac{1}{N}}}$$

1.3. Output file

A simulation in ***attenuation*** example consists of a series of 50 tests (runs) with different photon energy varying 0.001 MeV to 100 000 MeV for a given thickness of the sample. After a simulation, a ***AttenuationCoefficient.dat*** output file is generated (for the given material) containing 50 lines. Each line contains the following 17 values for the test with a given energy of photon (Fig. 1):

Column 1	Energy in MeV
Column 2	Calculated total mass attenuation coefficient in cm^2/g
Column 3	Number of transmitted photons *N*
Column 4	Number of incident photons N_0
Column 5	Target thickness *d* in cm
Column 6	Density ρ in g/cm^3
Column 7	Uncertainty
Column 8	Linear attenuation coefficient μ_l for photoelectric in cm^{-1} using ComputeCrossSectionPerVolume method
Column 9	Linear attenuation coefficient μ_l for Compton in cm^{-1} using ComputeCrossSectionPerVolume method
Column 10	Linear attenuation coefficient μ_l for gamma conversion in cm^{-1} using ComputeCrossSectionPerVolume method
Column 11	Linear attenuation coefficient μ_l for Rayleigh in cm^{-1} using ComputeCrossSectionPerVolume method
Column 12	Total linear attenuation coefficient μ_l in cm^{-1} using ComputeCrossSectionPerVolume method
Column 13	Linear attenuation coefficient μ_l for photoelectric in cm^{-1} using GetCrossSectionPerVolume method
Column 14	Linear attenuation coefficient μ_l for Compton in cm^{-1} using GetCrossSectionPerVolume method
Column 15	Linear attenuation coefficient μ_l for gamma conversion in cm^{-1} using GetCrossSectionPerVolume method
Column 16	Linear attenuation coefficient μ_l for Rayleigh in cm^{-1} using GetCrossSectionPerVolume method
Column 17	Total linear attenuation coefficient μ_l in cm^{-1} using GetCrossSectionPerVolume method

It should be noted that the linear attenuation coefficients obtained from the ***ComputeCrossSectionPerVolume*** () and ***GetCrossSectionPerVolume*** () methods are slightly different (<$1.3*10^{-3}$ in relative difference). For the calculation of mass attenuation coefficient, we used the values obtained from ***ComputeCrossSectionPerVolume*** ().

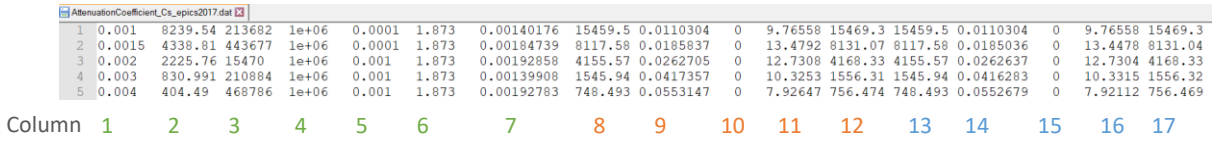


Fig. 1. Example of first 5 lines of the output file for cesium suing EPICS2017.

1.3. Composition of compact bone

The mass fraction in percent of G4_BONE_COMPACT_ICRU is defined in the ***G4NistMaterialBuilder.cc*** (Fig. 2). According to this, we calculated the atomic composition: $H_{117460}C_{42819}N_{3566}O_{47409}Mg_{152}P_{4181}S_{115}Ca_{6786}$. The subscript for each element is required to be an integer, because XCOM data for molecular compounds are only accessible by atomic composition with integers.

```
AddMaterial("G4_BONE_COMPACT_ICRU", 1.85, 0, 91.9, 8);
AddElementByWeightFraction( 1, 0.064);
AddElementByWeightFraction( 6, 0.278);
AddElementByWeightFraction( 7, 0.027);
AddElementByWeightFraction( 8, 0.410);
AddElementByWeightFraction(12, 0.002);
AddElementByWeightFraction(15, 0.07 );
AddElementByWeightFraction(16, 0.002);
AddElementByWeightFraction(20, 0.147);
```

*Fig. 2. Mass fraction of G4_BONE_COMPACT_ICRU defined in **G4NistMaterialBuilder.cc***

2. Analysis of simulated data

The simulation results for EPICS2017 and EPDL97 are saved in the ***Validation_final/epics2017_data*** directory and ***Validation_final/livermore_data*** directory respectively. The XCOM data are saved in ***Validation_final/XCOM_data directory***.

2.1. Uncertainty check

Once you have simulated results for all the materials mentioned above, the first thing to do is to check the uncertainty to ensure the statistical error on the attenuation coefficient for each test is always less than the maximal tolerated uncertainty value (in our study, 0.3%), otherwise the thickness of the sample should be adjusted.

UncertaintyCheck_EPICS2017.c and ***UncertaintyCheck_Livermore.c*** are designed for checking the uncertainty of simulated results based on EPICS2017 and EPDL97 respectively.

To use these two macros, firstly you should place these macros in the ***Validation_final*** folder. Then, type the following command in the Terminal:

```
root UncertaintyCheck_EPICS2017.c
```

2.2. Comparison and plot of mass attenuation coefficients

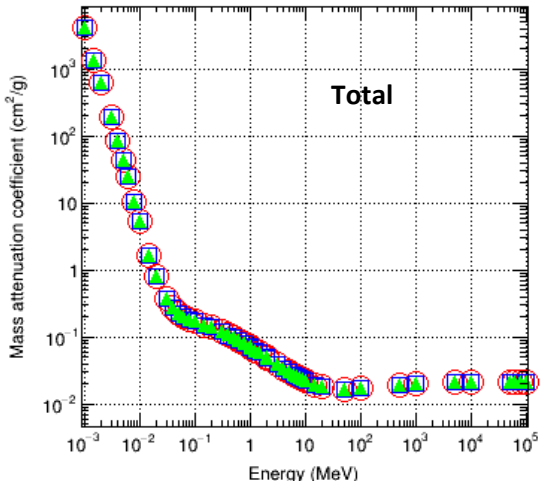
Analysis.c macro is developed to accomplish the following tasks:

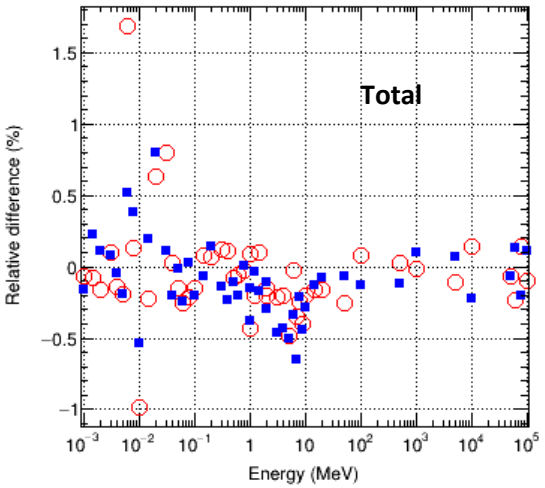
- Read the data in ***epics2017_data***, ***livermore_data***, ***XCOM_data*** directories
- Plot the mass attenuation coefficients (cm^2/g) of EPICS2017, EPDL97 and XCOM for total and each process for the selected materials. The figures are saved in the following directories:
    - ***MassAttenuationCoefficient_total*** for total interaction
    - ***MassAttenuationCoefficient_pair*** for gamma conversion process
    - ***MassAttenuationCoefficient_compt*** for Compton scattering
    - ***MassAttenuationCoefficient_phot*** for photoelectric effect
    - ***MassAttenuationCoefficient_Rayl*** for Rayleigh scattering
- Plot the relative difference of mass attenuation coefficients of EPICS2017 and EPDL97, compared to XCOM data for total and each process for the selected materials. The figures are saved in the following directories:
    - ***MassAttenuationCoefficient_total/RD*** for total interaction
    - ***MassAttenuationCoefficient_pair/RD*** for gamma conversion process
    - ***MassAttenuationCoefficient_compt/RD*** for Compton scattering
    - ***MassAttenuationCoefficient_phot/RD*** for photoelectric effect
    - ***MassAttenuationCoefficient_Rayl/RD*** for Rayleigh scattering
- Generate the files:
    - ***ratioMax_Average_epics2017.dat***, containing the maximal relative difference and average of absolute relative difference for EPICS2017 for all selected materials
    - ***ratioMax_Average_livermore.dat***, containing the maximal relative difference and average of absolute relative difference for EPDL97 for all selected materials

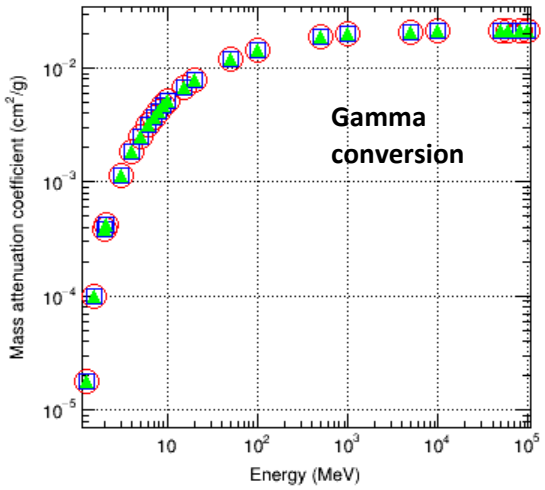
To use the macro, firstly you should place it in the ***Validation_final*** folder. Then, type the following command in the Terminal:

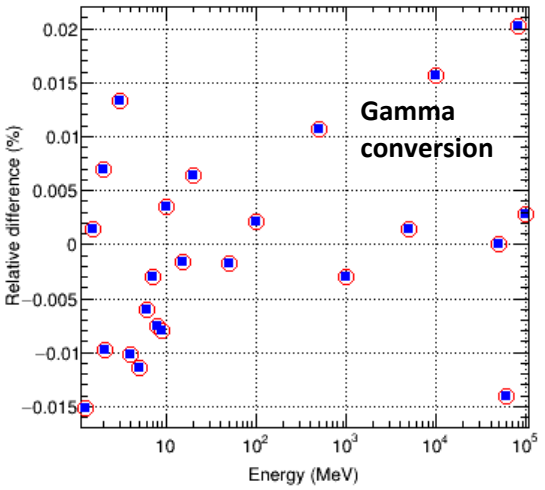
```
root Analysis.c
```

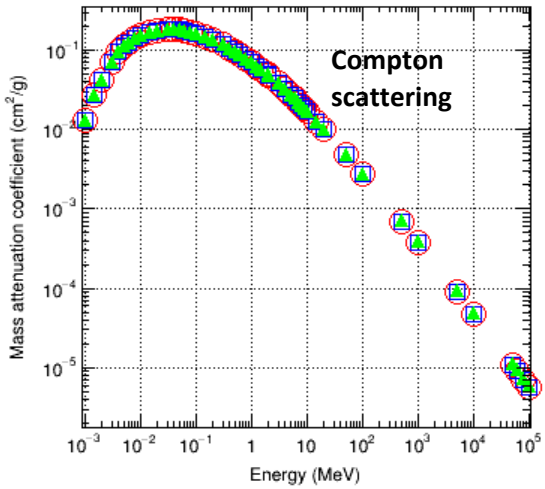
An example for water is shown in the Fig. 3.

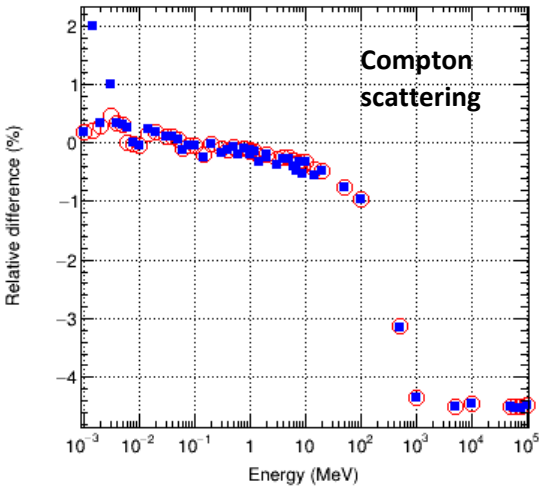

Total
Mass attenuation coefficient (cm²/g)
Energy (MeV)


Total
Relative difference (%)
Energy (MeV)


Gamma conversion
Mass attenuation coefficient (cm²/g)
Energy (MeV)


Gamma conversion
Relative difference (%)
Energy (MeV)


Compton scattering
Mass attenuation coefficient (cm²/g)
Energy (MeV)


Compton scattering
Relative difference (%)
Energy (MeV)

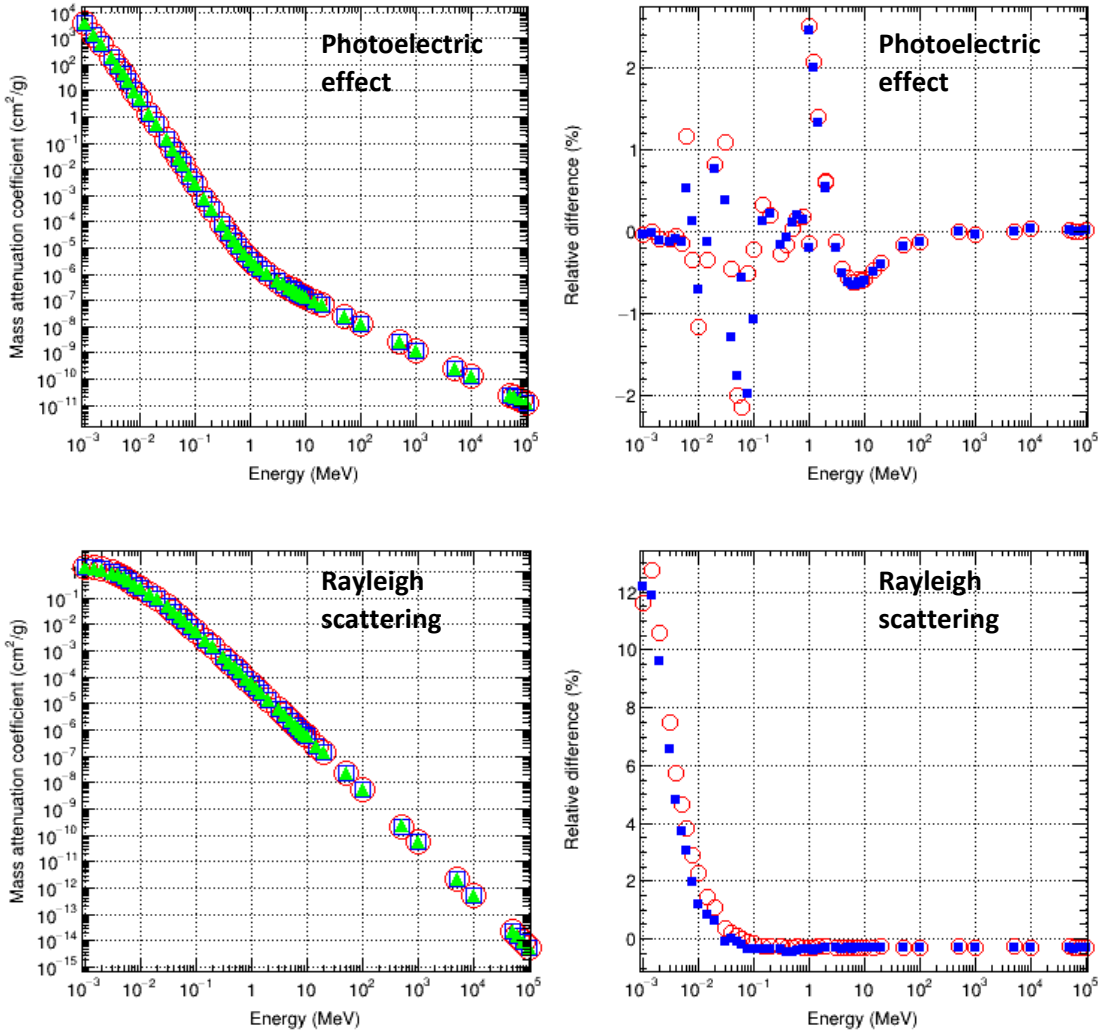


Fig. 3 (2 pages). Mass attenuation coefficient (left) calculated by Geant4 simulations for water based on EPICS2017 (open circles) and EPDL97 (filled squares) as well as XCOM data (filled triangles). Relative difference (right) compared to the XCOM database for both total and for each process; $Relative\ difference = \frac{Simulation - XCOM}{XCOM}$

Besides, ***plot_ratioMax_Average.c*** is used to plot the maximal relative difference and the average of absolute difference according to Z by reading ***ratioMax_Average_epics2017.dat*** and ***ratioMax_Average_livermore.dat*** (Fig. 4).

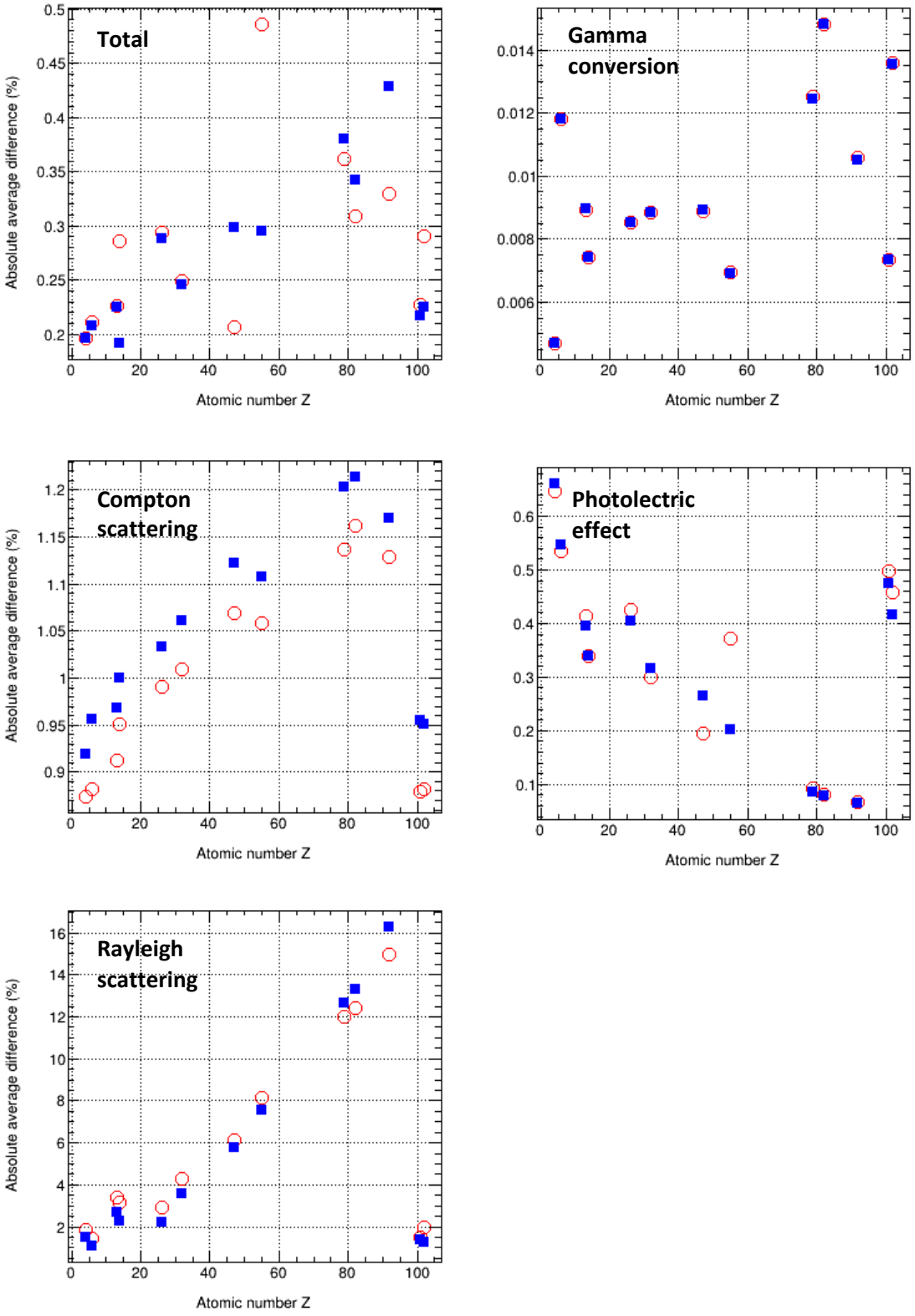


Fig. 4. Average of absolute relative difference of mass attenuation coefficient calculated by Geant4 simulations based on EPICS2017 (open circles) and EPDL97 (filled squares) compared to XOCM for total and each process. Z = 101 was arbitrarily chosen to represent water, Z = 102 to represent ICRU compact bone.

List of macro files

The ROOT macro files that are used:

1. ***total_X.mac***, X is the name of tested material. This macro is used for the execution of simulations. They are located in the ***Validation_final/Macros*** directory.
2. ***UncertaintyCheck_EPICS2017.c***, check the uncertainty of simulated results based on EPICS2017
3. ***UncertaintyCheck_Livermore.c***, check the uncertainty of simulated results based on EPDL97
4. ***Analysis.c***, plots:
    - mass attenuation coefficient among EPICS2017, EPDL97 and XCOM, for total and each process
    - comparisons of mass attenuation coefficient
5. ***plot_ratioMax_Average.c***, plot the maximal relative difference and the average of absolute difference between EPICS2017 and EPDL97 according to Z

Reference

[1] Berger MJ, Hubbell J. XCOM: Photon cross sections on a personal computer. National Bureau of Standards, Washington, DC (USA). Center for Radiation; 1987.

[2] Report 10b. Journal of the International Commission on Radiation Units and Measurements. 1964;os6:NP-NP.