Technical note 3: Compton scattering process

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Introduction

This technical note explains the implementation of EPICS2017 database for Compton scattering process, which includes the following parts:

- Section 1: description of Livermore cross section data format for Compton scattering process
- Section 2: format of original EPICS2017 data library
- Section 3: implementation of cross section in Geant4 11.0 version
- Section 4: cross section data difference between EPICS2017 and Livermore
- Section 5: implementation of scattering function fit in Geant4 11.0 version

1. Livermore model for Compton scattering

1.1. G4LivermoreComptonModel model class

For the Compton scattering process in Geant4, the **G4LivermoreComptonModel** class performs the following tasks:

- read the tabulated cross section data from Geant4 data library
- compute the interpolated cross section for the energy value of the incident gamma
- generate the final state (photon + electron).

1.2. Location of cross section data files

For the 10.7 version of Geant4, the Livermore total cross section data files that the class reads are contained in the directory:

$G4LEDATA/livermore/comp

The **G4EMLOW7.9 ($G4LEDATA)** directory contains the 7.9 version (October 2019) of the data files for low energy electromagnetic processes.

1.3. Format

Cross section files are composed of **two header lines** and **a series of "cross section" data** (energy – "cross section" points[1])

The file name is:

ce-cs-Z.dat   *("ce" is for "Compton effect")*

where *Z* is the atomic number of the element.

Fig. 1 presents an example of a part of total "cross section" data file *ce-cs-1.dat* for Hydrogen.

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[1] "cross section" refers to energy × cross section in this technical note

Fig. 1. Example of the beginning of the data file for Hydrogen for Livermore

1.3.1. Information in the header lines

The 3 figures (Fig. 1) in the first header line indicate the lowest and highest energy values in the table (in **MeV**), and the number of energy – "cross section" points.

The figure in the second header line repeats the number of energy – "cross section" points.

1.3.2. Information in the data lines

As illustrated in Fig. 1, the first column contains the energy values in **MeV**, from the lowest to highest energy value given in the first header line. The second column contains the corresponding "cross section" data, which is the product of energy and cross section instead of genuine cross section, in **MeV·barn** with 10 **significant digits**.

2. Format of original Compton scattering data in *EPDL2017.ALL*

In *EPDL2017.ALL*, as introduced in Technical note 1, we can simply locate the data lines relevant to the Compton scattering (incoherent scattering) process, by choosing **72** and **93 (for whole atom parameters)** for the reaction descriptor in the second header line (Fig. 2, line 2). In fact, four types of data relevant to Compton scattering process are given for each element:

       1) the cross section (Fig. 2)

       2) average energy of the scattered photon (Fig. 3)

       3) average energy of secondary electron (Fig. 4)

       4) scattering function (Fig. 5)

Fig. 2-5 present an example of the **data** tables relevant to the Compton scattering process for Hydrogen. Some of the parameters in the header lines are identical in these three tables (see Technical note 1):

The first header line specifies: Z = 1, A = 000, Yi = 7 (incident particle = photon) (Fig. 2, in red).

The second header line specifies: C =72 (reaction descriptor: Compton scattering) (Fig. 2, in red).

We are only interested in the cross section and scattering function data in this technical not (and not in the energy of scattered photon and electron) for the purpose of updating the Geant4 database. Nevertheless, we will still present all the available information.

2.1. Cross section

Fig. 2 presents an example of a part of **cross section data table relevant to the Compton scattering** process for Hydrogen.

In this example (Fig. 2, in blue):

- In the first header line: Yo = 0, means that the given information is not about the secondary particles
- In the second header line: I = 0, means that the data lines below are the cross section data

2 header lines →

```
   1000  7  0  1.00797    1807172 2  0.0         0.0         0.0
72  0   0  0.0           0.0          0.0         0.0         0.0
```

data lines →

```
  1.000000000E-06 9.562300000E-08
  1.059248390E-06 1.072900000E-07
  1.105977190E-06 1.169660000E-07
  1.142371710E-06 1.247910000E-07
  1.199221310E-06 1.375210000E-07
  1.258900000E-06 1.515500000E-07
  1.333502680E-06 1.700420000E-07
```

Energy of incident   Cross section (barn)
gamma (MeV)

Fig. 2. Example of cross section data table relevant to the Compton scattering process for Hydrogen in EPDL2017.ALL

2.2. Average energy of the scattered photon

Fig. 3 presents an example of **average energy of the scattered photon** for Hydrogen.

In this example (Fig. 3, in blue):

- In the first header line: Yo = 7, means secondary particles are photons.
- In the second header line: I = 10, means that the data lines indicate the average energy of secondary particles, namely photon in this case.

2 header lines →

```
   1000  7  7  1.00797    1807172 2  0.0         0.0         0.0
72 10   0  0.0           0.0          0.0         0.0         0.0
```

data lines →

```
  1.000000000E-06 9.999973000E-07
  1.258925000E-06 1.258921000E-06
```

Energy of incident   Energy of scattered
gamma (MeV)   photon (MeV)

Fig. 3. Example of average energy table of the scattered photon for Hydrogen in EPDL2017.ALL

2.3 Average energy of the secondary electron

Fig. 4 presents an example of **average energy of the secondary electron** for Hydrogen.

In this example,

- In the first header line: Yo = 9, means secondary particles are electrons.
- I = 10, means that the data lines indicate the average energy of secondary particles, namely electrons in this case.

2 header lines →

```
   1000  7  9  1.00797    1807172 2  0.0         0.0         0.0
72 10   0  0.0           0.0          0.0         0.0         0.0
```

data lines →

```
  1.000000000E-06 2.740270000E-12
  1.258925000E-06 4.343020000E-12
```

Energy of incident   Energy of secondary
gamma (MeV)   electron (MeV)

*Fig. 4. Example of average energy of the secondary electron
for Hydrogen in file EPDL2017.ALL*

2.4. Scattering function

Fig. 5 presents an example of a part of **scattering function data table relevant to the Compton scattering** process for Hydrogen.

In this example (Fig. 5, in blue):

- In the first header line: Yo = 0, means no information is given about the secondary particles.
- In the second header (red): C = 93, means that the data lines below are whole atom parameters
- In the second header line: I = 942, means that the data lines below are scattering function

*Fig. 5. Example of scattering function data table relevant to the Compton scattering process
for Hydrogen in EPDL2017.ALL*

2.5. Units

Energy used in *EPDL2017.ALL* is in **MeV**.

Cross section is in **barns**.

Momentum transfer is in 10^6 Å^{-1}, i.e. 10^{16} m^{-1}.

3. Implementation of cross section in Geant4

3.1. generate_ce_csE_2017.c macro

generate_ce_csE_2017.c is a ROOT macro, which is used to generate the total "cross section" data (product of energy and cross section) files from *EPDL2017.ALL* for elements (Z:1-100), these files will be added to Geant4 data library.

As explained in section 2, Compton scattering cross section data is distinguished by the header line:

72 0 0 0.0   0.0   0.0   0.0   0.0

This function produces respectively 100 "cross section" data files (one file for one element), saved in the directory called *epics2017/comp*

The output file is named: *ce-cs-Z.dat*

where *Z* is the atomic number of the element.

The units for energy and "cross section" in the generated data files are in **MeV** and in **MeV·barn**.

Command

To use the *generate_ce_csE_2017.c* macro, firstly you should place this macro and the *EPDL2017.ALL* file in the same directory. Secondly, type the following command in the Terminal:

```
root generate_ce_csE_2017.c
```

3.2. Format

The format of the implemented total cross section data files obtained from *EPDL2017.ALL* follows the format of Geant4 Livermore data files contained in the directory *$G4LEDATA/livermore/comp* (as detailed in section 1).

It is composed of **2 header lines** followed by **a series of physical data lines** with 2 columns (energy in **MeV** and "cross section" in **MeV·barn**). A major difference compared to Livermore data is the number of significant digits. **We kept 10 significant digits for both energy and "cross section" data** *(However, we noticed that not all the significant digits are actually used for Compton scattering cross section data in **EPDL2017.ALL**).*

The format of the total cross section data files is illustrated in Fig. 6.

Fig. 6. Example of a part of "cross section" data file for Hydrogen for EPICS2017

3.2.1. Information in the header lines

Just as the data files of Livermore, the three figures in the first header line indicate the lowest and highest energy values in the table (in **MeV**), and the number of data points. The figure in the second header line repeats the number of data points.

3.2.2. Information in the data lines

As illustrated in Fig. 6, the first column contains the energy values of the incident gamma in **MeV** with **10 significant digits**, from the lowest to highest energy value given in the first header line. The second column contains the corresponding "cross section" data in **MeV·barn** with **10 significant digits**.

4. Comparison of cross section data between EPICS2017 and Livermore

Before implementing the new database in Geant4, we have compared cross section data between EPICS2017 and Livermore using *plot_cs.c* macro.

4.1. plot_cs.c

The *plot_cs.c* ROOT macro reads data files in

- *epics2017/compCS/ce-cs-Z.dat* extracted by *generate_ce_cs_2017.c*
- *epics2014/compCS/ce-ce-Z.dat* extracted by *generate_ce_cs_2014.c*

It then plots the following figures for cross section data. There is one figure per element.

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- cross section data of EPICS2017 (Z: 1-100) (example in Fig. 7, for Hydrogen)
- cross section data of Livermore (Z: 1-100) (example in Fig. 8, for Hydrogen)
- comparison of cross section data between EPICS2017 and Livermore (Z: 1-100) (example in Fig. 9, for Hydrogen)

The generated figures are saved in the corresponding directories:

- *plots/epics2017*
- *plots/epics2014*
- *plots/comparison*

Command

To use the *plot_cs.c* macro, you should put it in the same directory as the data file directories *epics2017* and *epics2014* are, so that it can read the files contained inside. The *plots/* directories above are automatically generated when the macro runs, by the command:

```
root plot_cs.c
```

The figure presenting the comparison of cross section data between EPICS2017 and Livermore is composed of two graphs:

1. Comparison of cross section between EPICS2017 and Livermore

2. Relative difference (%) of cross section for EPICS2017 compared to Livermore:

$$RD = \frac{CS_{EPICS2017} - CS_{Livermore}}{CS_{Livermore}} \times 100\%$$

where $CS_{EPICS2017}$ and $CS_{Livermore}$ are the cross section at a given energy for EPICS2017 and Livermore.

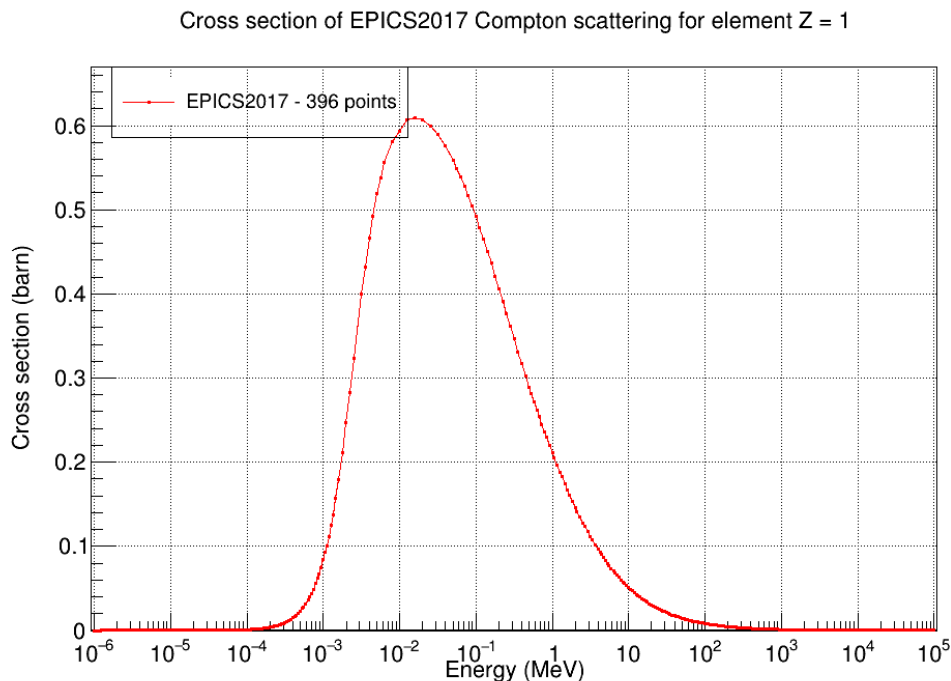The figures below (Fig. 7-9) display examples for Hydrogen.

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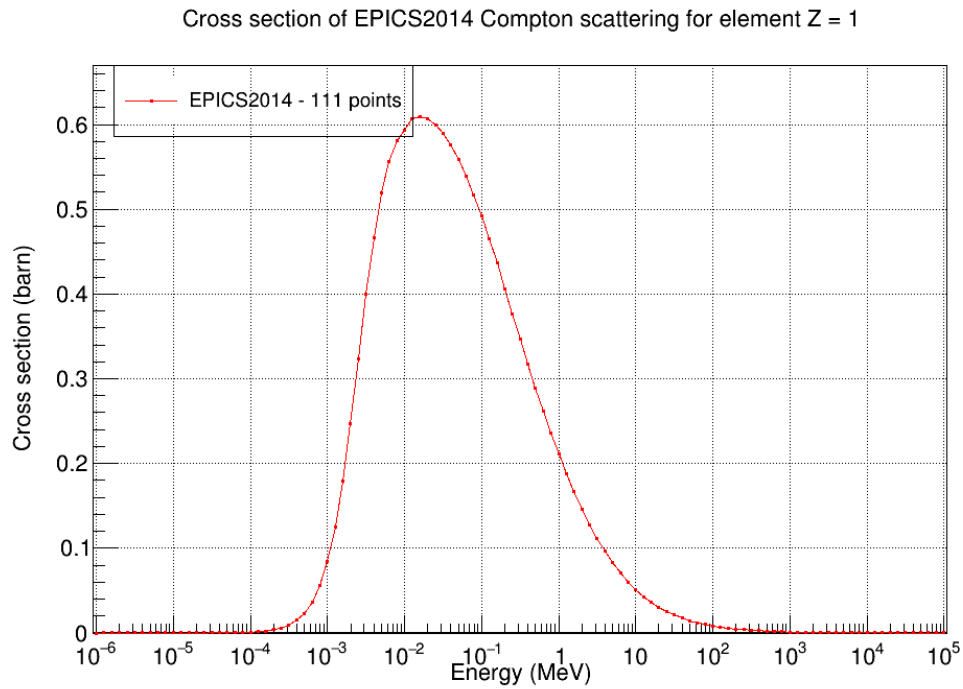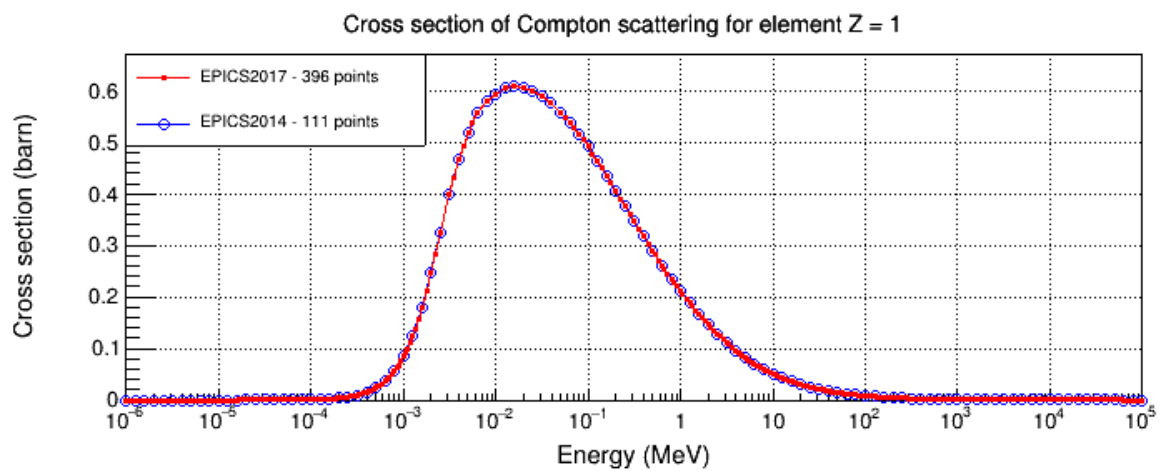*Fig. 7. An example of "cross section" data of EPICS2017 for Hydrogen*

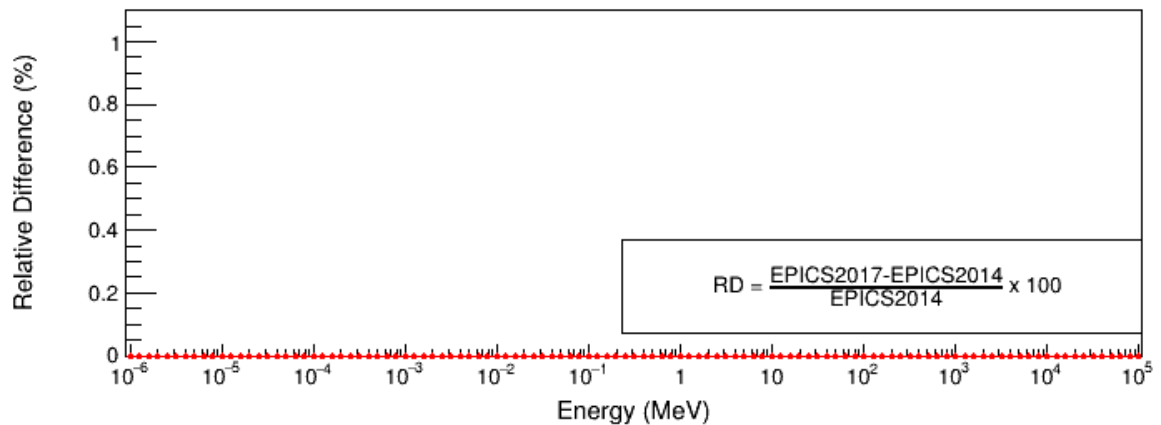*Fig. 8. An example of cross section data of Livermore for Hydrogen*

Fig. 9. An example of comparison of cross section data between EPICS2017 and Livermore for Hydrogen

4.2. Discussion

For each element, EPICS2017 contains more energy – "cross section" points than Livermore does. For example, Hydrogen has 396 points for EPICS2017 (Fig. 7) while only 111 for Livermore (Fig. 8). Besides, all the points of Livermore are included in EPICS2017 with exactly same "cross section" values, thus there is no difference in the comparison of "cross section" between EPICS2017 and Livermore (Fig. 9, bottom graph).

5. Scattering function fit

For low energy incident photons, the simulation of the Compton scattering process is performed according to the product of the Klein-Nishina formula and the scattering function SF(q) [1, 2], where q is the momentum transfer.

In previous **G4LivermoreComptonModel**, scattering function data was derived from EPDL97 and fitted with 3 functions in three regions:

- polynomial of degree 1 (region 1)
- polynomial of degree 3 (region 2)
- Z value (region 3)

Scattering function data is now extracted from EPICS2017 and fitted with 4 functions:

- polynomial of degree 1 (region 1)
- polynomial of degree 4 (first part of region 2)
- polynomial of degree 4 (second part of region 2)
- Z value (region 3)

A more detailed information is given in section 5.3.

5.1. generate_scatteringFunction_2017.c macro

generate_ scatteringFunction_2017.c is a ROOT macro, which is used to generate the scattering function files from **EPDL2017.ALL** for elements (Z:1-100), these files will be used to make a fit (using four functions) for scattering function which will be eventually adopted in **G4LivermoreComptonModel**.

Command

To generate scattering function from **EPDL2017.ALL**, make sure you put this macro and **EPDL2017.ALL** in the same directory, and then type the following command in the Terminal:

```
root generate_ scatteringFunction_2017.c
```

The output files are named: **sf-Z.dat**

where *Z* is the atomic number of the element.

They are saved in **epics2017/scatteringFunction** directory.

Note that another macro **generate_scatteringFunction_2014.c** is also provided if you want to extract scattering function from EPDL2014.

5.2. plot_scatteringFunction.c

plot_scatteringFunction.c is meant to plot the comparison of scattering function between EPICS2017 and Livermore given that scattering function data files have been prepared as described in section 5.1. It generates one figure for each element.

Command

To run this macro, make sure you put it and the scattering function data files that you extracted and prepared as explained in section 5.1 in the same directory. Then type the following command in the Terminal:

```
root plot_scatteringFunction.c
```

An example of comparison for Hydrogen is illustrated in Fig. 10.

The figure is composed of two graphs:

1. Comparison of scattering function between EPICS2017 and Livermore
2. Relative difference (%) of scattering function for EPICS2017 compared to Livermore:

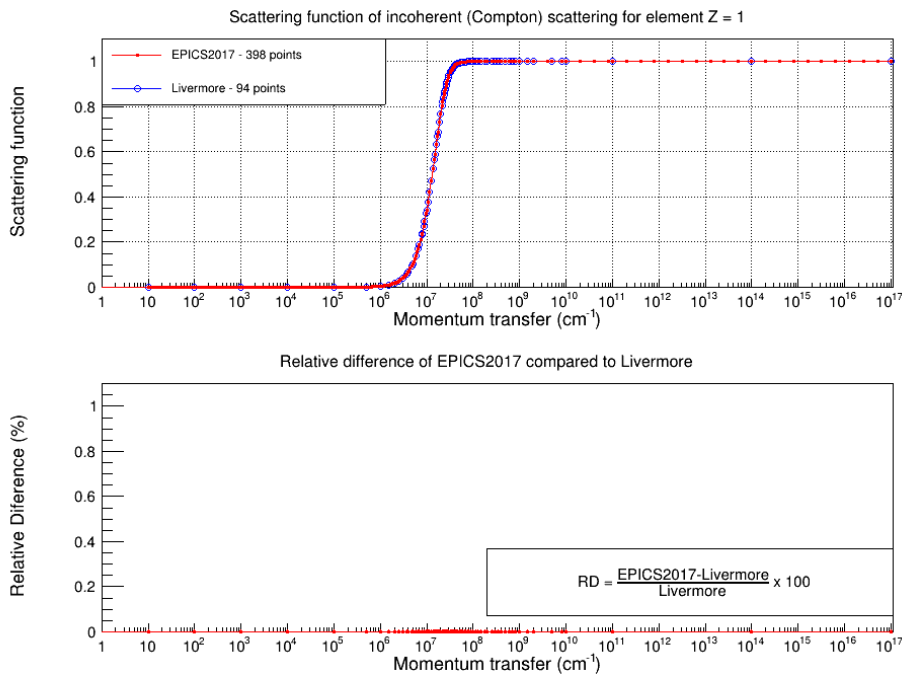$$RD = \frac{SF_{EPICS2017} - SF_{Livermore}}{SF_{Livermore}} \times 100\%$$

Fig. 10. An example of comparison of scattering function data between EPICS2017 and Livermore for Hydrogen

Discussion

For each element, EPICS2017 contains more momentum transfer – scattering function points than Livermore does. For example, Hydrogen has 398 points for EPICS2017 while only 94 for Livermore. Besides, all the points of Livermore are included in EPICS2017 with exactly same scattering function values, thus there is no difference in the comparison of scattering function between EPICS2017 and Livermore (Fig. 10, bottom graph).

5.3. *fit_scatteringFunction_Poly1_Poly4_Poly4.c* macro

fit_scatteringFunction_Poly1_Poly4_Poly4.c is used to make the fit for scattering function data extracted from *EDPL2017.ALL* (section 5.1).

5.3.1. Previous fitting method

The fit of scattering function (SF) was composed of 3 functions given the values of momentum transfer (q):

1) polynomial of degree 1: $\lg(q) < a$ (region 1),
   $\lg(SF) = a_0 + a_1 \cdot \lg(q)$

2) polynomial of degree 3: : $a \leq \lg(q) \leq b$ (region 2),
   $\lg(SF) = b_0 + b_1 \cdot \lg(q) + b_2 \cdot \lg(q) \cdot \lg(q) + b_3 \cdot \lg(q) \cdot \lg(q) \cdot \lg(q)$

3) Z value: $\lg(q) > b$ (region 3)
   SF = Z, Z is the atomic number of the current element

Where:

- a and b are limits of three regions,
- a_0, a_1, b_0, b_1, b_2, b_3 are fitting parameters.

The limits and fitting parameters can be accessed by reading **G4LivermoreComptonModel** code.

5.3.2. Current fitting method

Based on the previous fitting method, the current fitting method improves the accuracy of such parameterization by two steps:

- Narrowing the interval of region 1 with respect to the fitting function polynomial of degree 1
- Dividing region 2 into two parts and fitting each part with a polynomial of degree 4 instead of one polynomial of degree 3.

Therefore, the new fit of scattering function is now made of 4 functions:

1) polynomial of degree 1: $\lg(q) < A$ (region 1),
   $\lg(SF) = A_0 + A_1 \cdot \lg(q)$

2) polynomial of degree 4: $A \leq \lg(q) < B$ (first part of region 2),
   $\lg(SF) = B_0 + B_1 \cdot \lg(q) + B_2 \cdot \lg(q) \cdot \lg(q) + B_3 \cdot \lg(q) \cdot \lg(q) \cdot \lg(q) + B_4 \cdot \lg(q) \cdot \lg(q) \cdot \lg(q) \cdot \lg(q)$

3) polynomial of degree 4: $B \leq \lg(q) \leq C$ (second part of region 2),
   $\lg(SF) = C_0 + C_1 \cdot \lg(q) + C_2 \cdot \lg(q) \cdot \lg(q) + C_3 \cdot \lg(q) \cdot \lg(q) \cdot \lg(q) + C_4 \cdot \lg(q) \cdot \lg(q) \cdot \lg(q) \cdot \lg(q)$

4) Z value: $\lg(q) > C$ (region 3),
   SF = Z, Z is the atomic number of the current element

Where:

- A, B and C are limits of three regions
- $B = 0.5 \times (A + C)$
- C = b in previous fitting method, because only the limit of region 1 and region 2 is modified
- A_0, A_1, B_0, B_1, B_2, B_3, B_4, C_0, C_1, C_2, C_3, C_4 are fitting parameters.

fit_scatteringFunction_Poly1_Poly4_Poly4.c thus firstly reads the existing limits of three regions from *ScatteringFunctionFitsParamsTable_2014.txt* file obtained from **G4LivermoreComptonModel** (10.7 version of Geant4). Then it performs the fitting process generating the output file *ScatteringFunctionFitsParamsTable_Poly1_Poly4_Poly4 .txt* in which the new limits and fitting parameters are written.

Command
To use the ***fit_scatteringFunction_Poly1_Poly4_Poly4.c*** macro, make sure that

- the scattering function data files have been extracted and prepared as explained in section 5.1
- the file ***ScatteringFunctionFitsParamsTable_2014.txt*** which contains the limits and fitting parameters is placed in the same directory as *fit_scatteringFunction_Poly1_Poly4_Poly4.c*

Then just type the following command in the Terminal:

```
root fit_scatteringFunction_Poly1_Poly4_Poly4.c
```

Besides, this macro also generates another output ***MaximalDifferenceOfSFFits_2017_2014.dat***, which contains the maximal difference respectively using previous fit and new fit compared to tabulated scattering function values for all the elements. This file is read to plot the maximal difference according to Z value, which is discussed in section 5.4.

5.4 *plotMaximalDifferenceOfFittedScatteringFunctionWithZ_2017_2014.c* macro

Once ***MaximalDifferenceOfSFFits_2017_2014.dat*** is generated, we can make use of *plotMaximalDifferenceOfFittedScatteringFunctionWithZ_2017_2014.c* macro to plot the distribution of maximal difference of fits in different regions according Z value.

Fig. 11 shows the figure produced by this macro.

It is composed of 2 graphs:

- The left graph is the maximal difference using previous fit (EPDL2014) and new fit (EPDL2017) in region 1 as a function of Z value.
- The right graph is the maximal difference using two fits in region 2. Remember that new fit has two parts for region 2, thus we selected the maximal difference in the whole region 2.
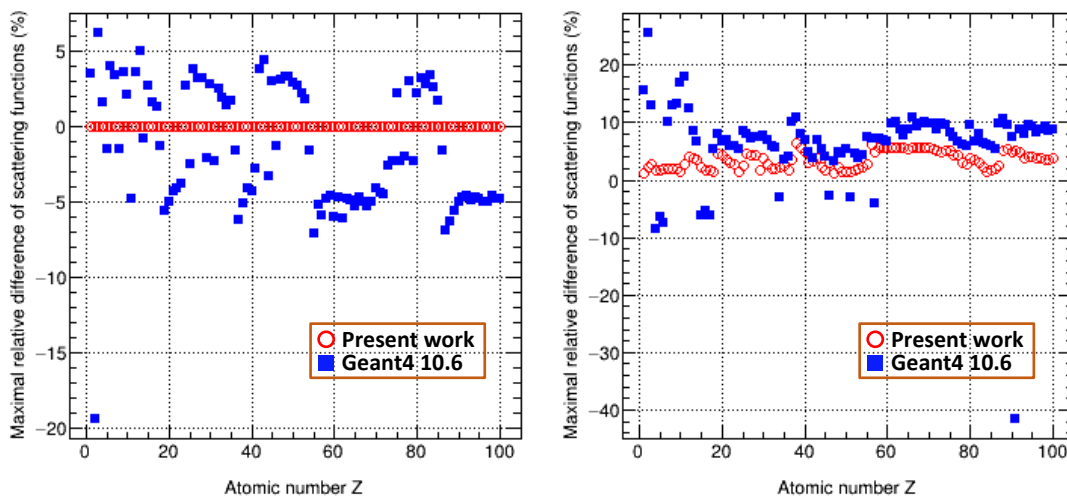
s

Fig. 11. Maximal difference using previous fit and new fit according to Z value

Based on the absolute maximal difference values, this new fitting procedure improves the precision of fit by a factor of 1000 for region 1 and 2.8 for region 2. The improved precision (IP) is calculated according to the following formula:

$$\text{IP} = \frac{\sum_{Z=1}^{Z=100} \frac{R_{old}(Z)}{R_{new}(Z)}}{100}$$

where $R_{new}(Z)$ and $R_{old}(Z)$ are the maximal relative difference of new fit and previous fit of scattering functions for the element Z.

List of macro files

The ROOT macro files that can be useful:

1. ***generate_ce_csE_2017.c***, generates "cross section" data files from ***EPDL2017.ALL***
2. ***generate_ce_csE_2014.c***, generates "cross section" data files from ***EPDL2014.ALL***
3. ***plot_ceE.c***, plots the comparison of "cross section" data between EPICS2017 and Livermore
4. ***generate_scatteringFunction_2017.c***, generates scattering function data files from ***EPDL2017.ALL***
5. ***generate_scatteringFunction_97.c***, generates scattering function data files from ***EPDL2014.DAT***
6. ***plot_scatteringFunction.c***, plots the comparison of scattering function data between EPICS2017 and Livermore
7. ***fit_scatteringFunction_Poly1_Poly4_Poly4.c***, makes the new fit for scattering function of EPICS2017
8. ***plotMaximalDifferenceOfFittedScatteringFunctionWithZ_2017_2014.c***, plots the maximal difference of fits according to Z value

Reference

[1] Hubbell JH. Summary of existing information on the incoherent scattering of photons, particularly on the validity of the use of the incoherent scattering function. Radiation Physics and Chemistry. 1997;50:113-24.

[2] Cullen DE. A simple model of photon transport. Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms. 1995;101:499-510.