New PhotoElectric effect model for GeantV/Geant4

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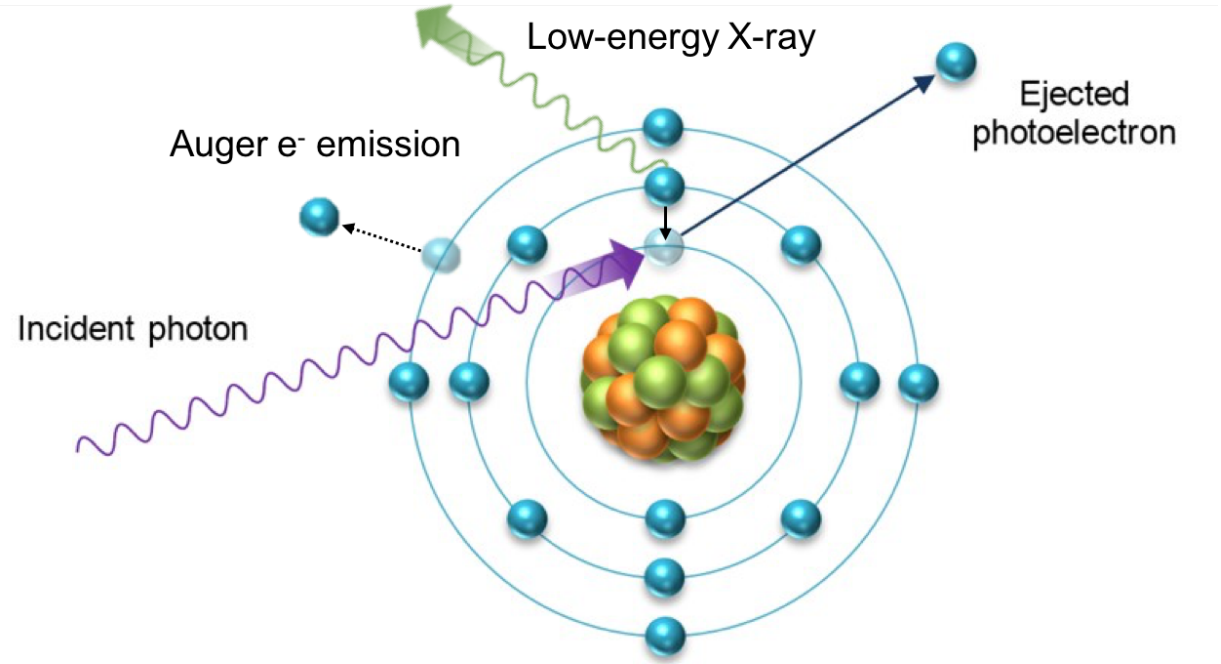
Overview

Introduction

In the photo-electric absorption process a **photon is absorbed** by an atom and an **electron is emitted** with an energy:

$$E_{photoelectron} = E_{\gamma} - B_{shell}(Z_i) \tag{1}$$

The atom, left in an excited state with a vacancy in the ionized shell, decays to its ground state through a cascade of radiative and non-radiative transitions with the **emission of characteristic x-rays** and **Auger and Coster-Kronig electrons**.



PhotoElectric effect in Geant4

Geant4 photoelectric package

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Geant4 photoelectric package

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- Models developed for HEP applications: **standard electromagnetic package**
  - *G4PEEffectFluoModel*: V. Grichine, M. Mairie and V. Ivanchenko
- Models based on the **Livermore** evaluated data Library
  - *G4LivermorePhotoElectricModel*: A Ivanchenko and V. Ivanchenko
  - *G4LivermorePolarizedPhotoElectricModel*: Sebastien Incerti, A.Forti, M.G.Pia, A. Mantero and V. Ivanchenko
- C++ implementation of the **Penelope** 2001 models
  - *G4PenelopePhotoElectricModel*: L. Pandola

If photon energy is below the lowest available energy, the cross section is computed for this lowest energy, to ensure the **gamma is absorbed by photoabsorption at any energy**.

- This is done for transport reasons in HEP
- As a result, all media is non-transparent to low-energy gamma rays

Standard electromagnetic package: G4PEEffectFluoModel

- **The atomic cross sections.** Biggs et al. parameterization from SANDIA tables, with separate fit of coefficients, is used :

$$\sigma(Z, E_\gamma) = \frac{a(Z, E_\gamma)}{E_\gamma} + \frac{b(Z, E_\gamma)}{E_\gamma^2} + \frac{c(Z, E_\gamma)}{E_\gamma^3} + \frac{d(Z, E_\gamma)}{E_\gamma^4} \quad (2)$$

- **The sub-shell** it's chosen in a **deterministic way**, not sampled:
  - the first inner shell having a binding energy $B_{shell} < E_\gamma$
- Shell atomic energies are taken from *G4AtomicShells* data
- **The photoelectron angle** is calculated according to the Sauter-Gavrila distribution for K shell, which is correct only to zero order in αZ

Low Energy Package: G4LivermorePhotoElectricModel

- The **total photoelectric and single shell cross-sections** are tabulated from threshold to 600keV. Above 600keV EPDL97 cross sections are parameterised as following:

$$\sigma(E) = \frac{a_1}{E} + \frac{a_2}{E^2} + \frac{a_3}{E^3} + \frac{a_4}{E^4} + \frac{a_5}{E^5} \tag{3}$$

  - The accuracy of such parameterisation is better than 1%.
- The **sub-shell** is sampled according to the relative cross-sections of all sub-shells.
- Two **angular generators**:
  - *G4SauterGavrilaAngularDistribution*: same as in the standard model - default option
  - *G4PhotoElectricAngularGeneratorPolarized*: double differential cross section generator derived from Gavrila's calculations, which can also handle polarized photons.

Low Energy Package: G4PenelopePhotoElectricModel

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- The **direction of the electron** is sampled according to the Sauter distribution. Introducing the variable $\nu = 1 - cos\theta_e$, the angular distribution can be expressed as:

$$p(\nu) = (2-\nu)[\frac{1}{A+\nu} + \frac{1}{2}\beta\gamma(\gamma-1)(\gamma-2)]\frac{\nu}{(A+\nu)^3} \tag{4}$$

where

$$\gamma = 1 + \frac{E_e}{m_e c^2},\ A = \frac{1}{\beta} - 1 \tag{5}$$

where E_e is the electron energy, m_e its rest mass and β its velocity in units of the speed of light c.

New G4/GV photoelectric models development

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  - Accuracy of cross-sections with new available data (livermore/epics2014)
  - CPU perfomance
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  - **Move to Ebel's parametrization**: K- shell cross sections based on Ebel's parameterisation produce more accurate results than EPDL in some test cases close to absorption edges for energy range [1KeV- 300 KeV]

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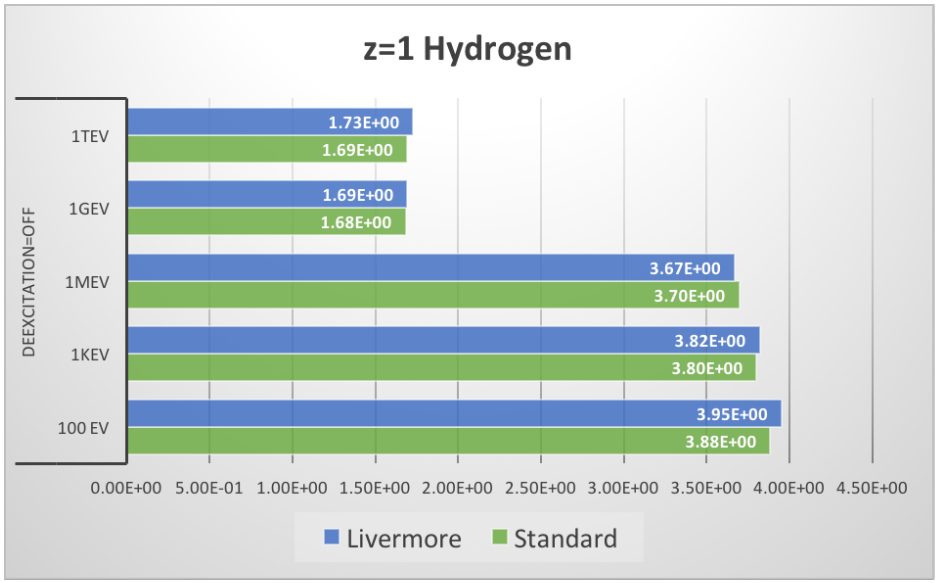
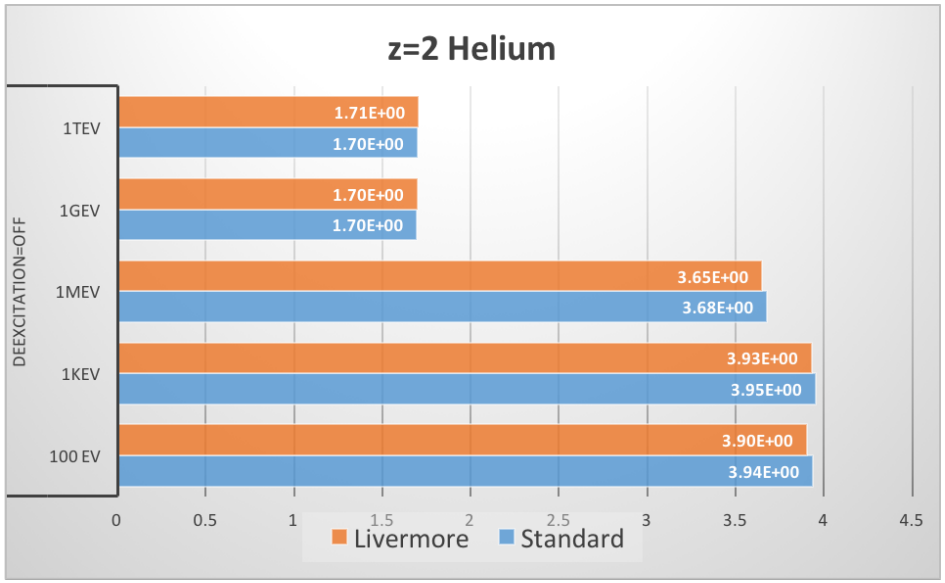
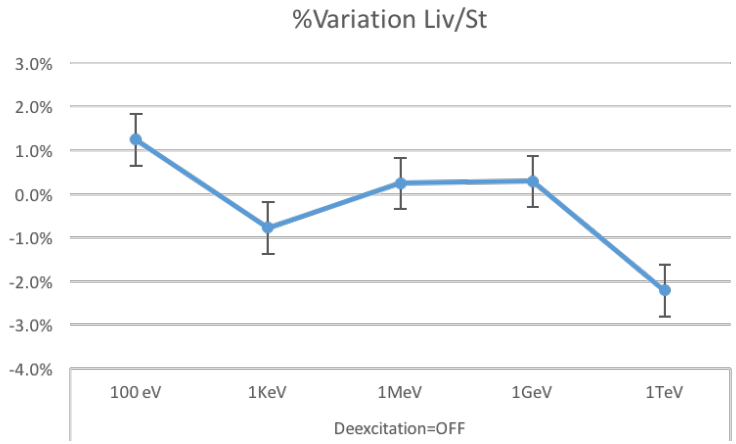
  - **Salvat and Sabatucci** new formulation (Penelope 2015 version):uses the same theory as in Scofield (1973) of the EPDL tables, but more accurate numerical algorithms.

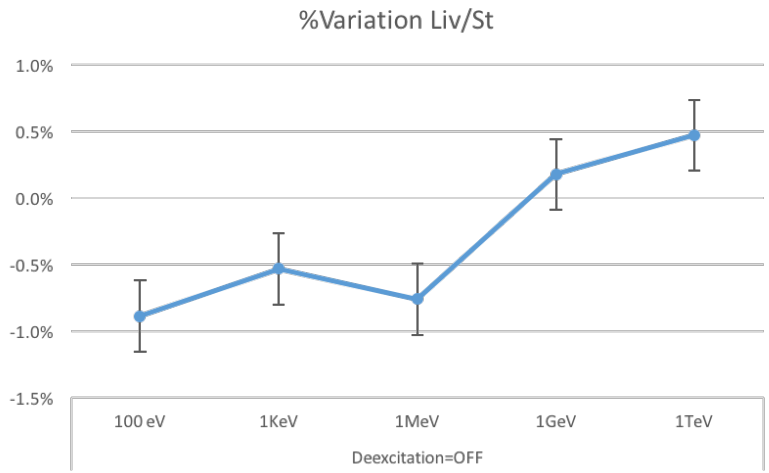
Livermore vs Standard - execution time

Model level test, $\#particles = 10^7$, $\#repetitions = 10$









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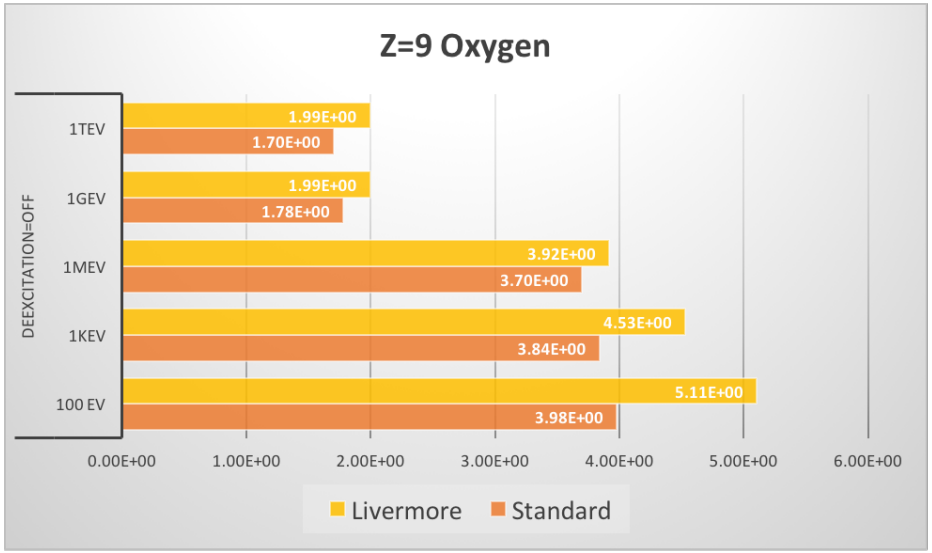

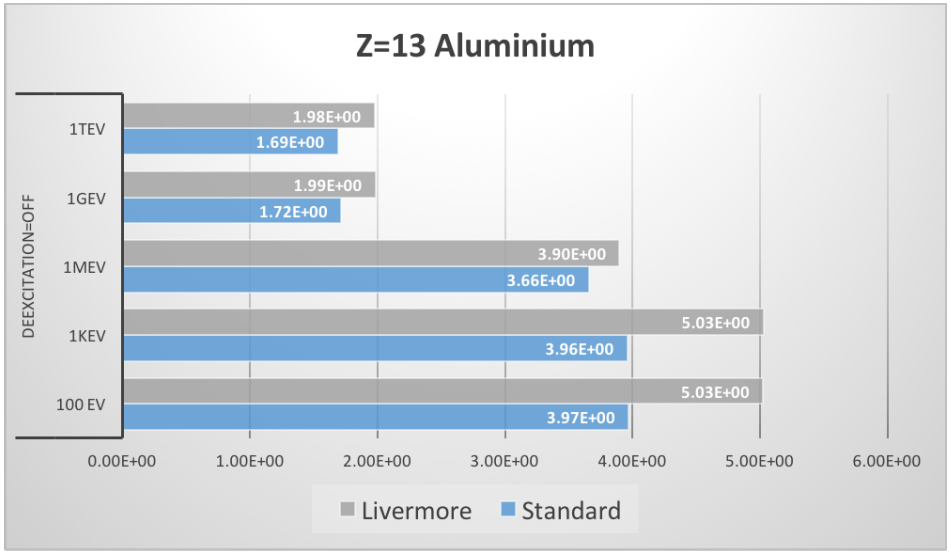

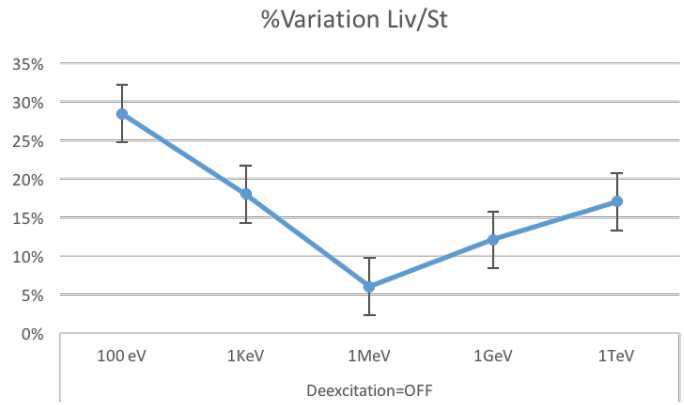

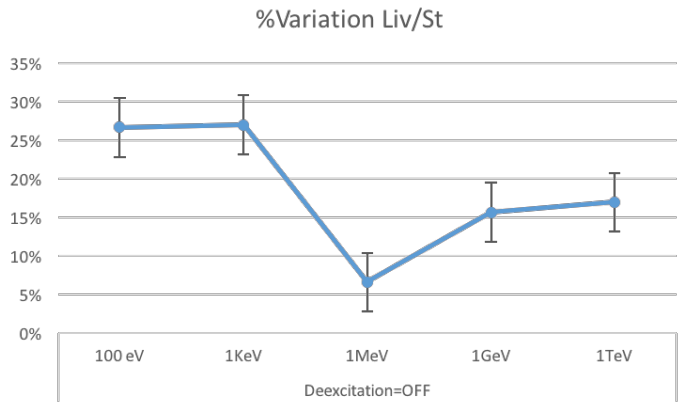

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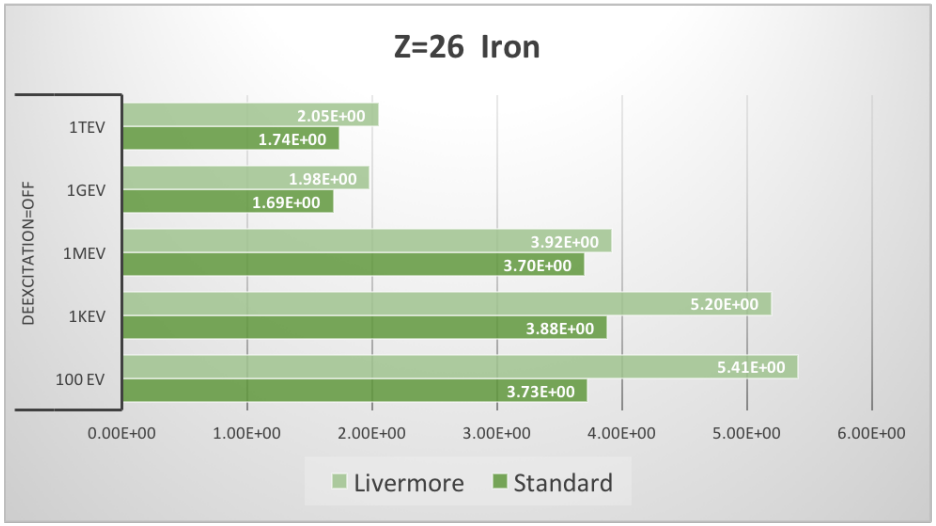
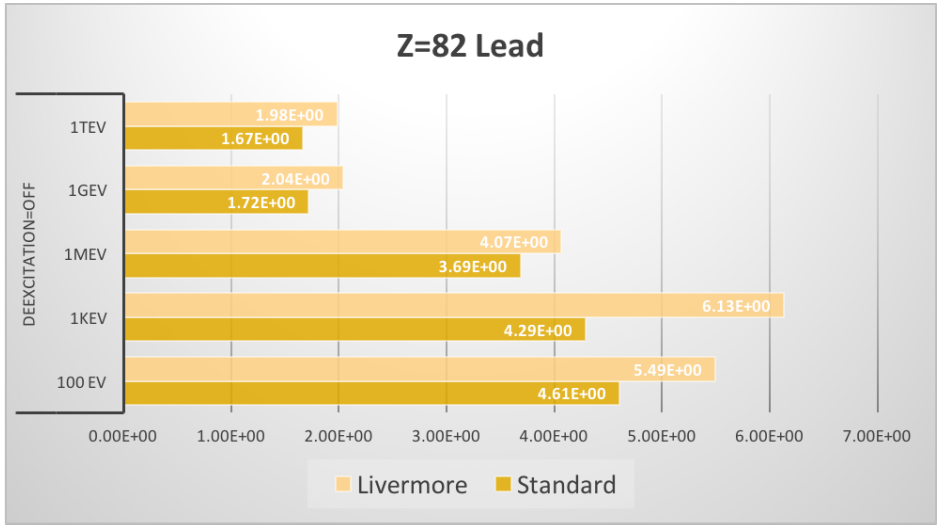
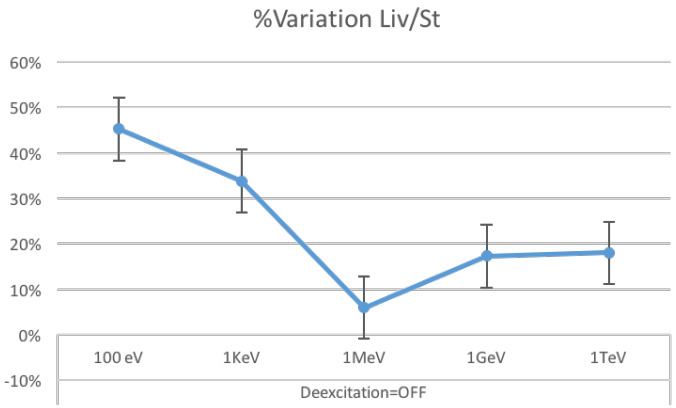
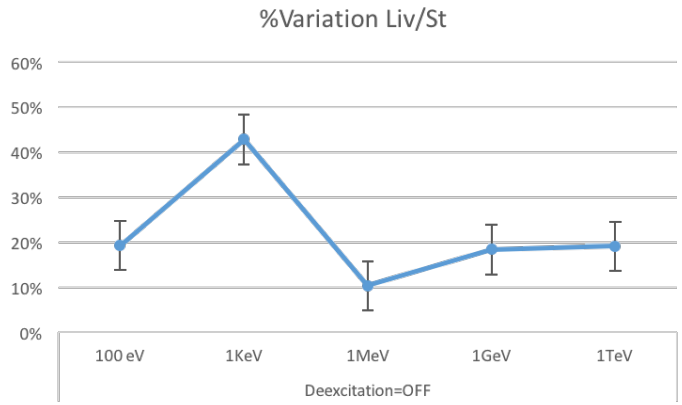


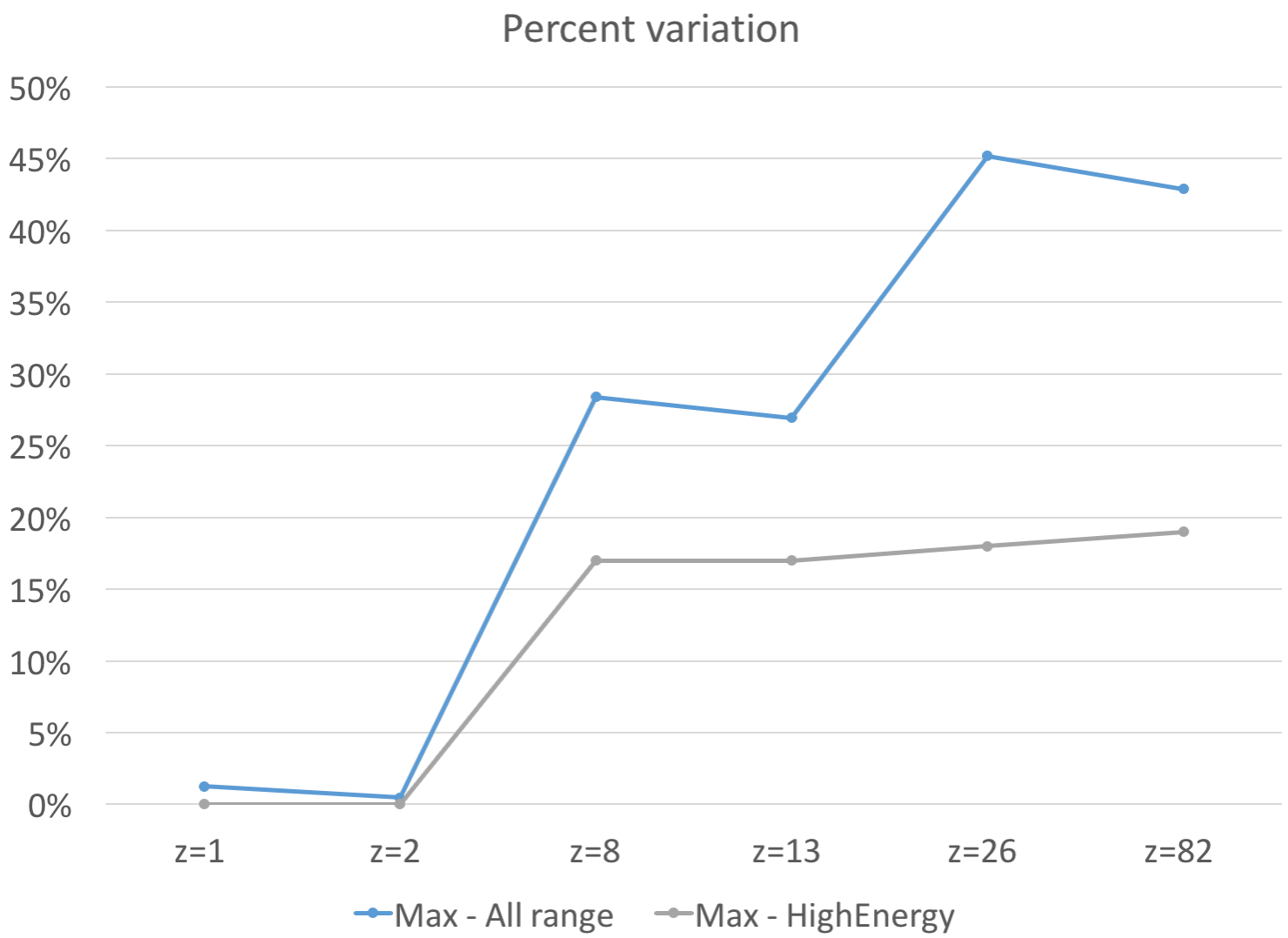




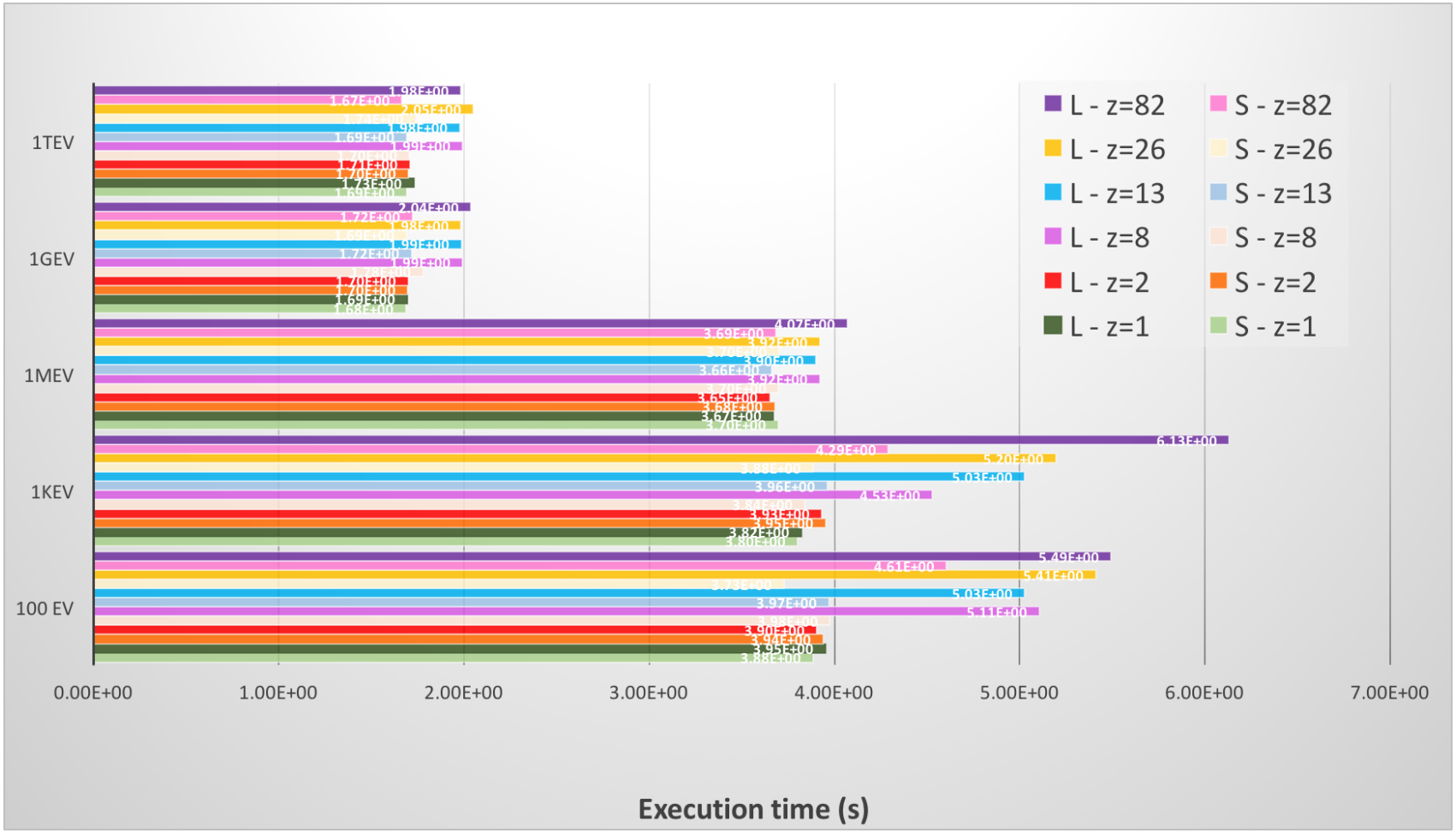


Livermore vs Standard percent variation

Max percent variation: all energies vs $E >= 1MeV$

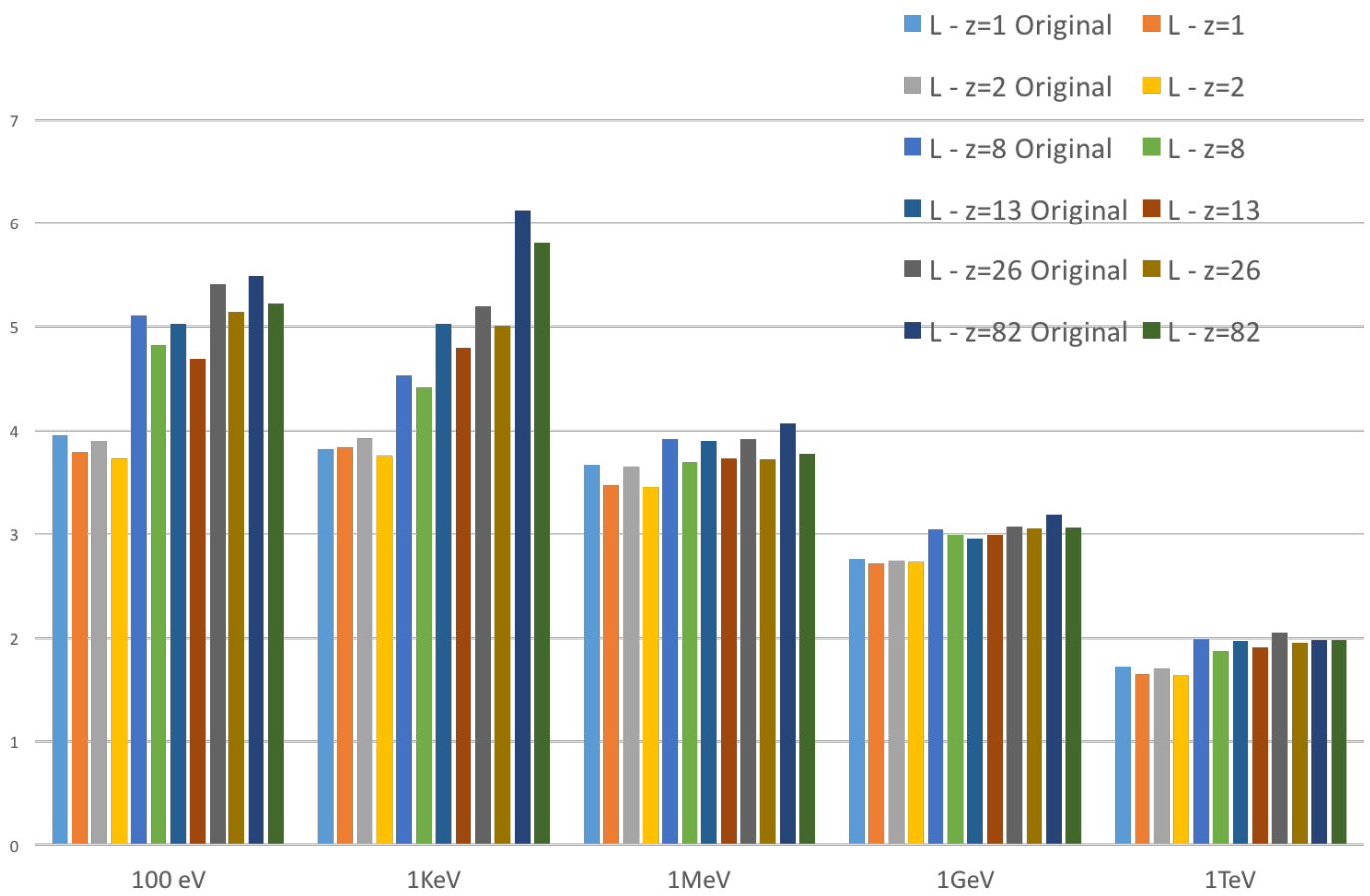


Livermore vs Standard - Angular distribution ON



- The standard angular distribution has a threshold at $\sim 26 MeV$
- Greater differences are observable at low energies and for heavier elements

New Penelope-like angular distribution



Achievements:

- Increased threshold from 26MeV to 100MeV
- Speedup between 4% and 10% in most cases

Unit test and benchmark of improved PELivermore model

The improved Livermore model has been included in 10.3ref04 and tested:

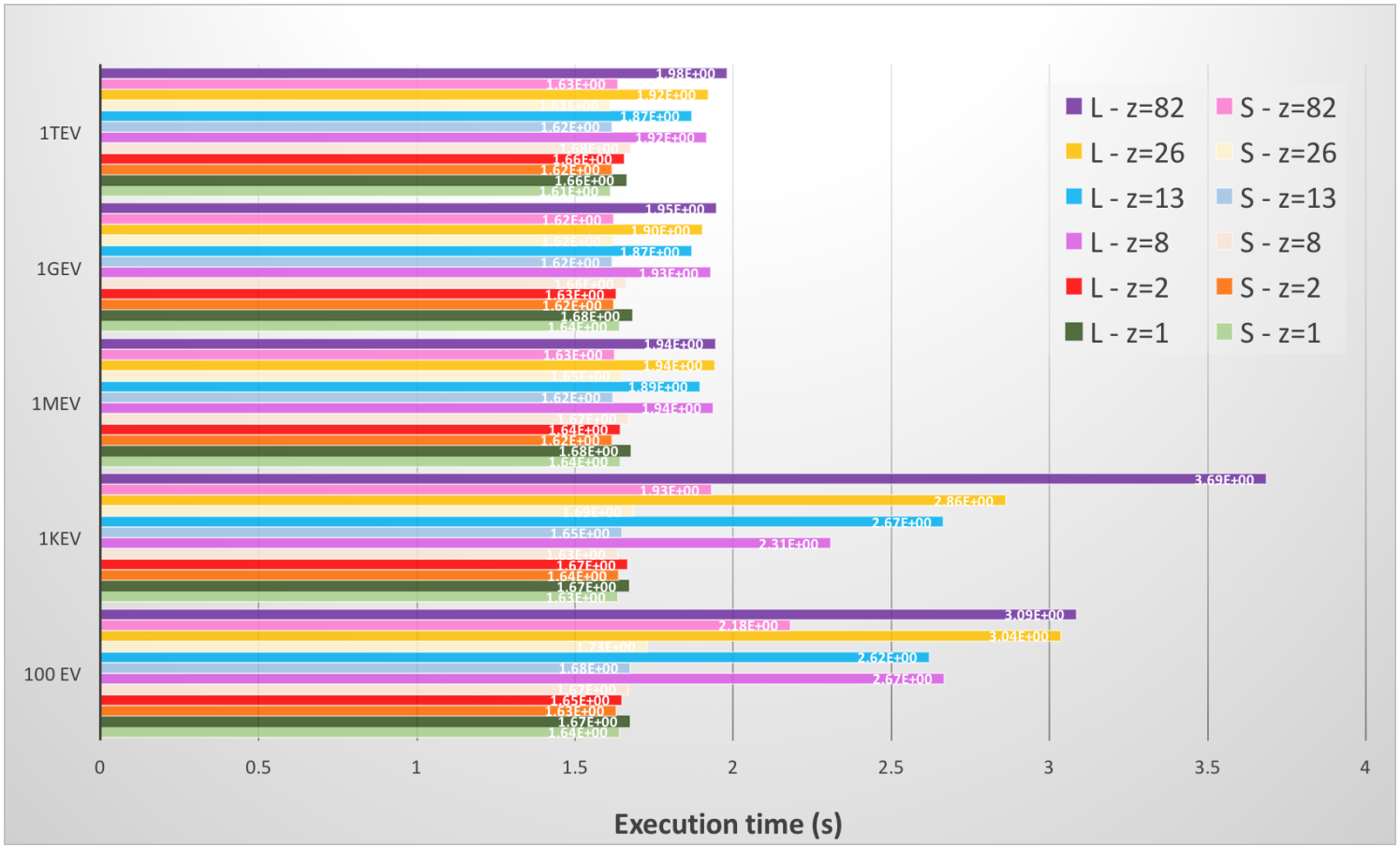
- Results for 10.3ref04 are **stable** compared to 10.3ref03
- No visible degradation of any result
- Validation results available at https://geant4-tools.web.cern.ch/geant4-tools/emtesting/

Version 10.3ref04 with Livermore model for Rayleigh and Photo-effect used as default in Em physics list, to check **CPU performance**:

- Improved quality of photon cross sections that may slightly affect shower shape
- 1% slowdown for Higgs sample
- 2% slowdown for e- showers

$->$ Optimization on photoelectric model might recover CPU performance.

Livermore vs Standard - Angular distribution OFF

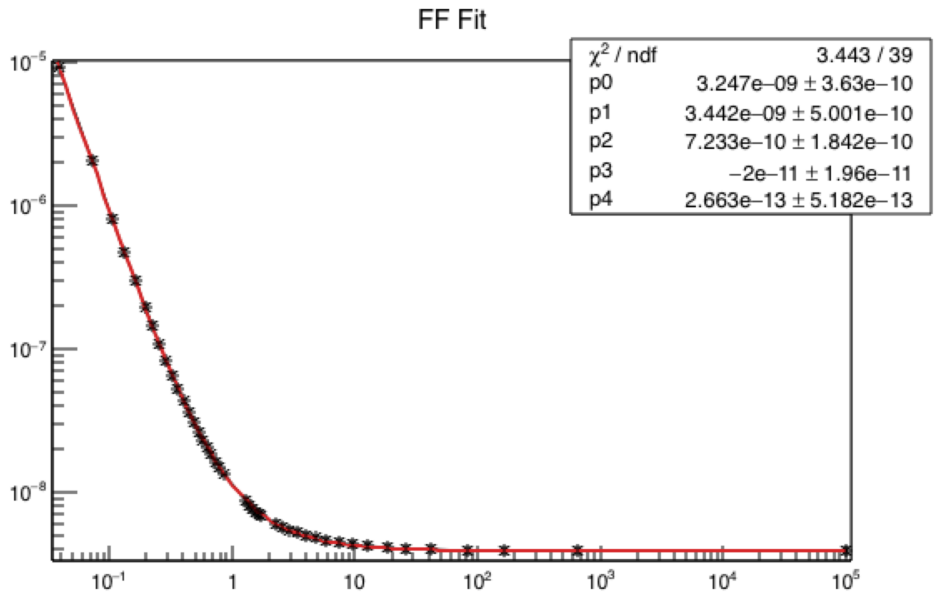


- Switching off the angular distribution we clearly see a dependency on the **energy** and on the **Z** of the material.
- This is dependent on a $600 KeV$ threshold between tabulated and parameterised cross sections (EPDL97)

New parameterisation - livermore/epics2014 data

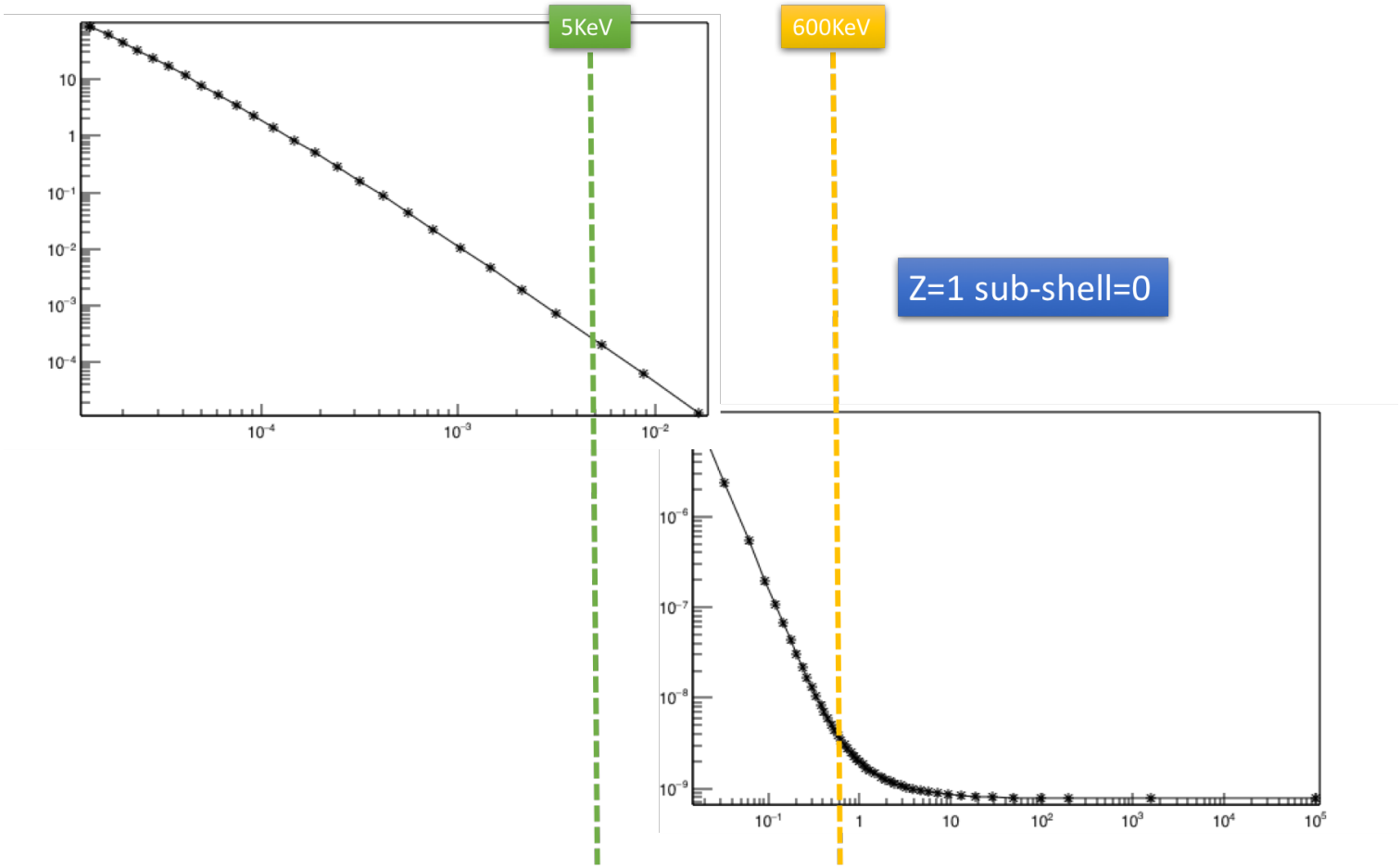
- New cross sections data recently introduced in Geant4: livermore/epics2014 (S. Incerti)
- New fit: adding one more parameter and performing two separate fits we can reduce the threshold from 600KeV to 5KeV.

$$\sigma(E) = \frac{a_1}{E} + \frac{a_2}{E^2} + \frac{a_3}{E^3} + \frac{a_4}{E^4} + \frac{a_5}{E^5} + \frac{a_6}{E^6} \tag{6}$$



- $E_\gamma >= 5KeV$: Two new fits in two different energy ranges
  - $E_\gamma \in [5KeV - 50KeV]$
  - $E_\gamma > 50KeV$
- $E_\gamma < 5KeV$:
  - Keep the parameterisation (under evaluation): high-energy physics simulations
  - Tabulated cross sections: low-energy physics simulations

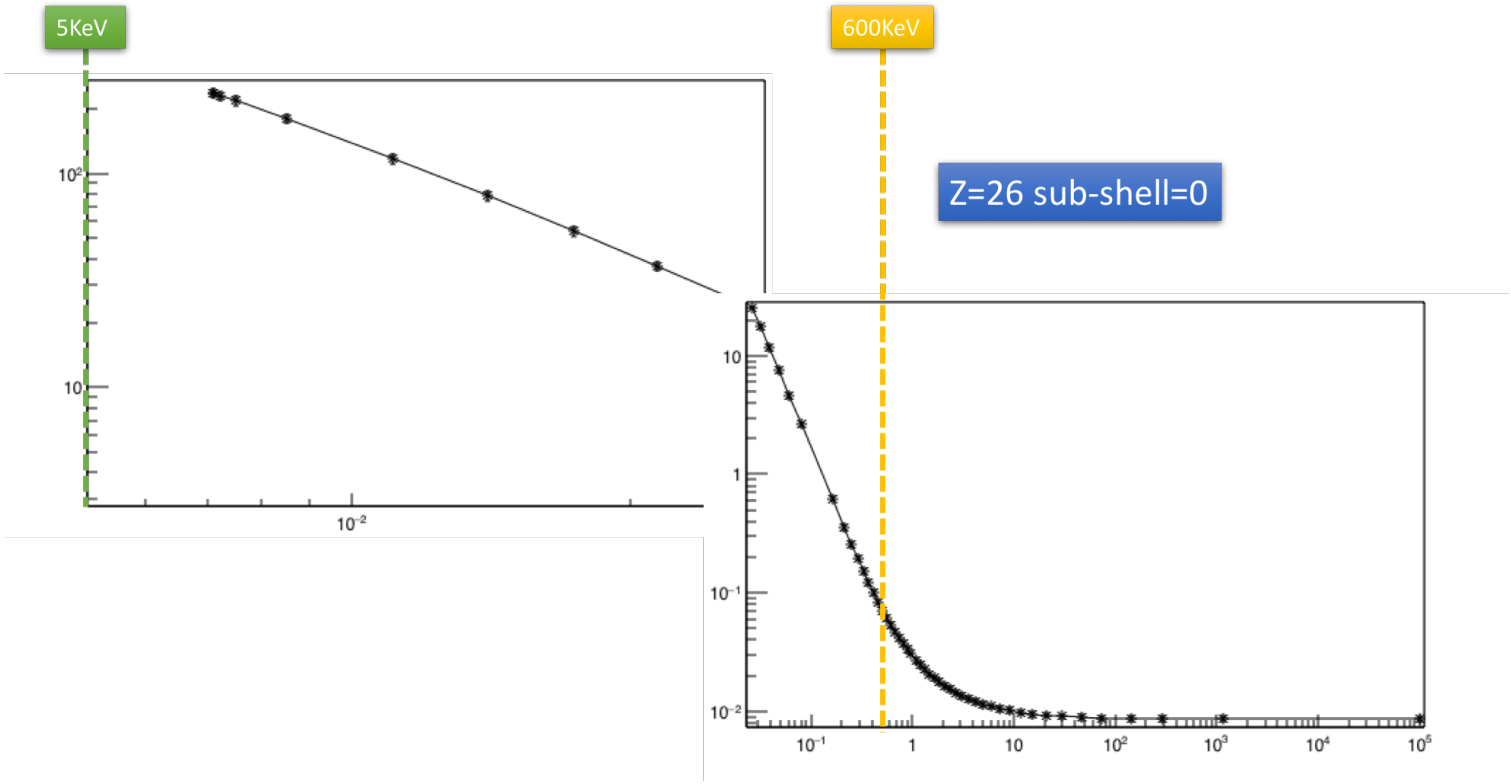
Two separate fits - new data



Achievements:

- Threshold moved from 600KeV to 5KeV
- Speedup measured (following slides)

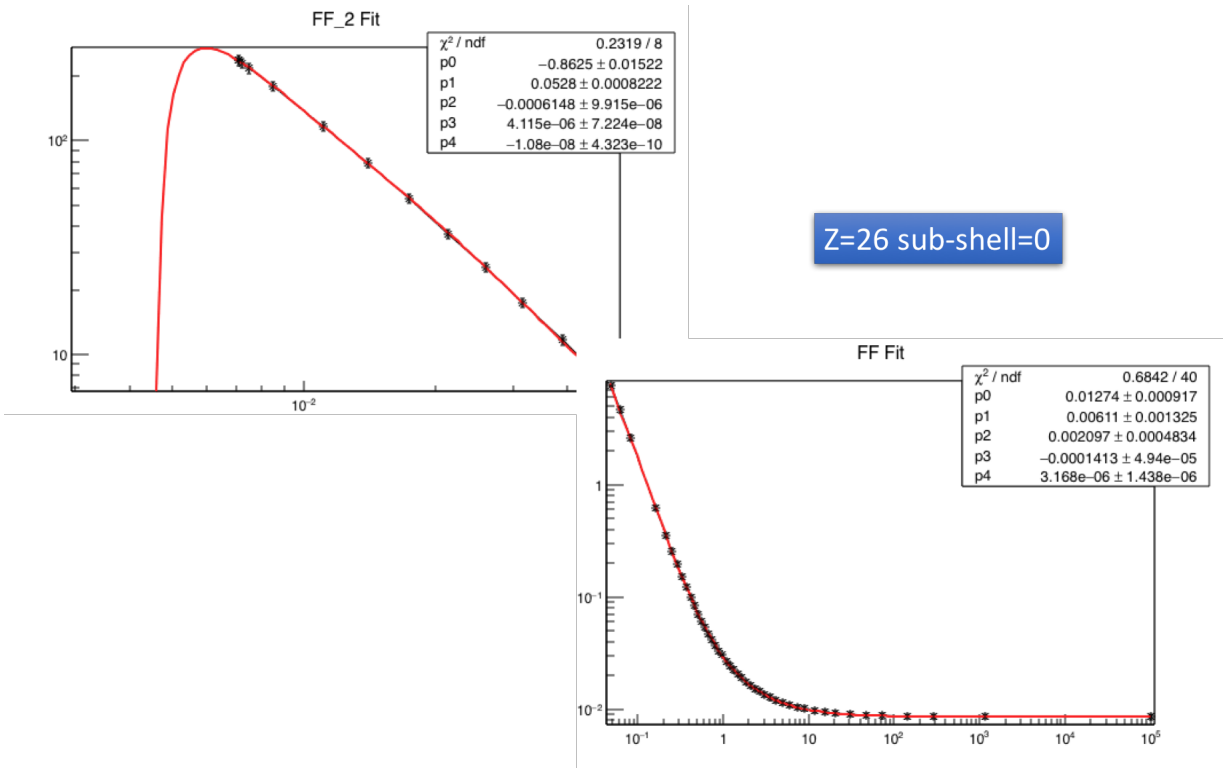
Two separate fits - new data



- In some cases we are able to cover all the spectrum with parameterization
- Especially for inner shells

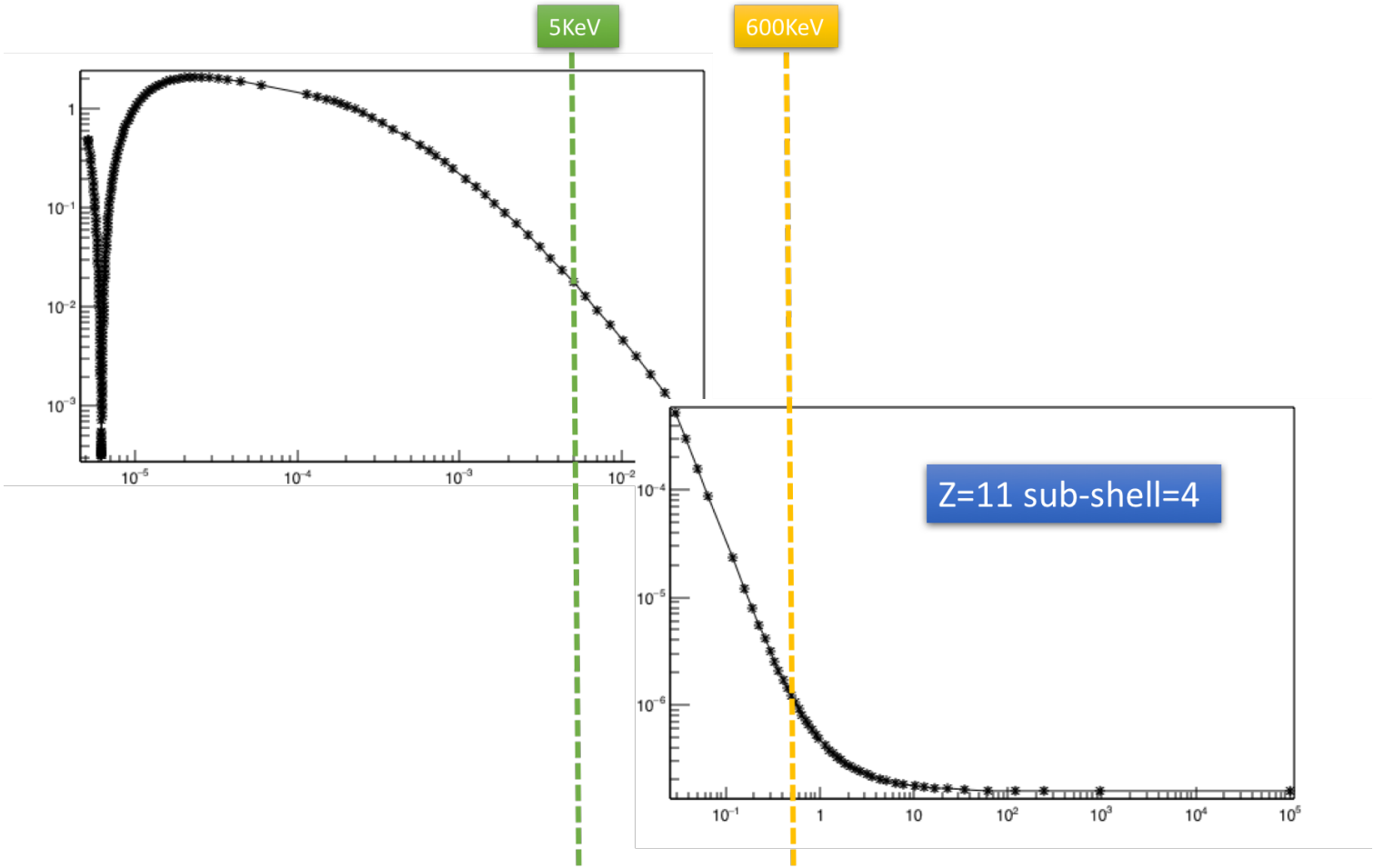
New parameterisation: example

- Two threshold limits: lowLim and highLim dynamically set.
- The continuity is assured fixing one parameter of the low energy fit, forcing it to be equal to the first point of the high-energy fit.
- HighLim threshold is then set to the closest real point available in the cross-section file.



Two separate fits - new data: special cases

- Outer shells present a non-monotonic behaviour, significantly at very low energies



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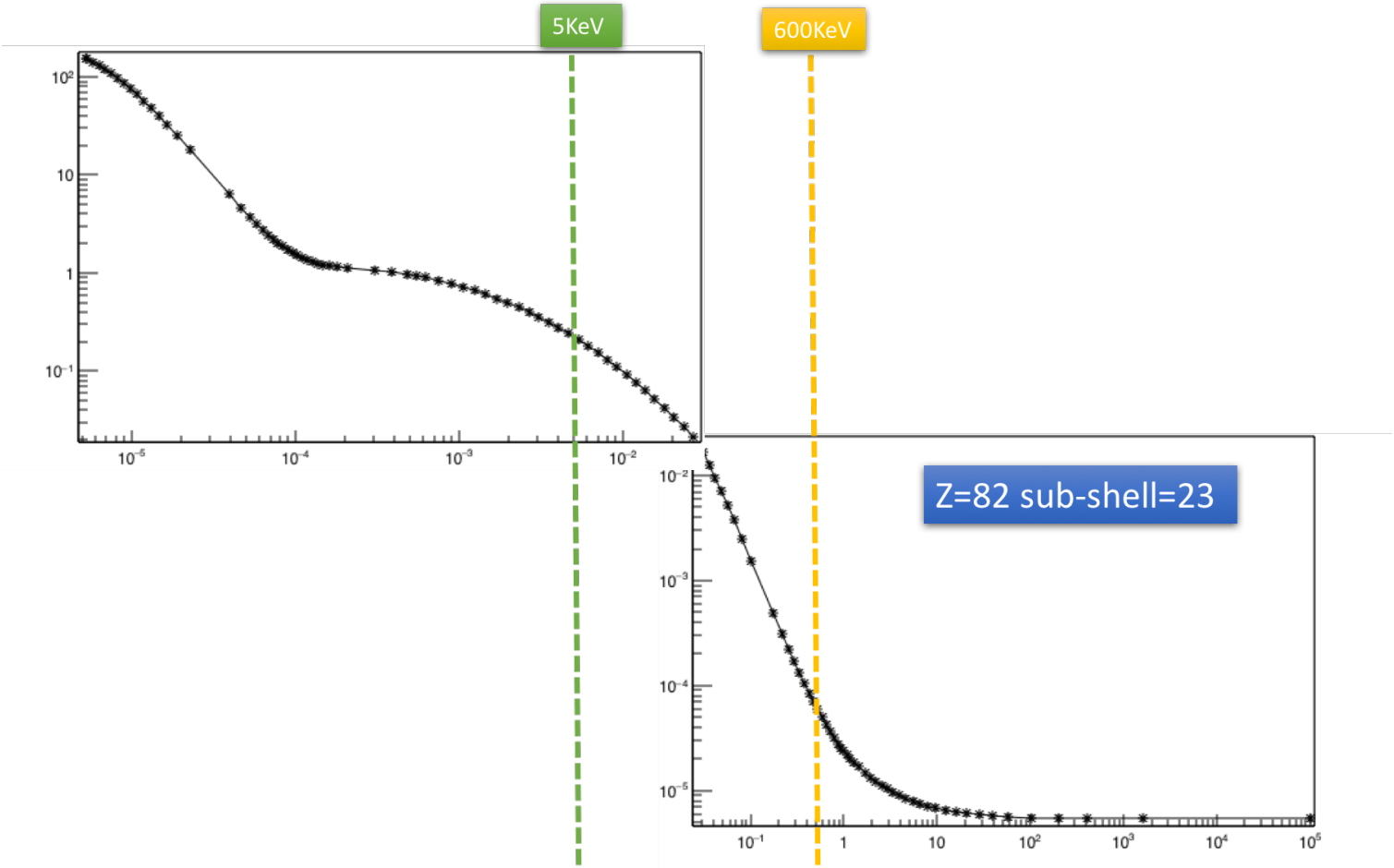
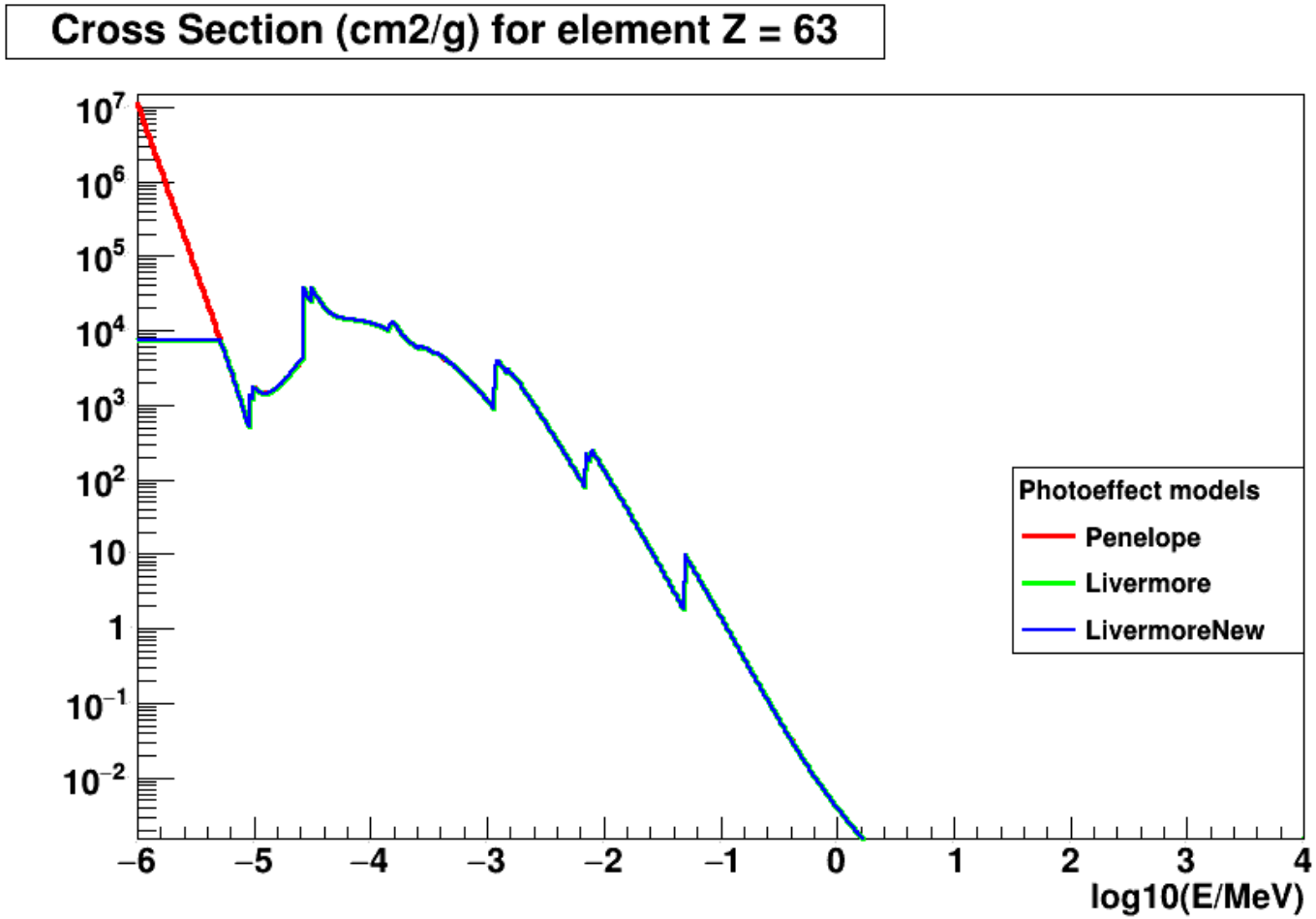


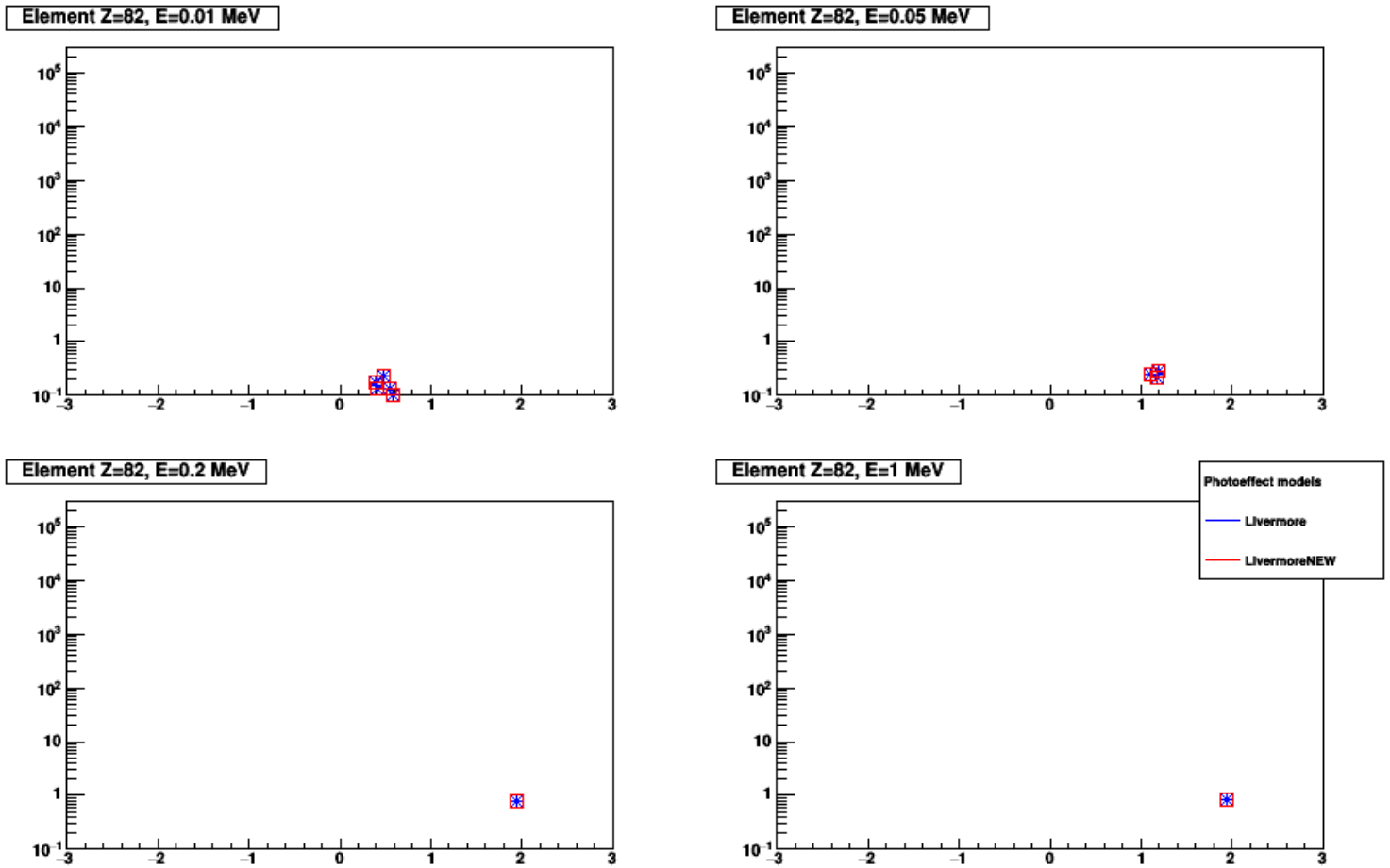
Geant4 models Cross-sections comparison

Observed cross-sections in respect with Penelope within 5%.

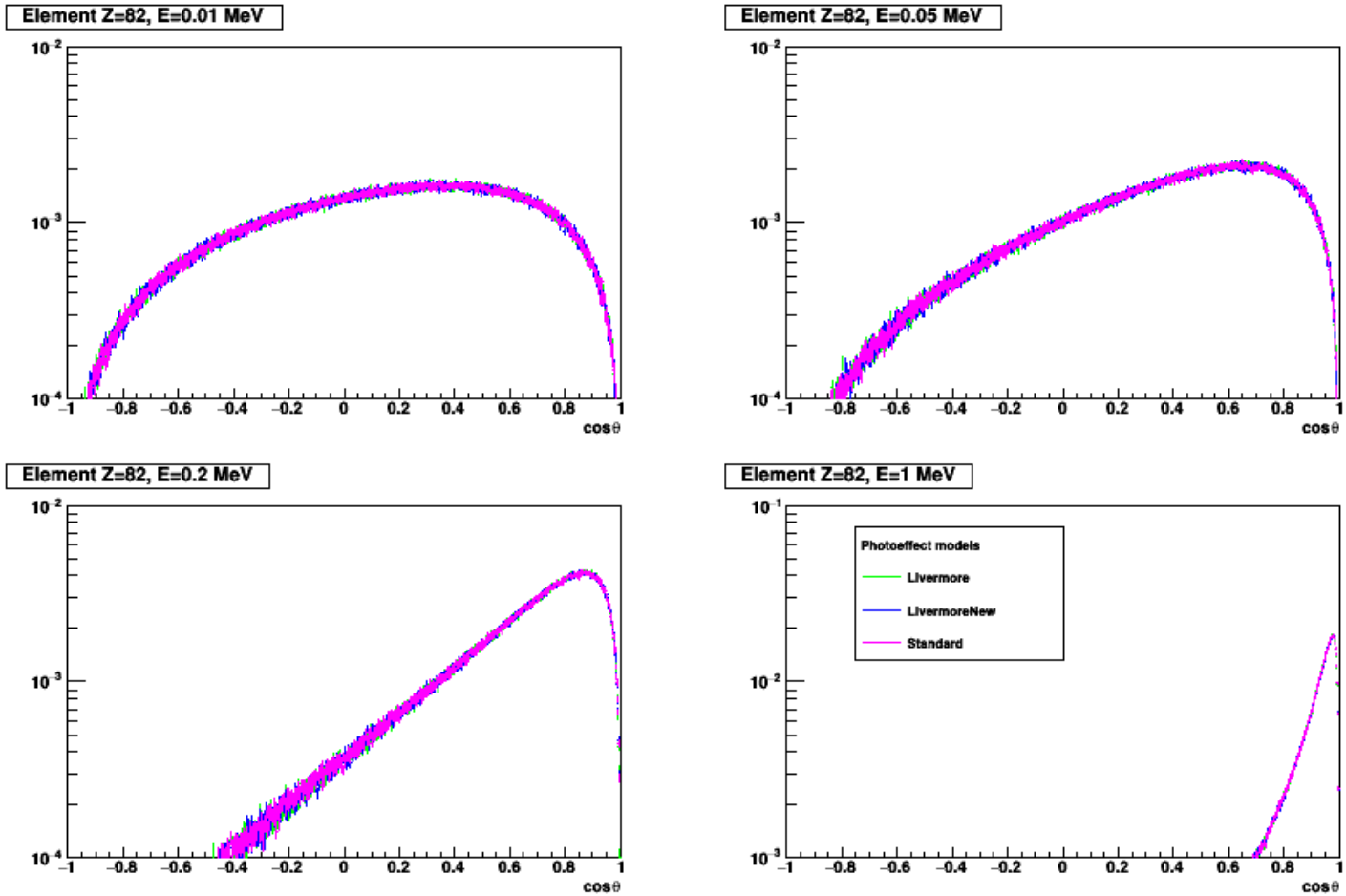


Geant4 models photoelectron energy comparison

Electron Energy Spectra Livermore respective to beam energy (i.e. $log10((energy - E1)/keV)$)

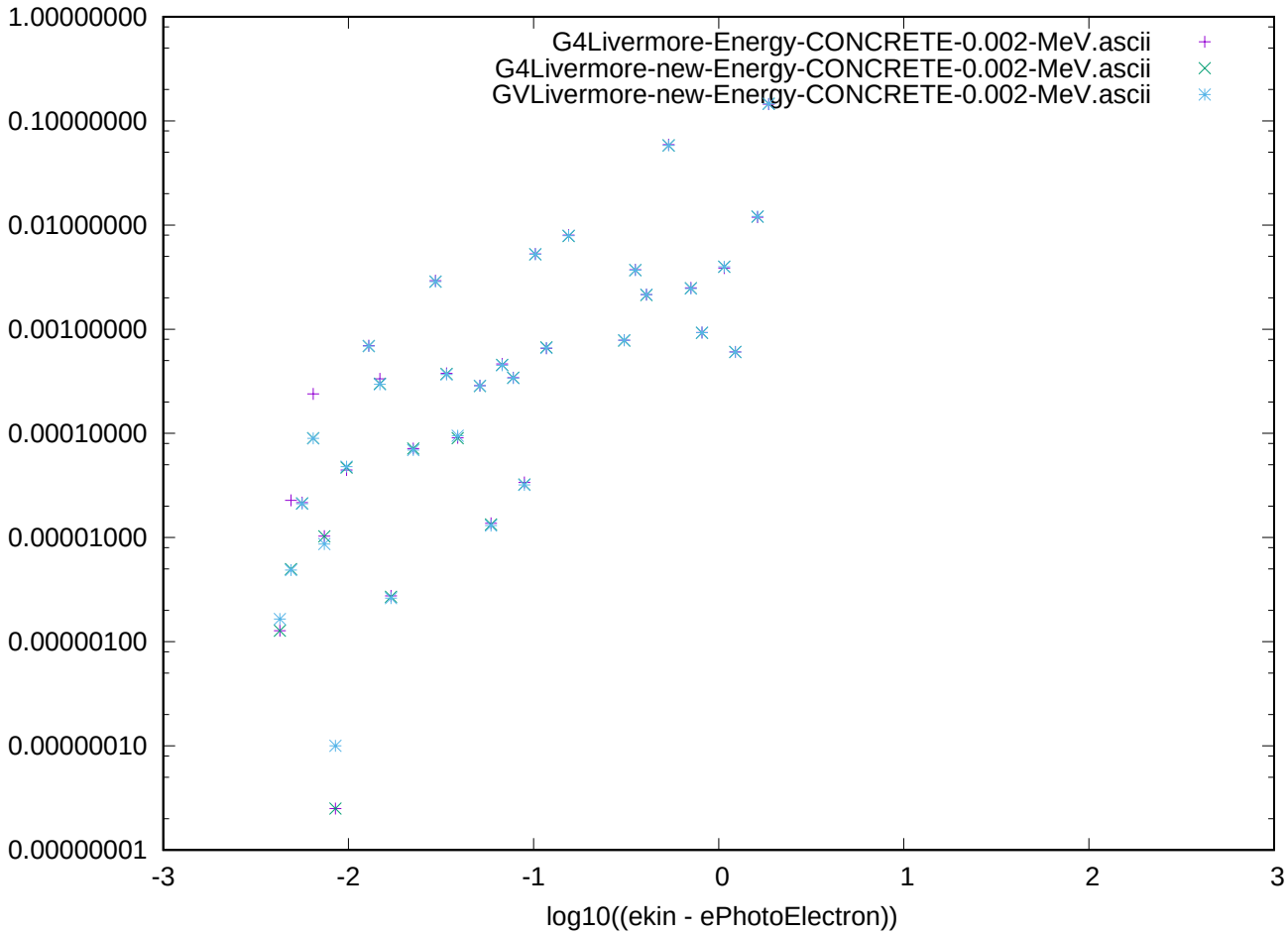


Geant4 models photoelectron angular comparison



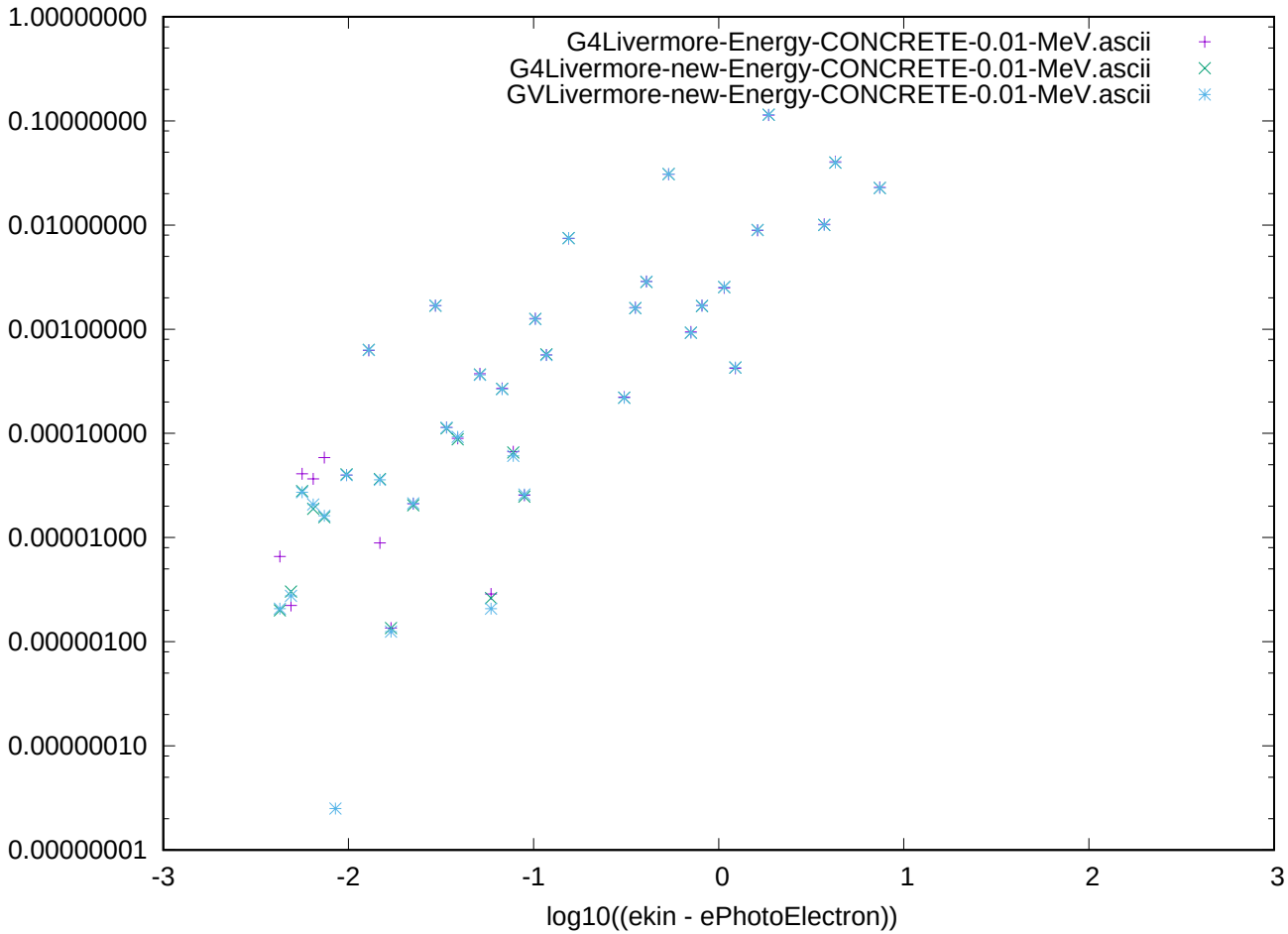
Geant4 and GeantV models photoelectron energy comparison

Test on CONCRETE, $E_\gamma = 0.002 MeV$, $\#particles = 10^7$



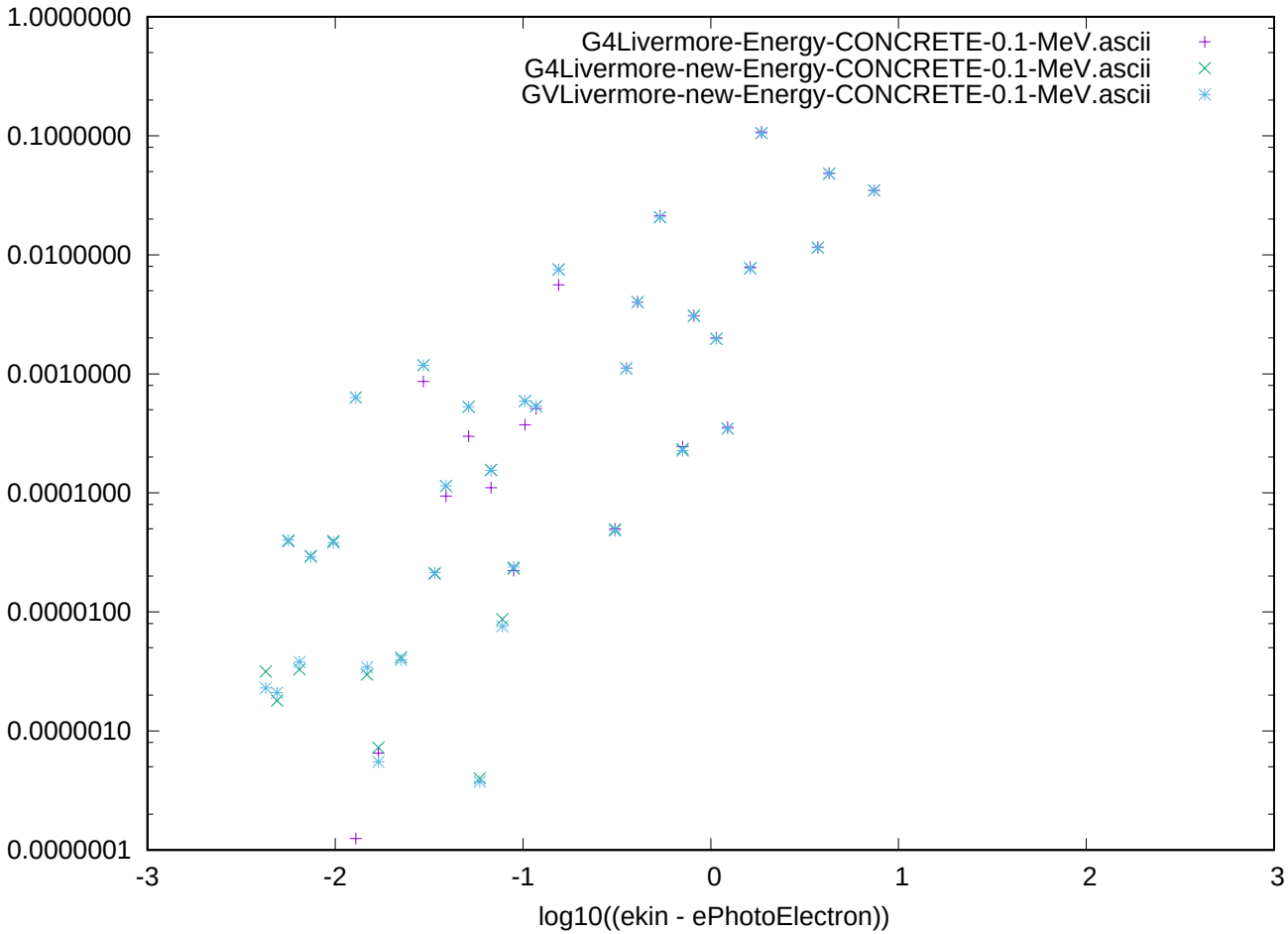
Geant4 and GeantV models photoelectron energy comparison

Test on CONCRETE, $E_\gamma = 0.01 MeV$, $\#particles = 10^7$



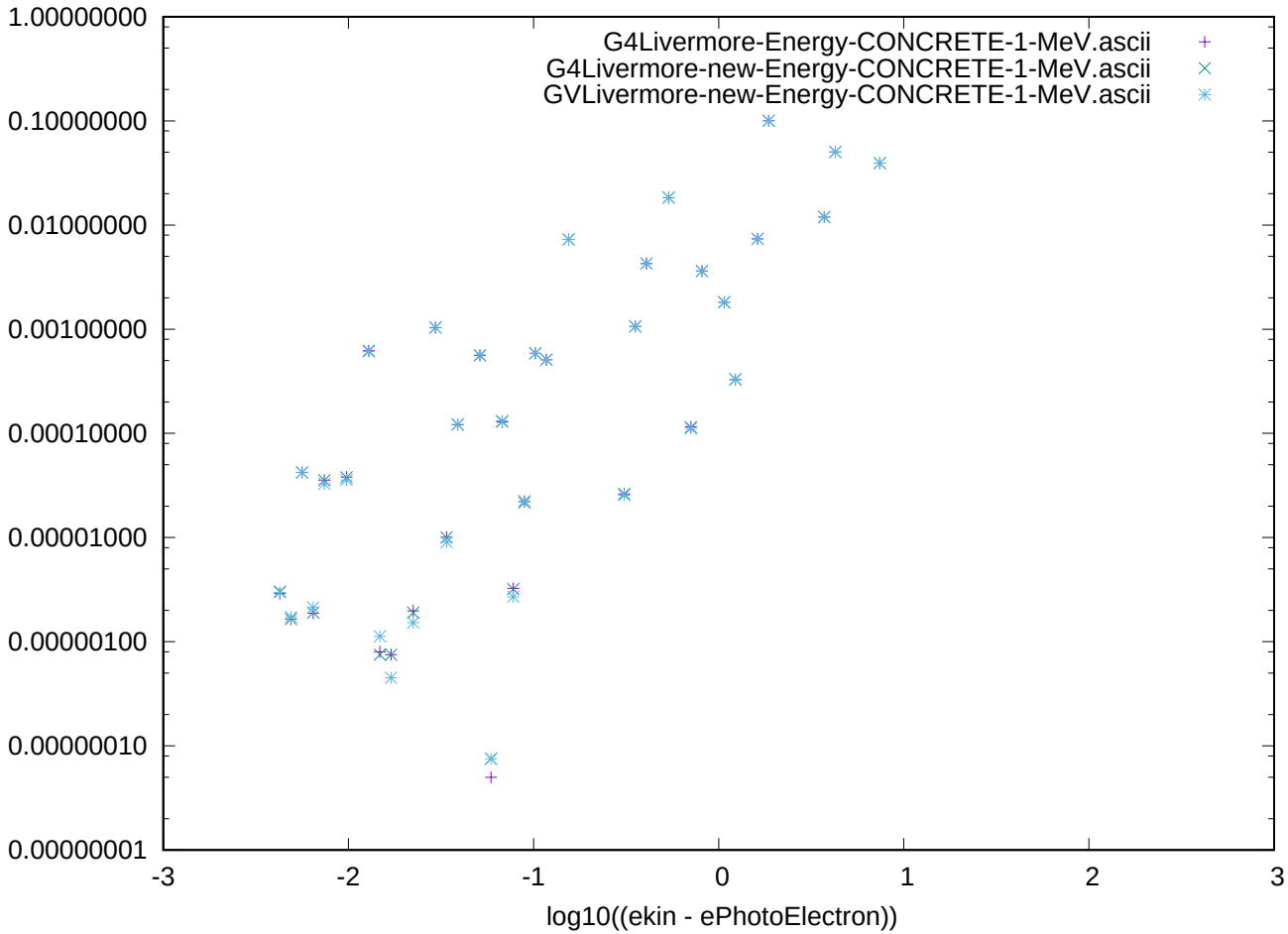
Geant4 and GeantV models photoelectron energy comparison

Test on CONCRETE, $E_\gamma = 0.1 MeV$, $\#particles = 10^7$



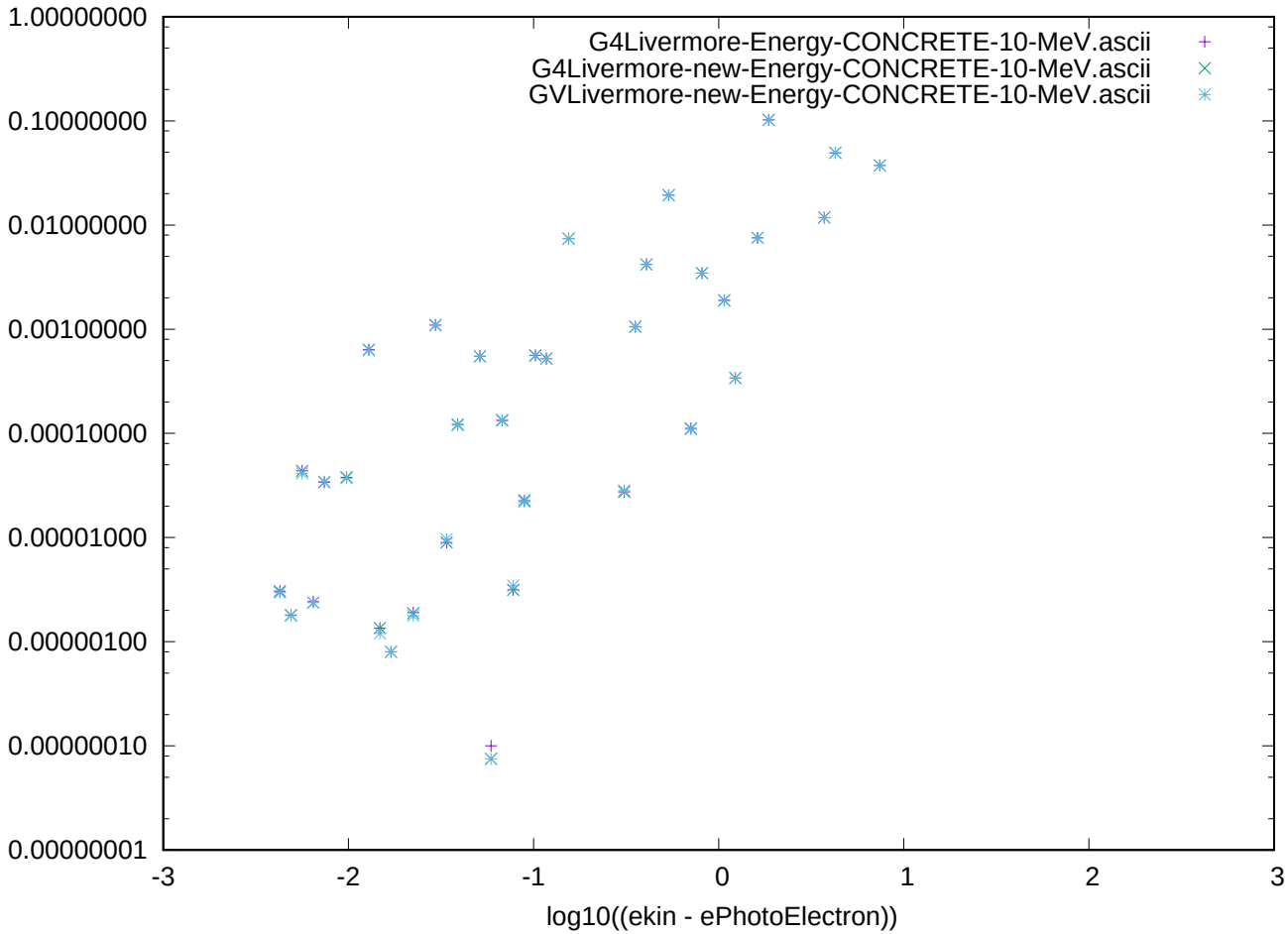
Geant4 and GeantV models photoelectron energy comparison

Test on CONCRETE, $E_\gamma = 1MeV$, $\#particles = 10^7$



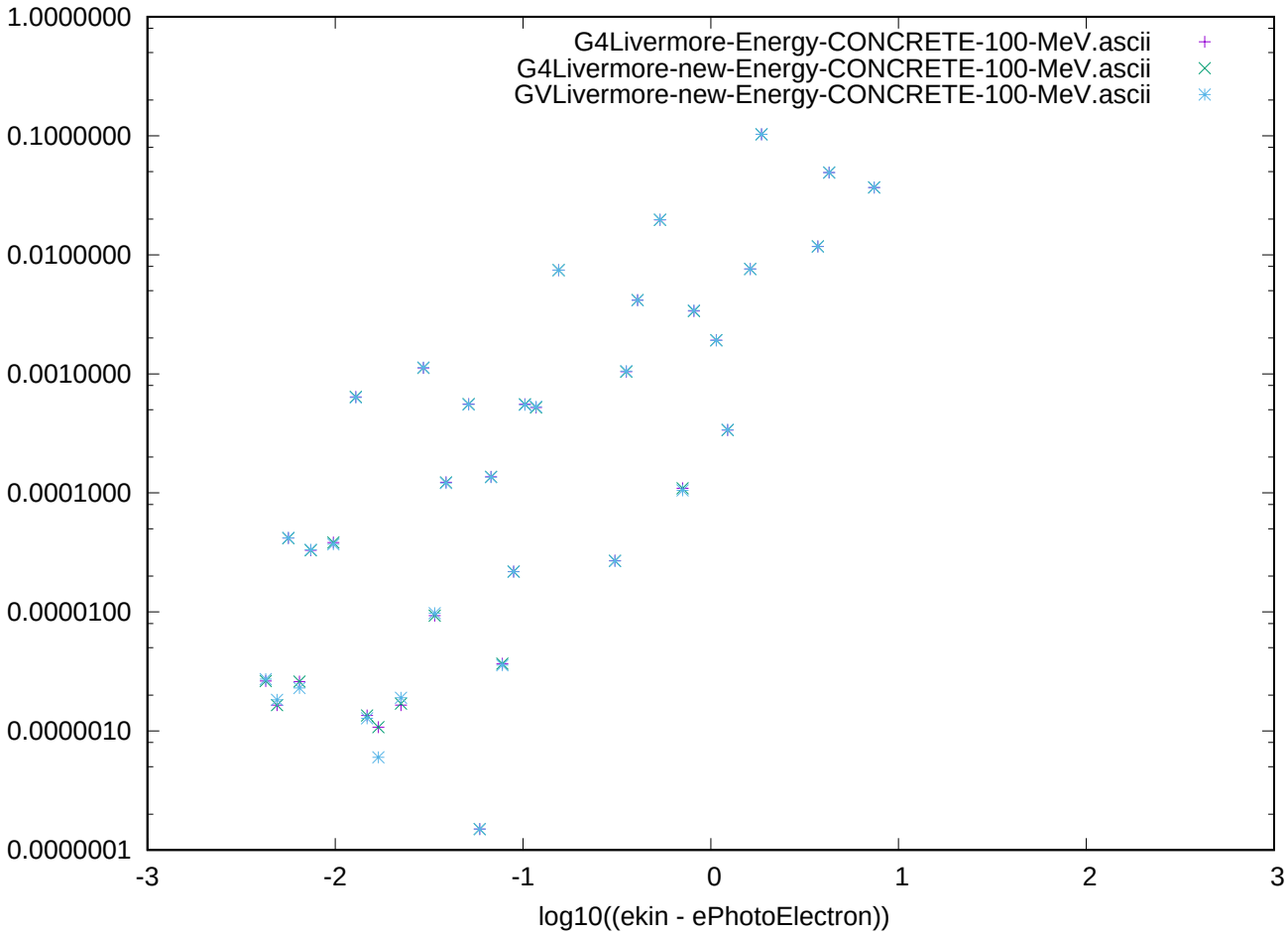
Geant4 and GeantV models photoelectron energy comparison

Test on CONCRETE, $E_\gamma = 10 MeV$, $\#particles = 10^7$



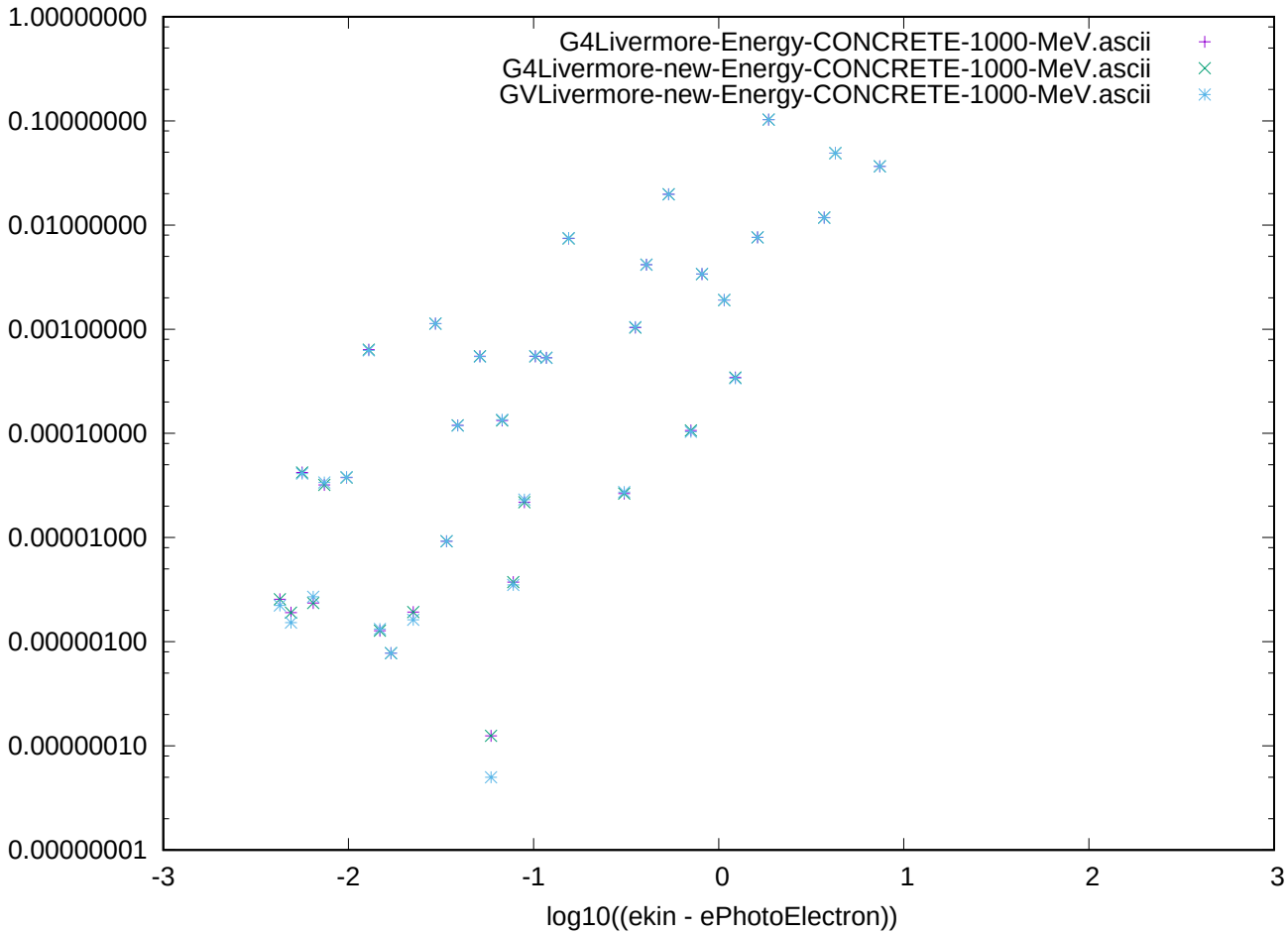
Geant4 and GeantV models photoelectron energy comparison

Test on CONCRETE, $E_\gamma = 100 MeV$, $\#particles = 10^7$



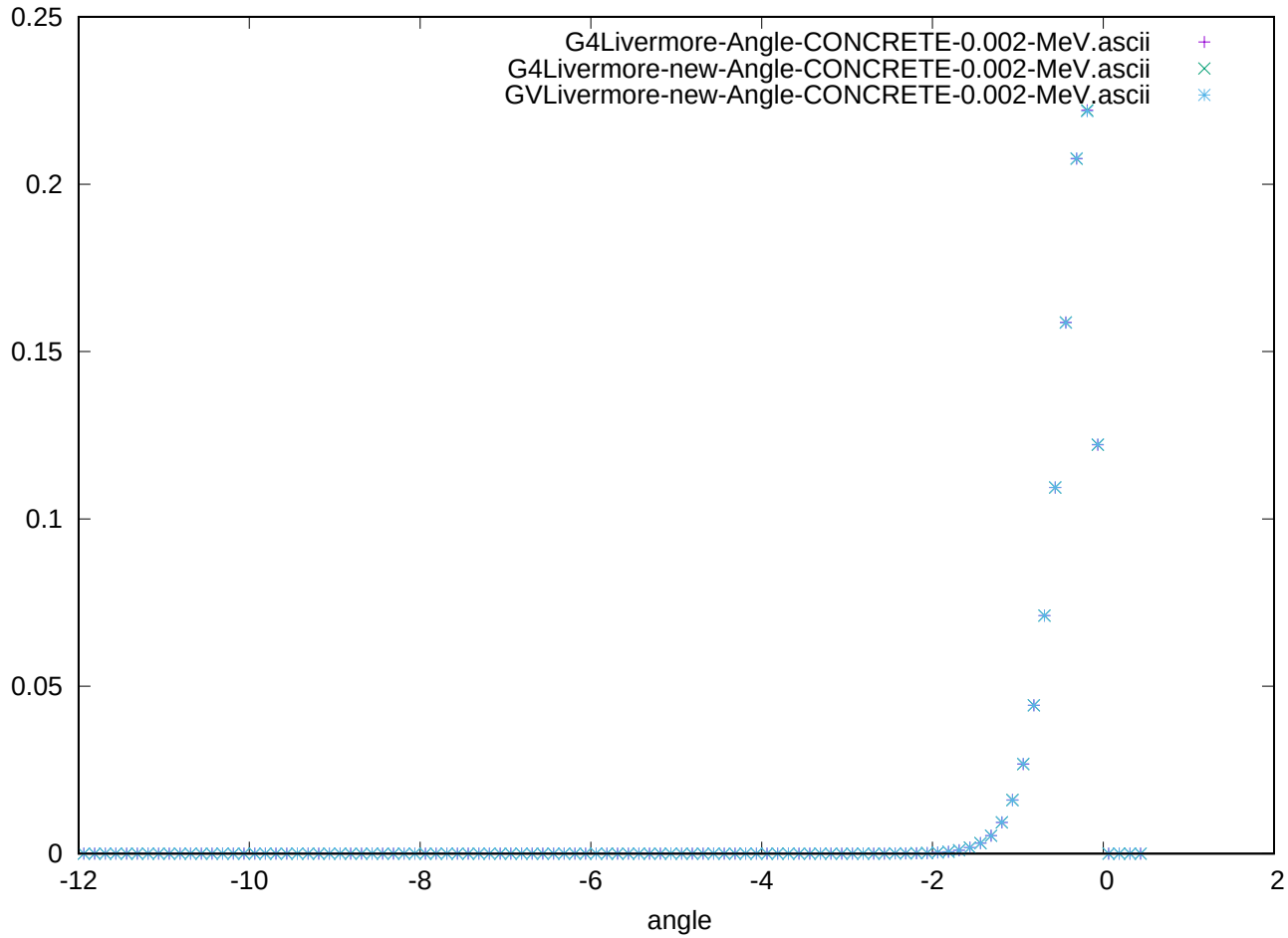
Geant4 and GeantV models photoelectron energy comparison

Test on CONCRETE, $E_\gamma = 1000 MeV$, $\#particles = 10^7$



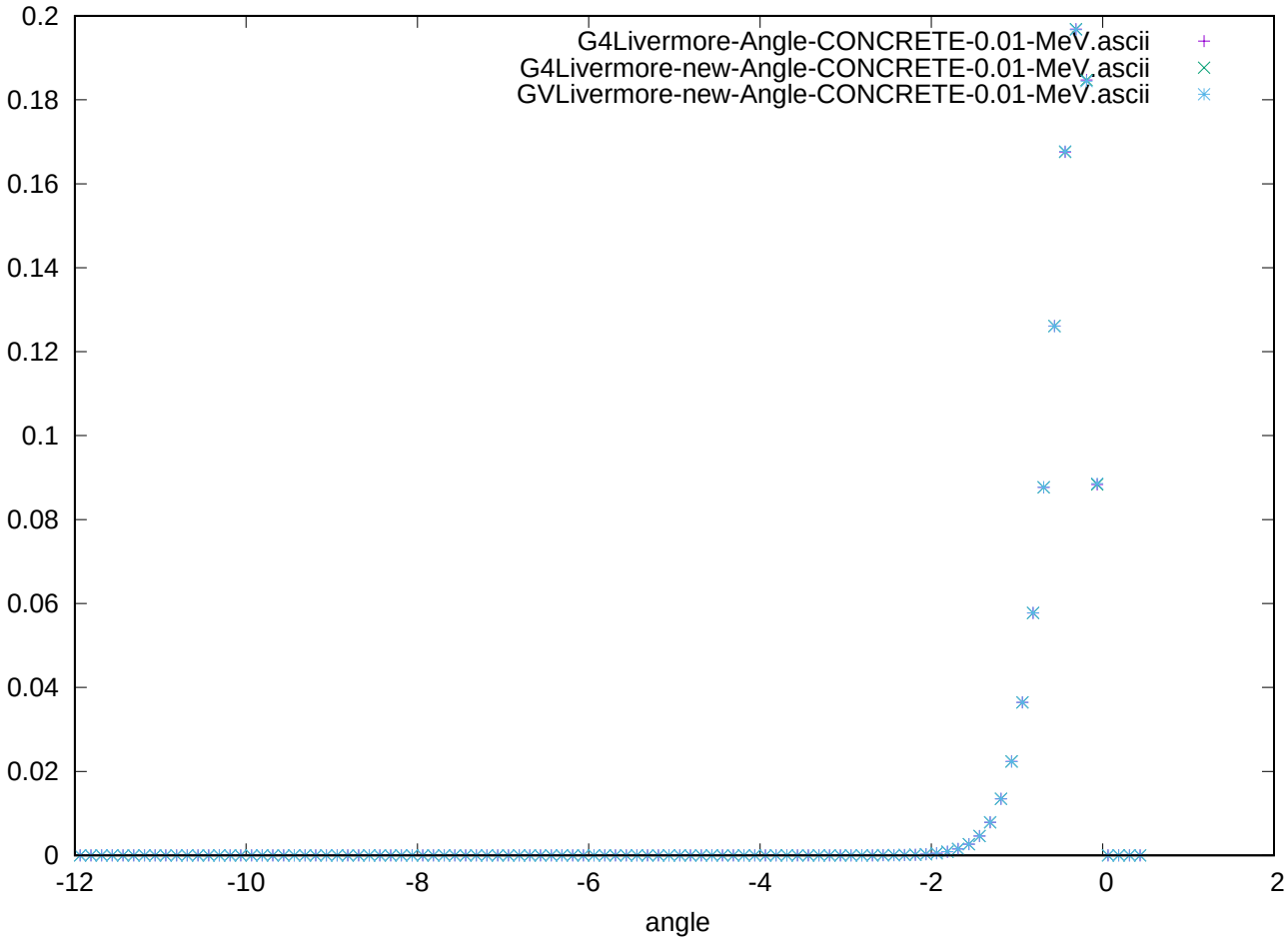
Geant4 and GeantV models photoelectron angular distribution

Test on CONCRETE, $E_\gamma = 0.002 MeV$, $\#particles = 10^7$



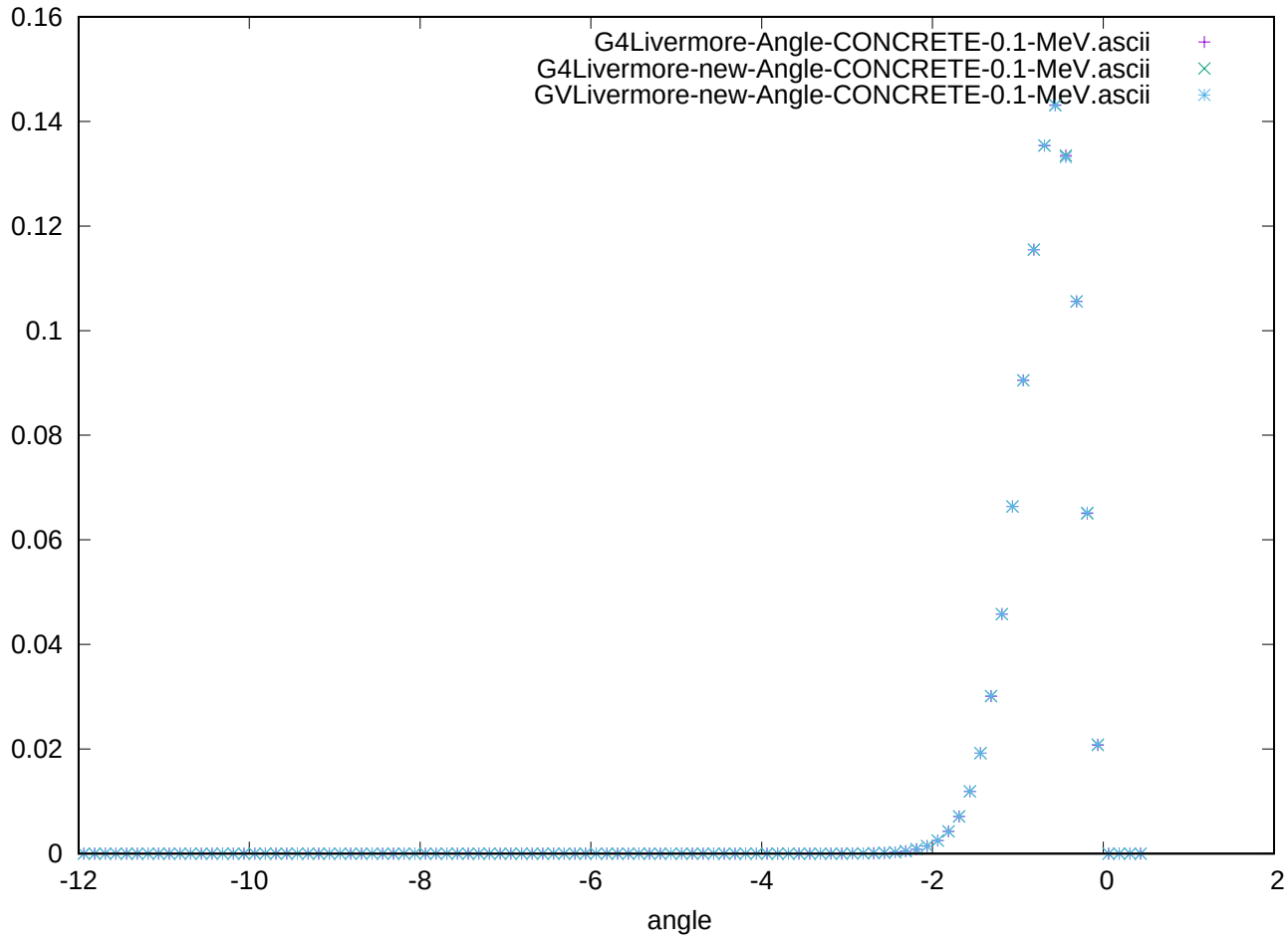
Geant4 and GeantV models photoelectron angular distribution

Test on CONCRETE, $E_\gamma = 0.01 MeV$, $\#particles = 10^7$



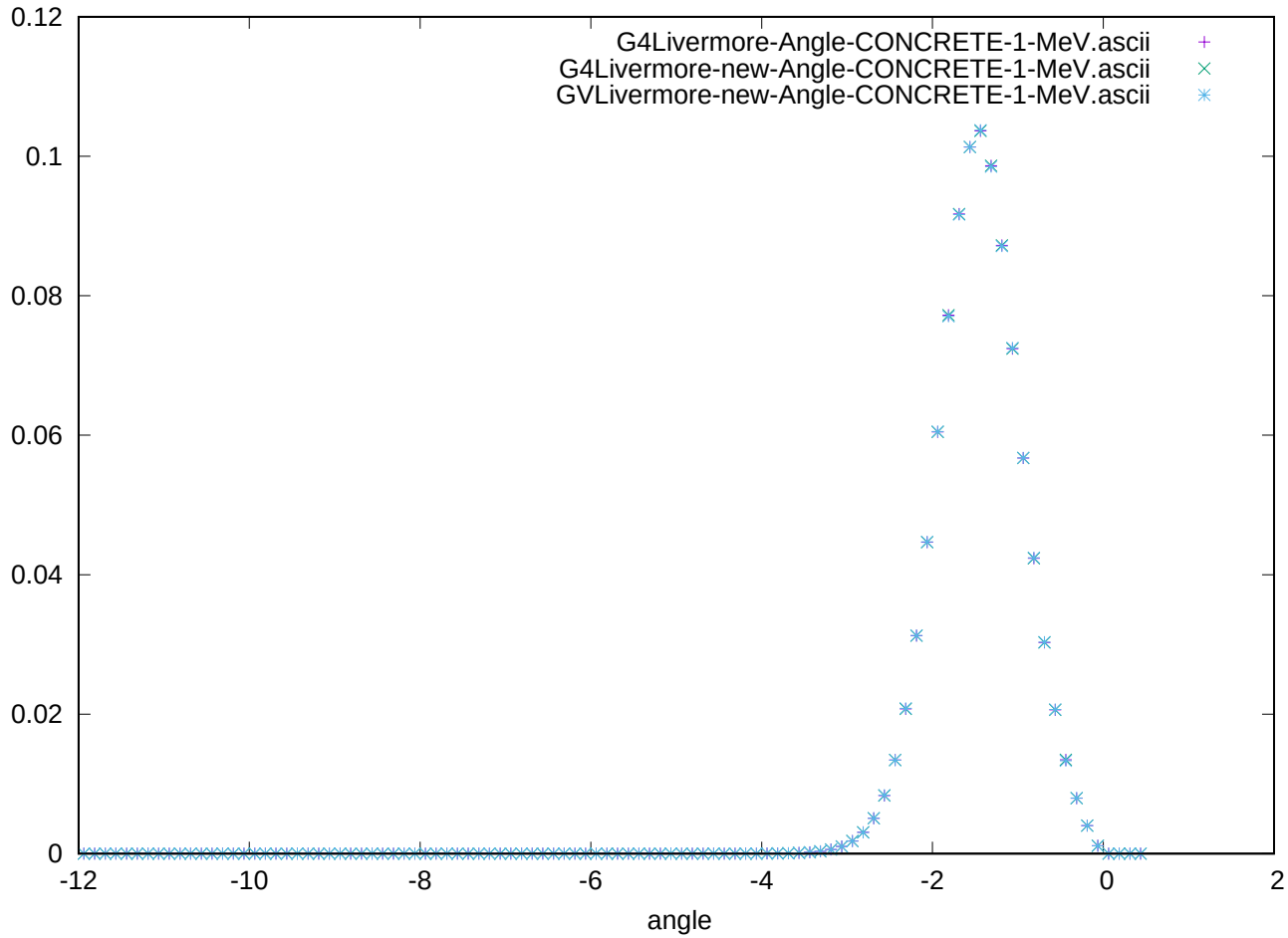
Geant4 and GeantV models photoelectron angular distribution

Test on CONCRETE, $E_\gamma = 0.1 MeV$, $\#particles = 10^7$



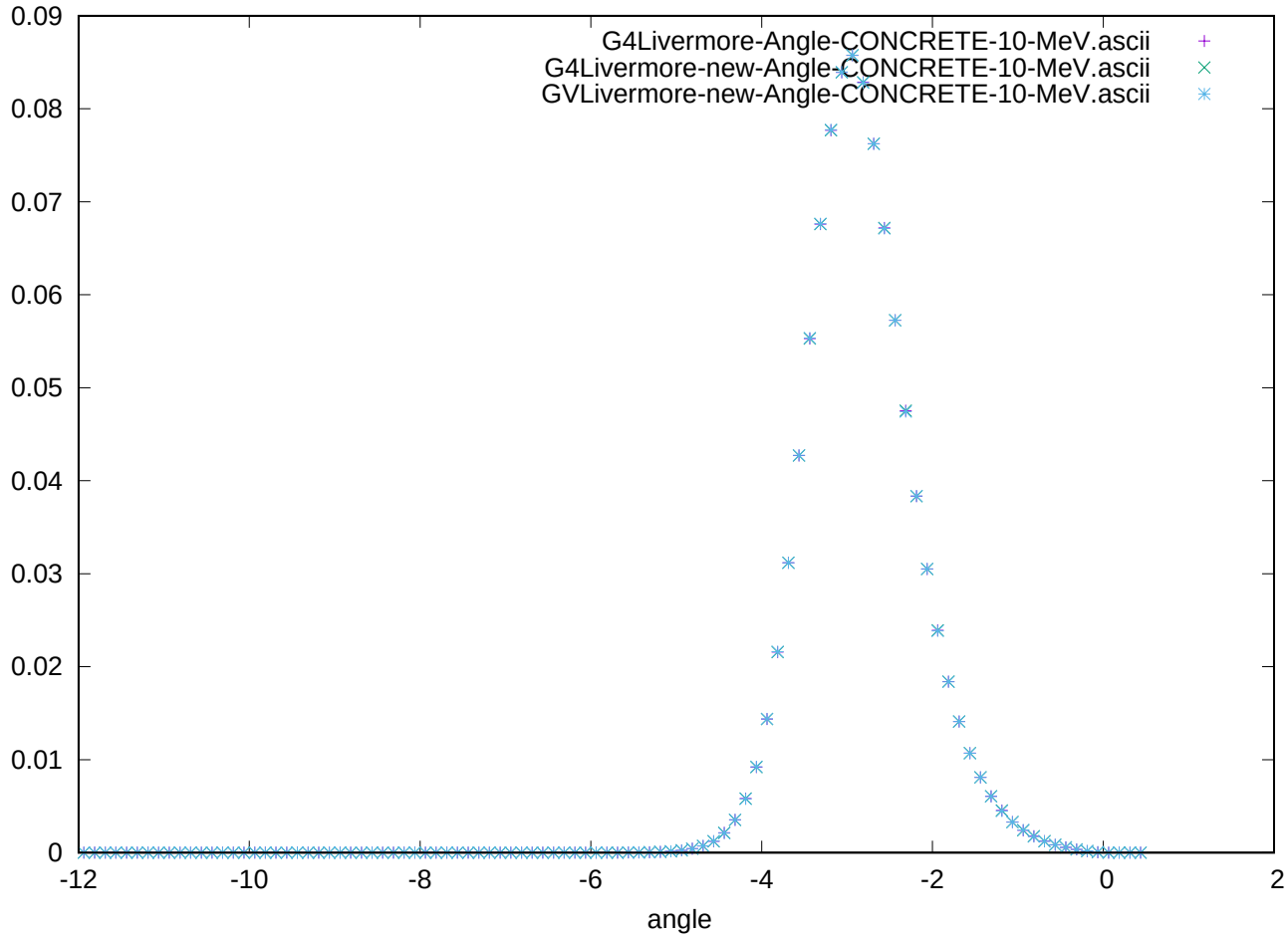
Geant4 and GeantV models photoelectron angular distribution

Test on CONCRETE, $E_\gamma = 1MeV$, $\#particles = 10^7$



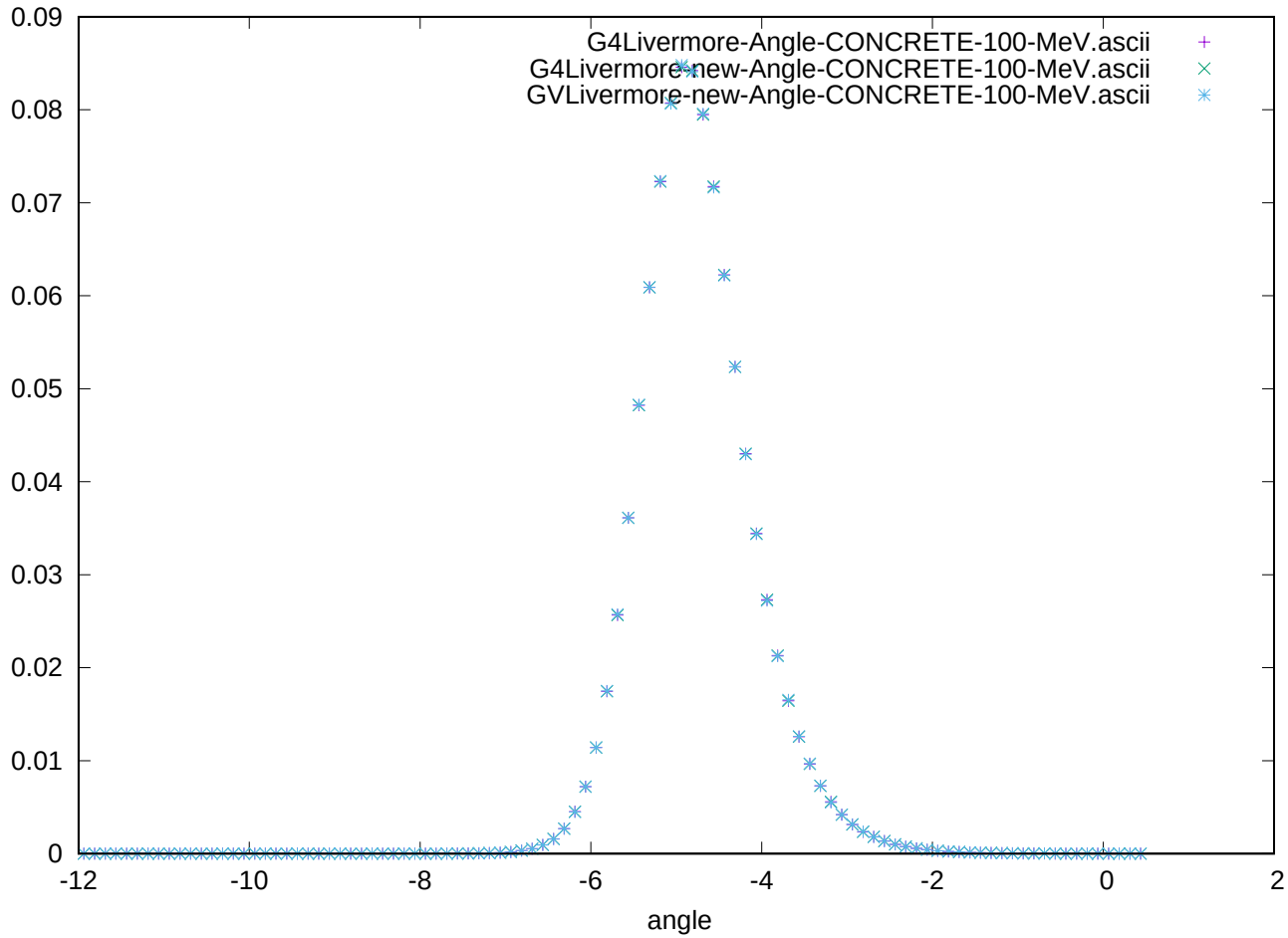
Geant4 and GeantV models photoelectron angular distribution

Test on CONCRETE, $E_\gamma = 10MeV$, $\#particles = 10^7$



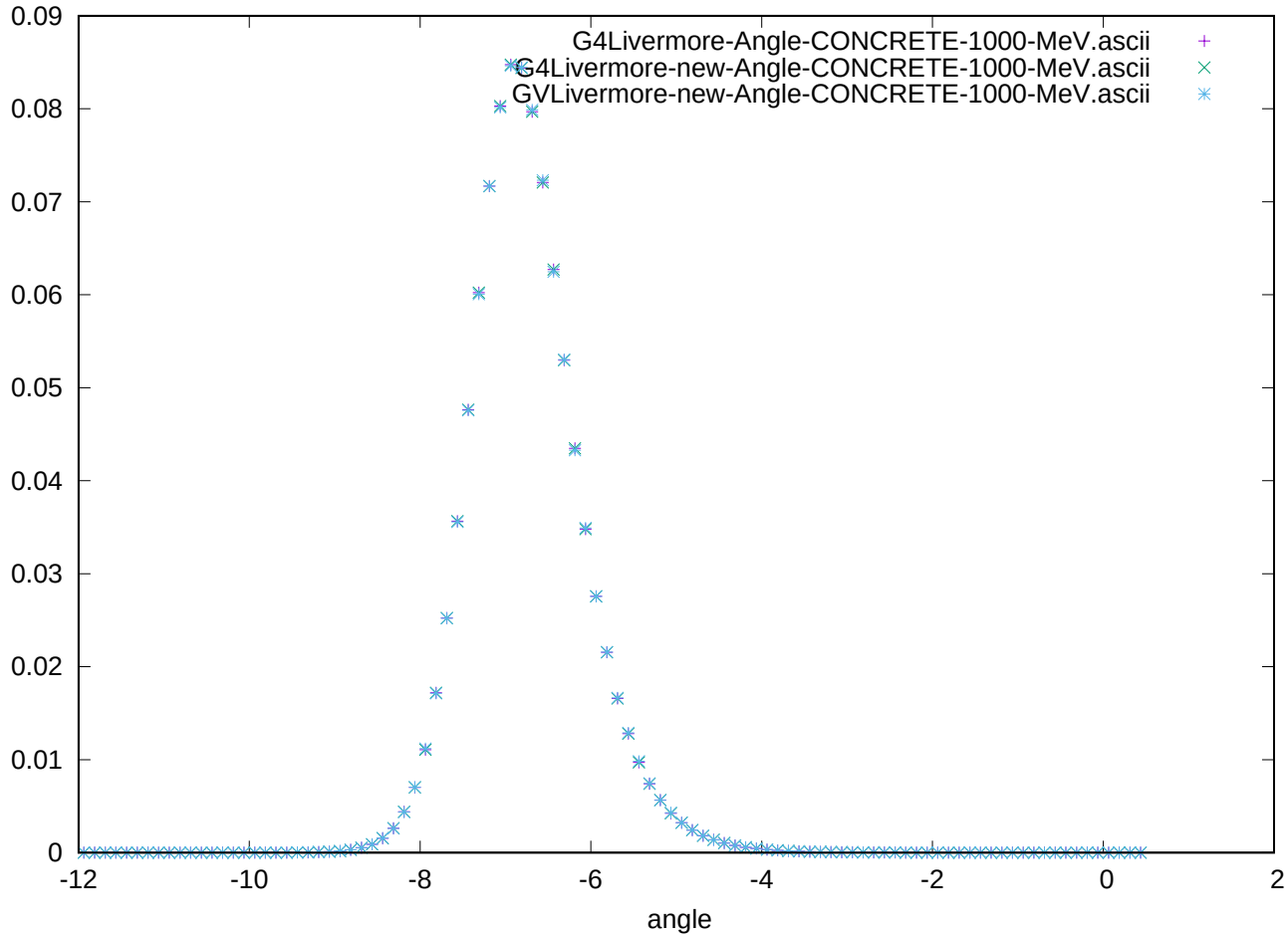
Geant4 and GeantV models photoelectron angular distribution

Test on CONCRETE, $E_\gamma = 100 MeV$, $\#particles = 10^7$

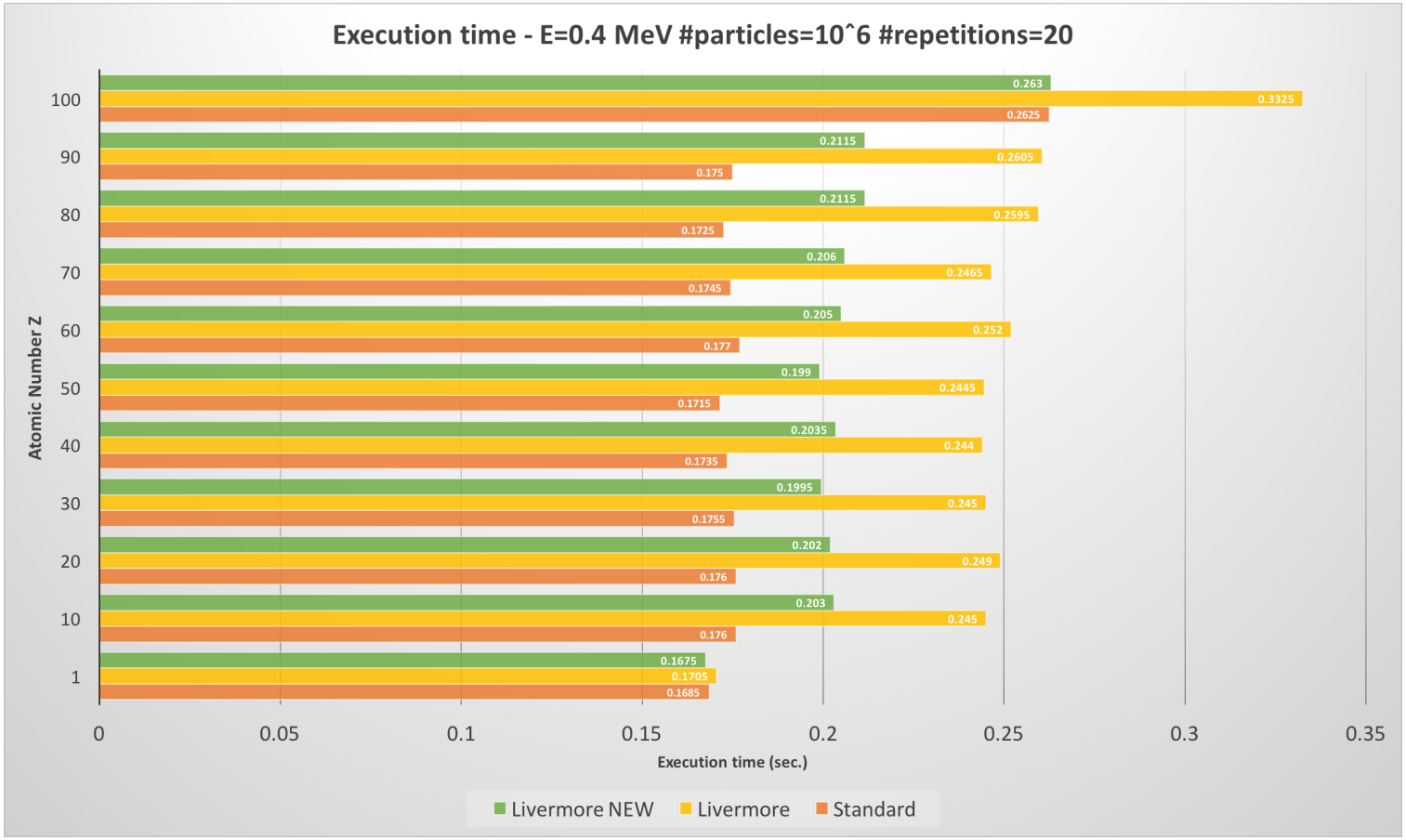


Geant4 and GeantV models photoelectron angular distribution

Test on CONCRETE, $E_\gamma = 1000 MeV$, $\#particles = 10^7$



New Livermore vs Standard and Livermore Execution times



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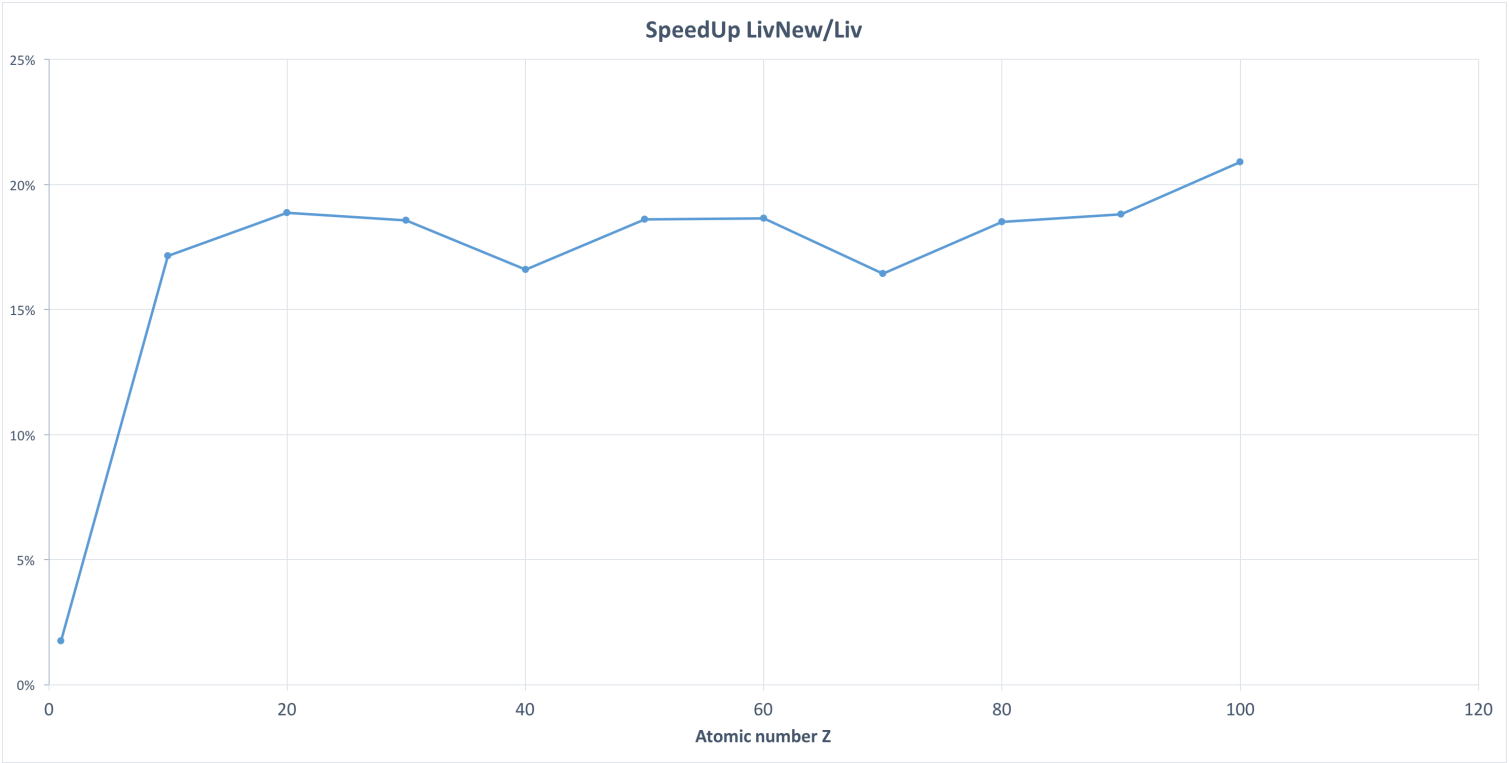

- Measured speed-up between 17% and 21%.

Conclusions and plans

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- Updated and improved Livermore model:
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  - A new fit (in two steps) on updated cross-sections data has been performed
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    - More efficiency: threshold from 600KeV to 5KeV
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    - More accuracy
    - More efficiency: threshold from 600KeV to 5KeV
  - The sampling of secondaries has been improved: speedup between 17% and 21%.
- This model can be an alternative to the standard model (Geant4):
  - More accurate parameterization (new data)
  - That take into account shells sampling
  - Fast 'enough'

Thanks for your attention.

Appendix

Experimental data: Total cross sections

TABLE II

SUMMARY OF THE EXPERIMENTAL TOTAL CROSS SECTION DATA USED IN THE VALIDATION ANALYSIS

Atomic Number	Element	Energy range (keV)	Sample size	References
1	H	0.0136 - 0.020	27	[102]–[104]
2	He	0.025 - 0.277	320	[105]–[112]
3	Li	0.046 - 0.400	93	[113]–[116]
7	N	0.015 - 0.4	73	[117], [118]
8	O	0.013 - 0.28	215	[103], [119]–[121]
10	Ne	0.022 - 2.952	448	[108], [110]–[112], [117], [122]
11	Na	0.046 - 0.246	17	[123]
13	Al	145.4	1	[124]
17	Cl	0.016 - 0.078	25	[125]
18	Ar	0.016 - 6	487	[105], [110]–[112], [117], [126]–[130]
19	K	0.004 - 0.005	12	[131]
22	Ti	59.54	1	[132]
23	V	59.54	1	[132]
24	Cr	59.54	1	[132]
25	Mn	59.54	1	[132]
26	Fe	0.008 - 59.54	25	[132]–[134]
27	Co	59.54	1	[132]
28	Ni	1.487 - 59.54	17	[132], [133]
29	Cu	59.54 - 661.6	9	[124], [132], [135]–[138]
30	Zn	59.54	1	[132]
33	As	59.54	1	[132]
34	Se	59.54	1	[132]
36	Kr	0.015 - 1.626	357	[105], [110], [112], [139], [140]
37	Rb	0.004 - 0.010	4	[141]
38	Sr	59.54	1	[132]
39	Y	279.2 - 661.6	2	[142]
40	Zr	59.54 - 661.6	7	[124], [135]–[137], [143]
41	Nb	59.54	2	[143]
42	Mo	59.54 - 661.6	7	[132], [138], [143]
43	Tc	59.54	1	[143]

Experimental data: Total cross sections

46	Pd	59.54	1	[143]
47	Ag	1.487 - 661.6	13	[124], [?], [135]–[137], [143]–[146]
48	Cd	59.54	2	[132], [143]
49	In	59.54	2	[143]
50	Sn	1 - 661.6	31	[124], [133], [135]–[137], [143], [144], [146]
51	Sb	59.54	1	[143]
52	Te	59.54	2	[143]
54	Xe	0.013 - 6	657	[110], [122], [128], [130], [147]
55	Cs	0.004 - 59.54	14	[132], [141], [148]
57	La	59.54	1	[149]
58	Ce	59.54 - 661.6	6	[142], [149]–[152]
59	Pr	59.54 - 661.6	3	[150]–[152]
60	Nd	59.54 - 661.6	2	[150], [152]
61	Pm	59.54	1	[152]
62	Sm	59.54 - 145.4	4	[149], [151], [152]
63	Eu	59.54	2	[149], [152]
64	Gd	59.54 - 661.6	5	[150]–[153]
65	Tb	59.54	3	[149], [152], [153]
66	Dy	59.54 - 661.6	8	[142], [149]–[153]
67	Ho	59.54	1	[152]
68	Er	59.54	3	[149], [152], [153]
70	Yb	279.2 - 661.6	2	[142]
72	Hf	65.839-68.547	25	[154]
73	Ta	1.487 - 661.6	31	[124], [133], [135]–[138], [144]
78	Pt	1 - 40	25	[133]
79	Au	0.93 - 661.6	33	[133], [135]–[137], [145]
80	Hg	1173	1	[155]
82	Pb	1.487 - 1173	36	[124], [133], [135]–[137], [144]–[146], [155], [156]
92	U	1.487 - 3	4	[133]

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M. C. Han and H. S. Kim and M. G. Pia and T. Basaglia and M. Batic and G. Hoff and C. H. Kim and P. Saracco (2016)

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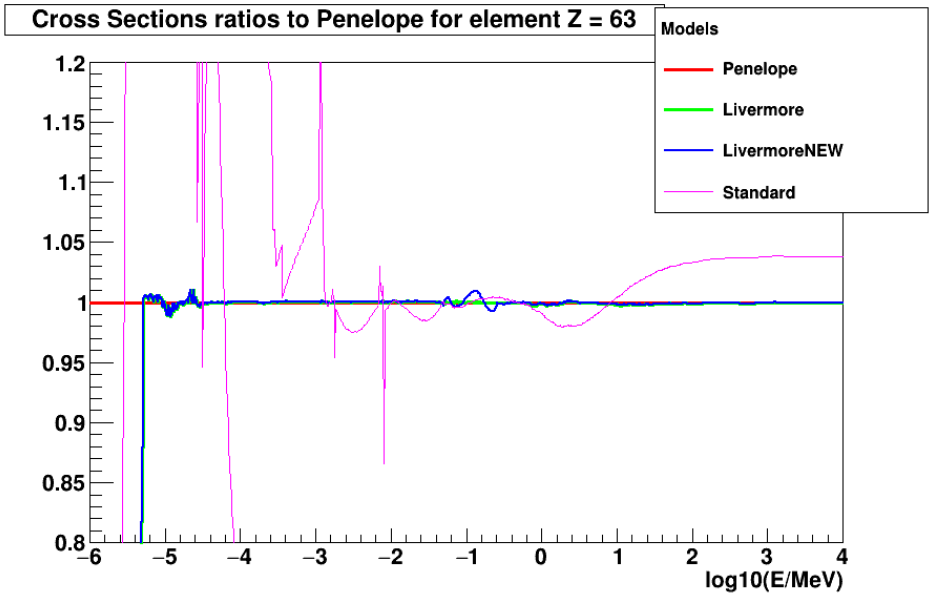
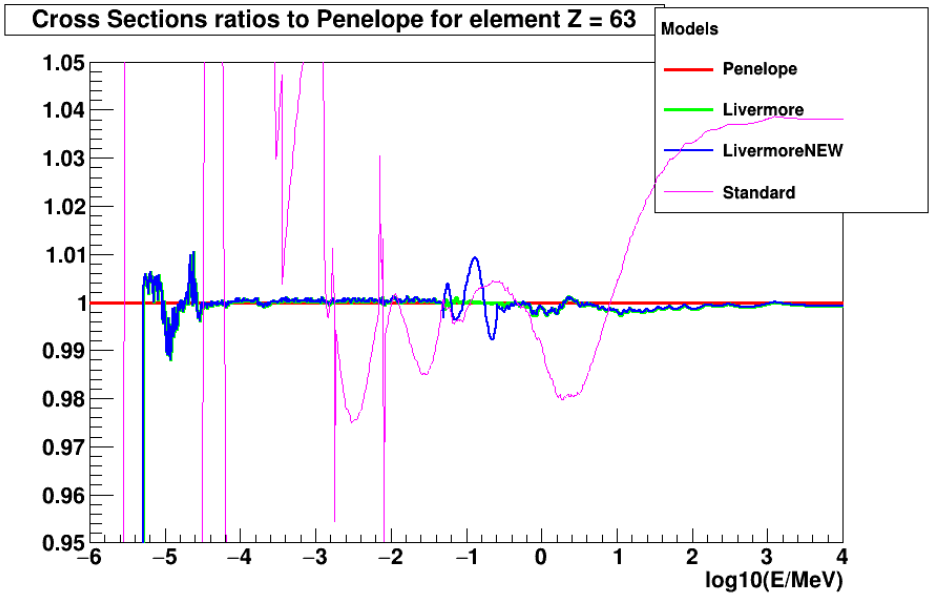
IEEE Transactions on Nuclear Science 63(2), 1117-1146.

The End

Backup slides

Geant4 models x-section ratio comparison





Standard electromagnetic package - Geant4-10.2 - Final state sampling

Differential Photoeffelectric cross section correct to first order αZ

$$\frac{d\sigma}{d\cos\theta} \simeq \frac{\sin^2\theta}{(1-\beta\cos\theta)^4}\left\{1+\frac{1}{2}\gamma(\gamma-1)(\gamma-2)(1-\beta\cos\theta)\right\} \tag{7}$$

where β and γ are the photoelectron Lorentz factors. $cos\theta$ is sampled from the probability density function :

$$f(\cos\theta) = \frac{1-\beta^2}{2\beta}\frac{1}{(1-\beta\cos\theta)^2} \tag{8}$$

so

$$\cos\theta = \frac{(1-2r)+\beta}{(1-2r)\beta+1} \tag{9}$$

The rejection function is :

$$g(\cos\theta) = \frac{1-cos^2\theta}{(1-\beta\cos\theta)^2}[1+b(1-\beta\cos\theta)] \tag{10}$$

with $b = \gamma(\gamma-1)(\gamma-1)/2$
It can be shown that $g(cos\theta)$ is positive for each $cos\theta \in [-1,+1]$, and can be majored by :

$$gsup = \begin{cases} \gamma^2[1+b(1-\beta)] & \text{if } \gamma \in]1,2] \\ \gamma^2[1+b(1+\beta)] & \text{if } \gamma > 2 \end{cases} \tag{11}$$

The efficiency of this method is $\sim 50\%$ if $\gamma < 2, \sim 25\%$ if $\in [2,3]$.

Standard electromagnetic package - Geant 10.2 - Macroscopic and atomic cross-sections

- Once the photoelectric process is selected, the model must choose **which atom** is involved. In compound materials the i^{th} element is chosen randomly according to the probability:

$$Prob(Z_i, E_\gamma) = \frac{n_i \sigma_i(Z_i, E_\gamma)}{\sum_i [n_i \sigma_i(E_\gamma)]} \tag{12}$$

  where n_i is the number of atom per volume of the i^{th} element composing the material.
- For each process the **total cross section** at a given energy E is obtained with a log-log interpolation of cross section data σ_1 and σ_2 available **in the data libraries** from the closest energies.

Macroscopic cross section and mean free path

- For compound materials (and also for mixtures) the molecular cross section $\sigma_{ph}(E)$ is evaluated by means of the **additivity approximation**.

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$$\sigma(E_\gamma) = \sum_i n_i \sigma(Z_i, E_\gamma) \tag{13}$$

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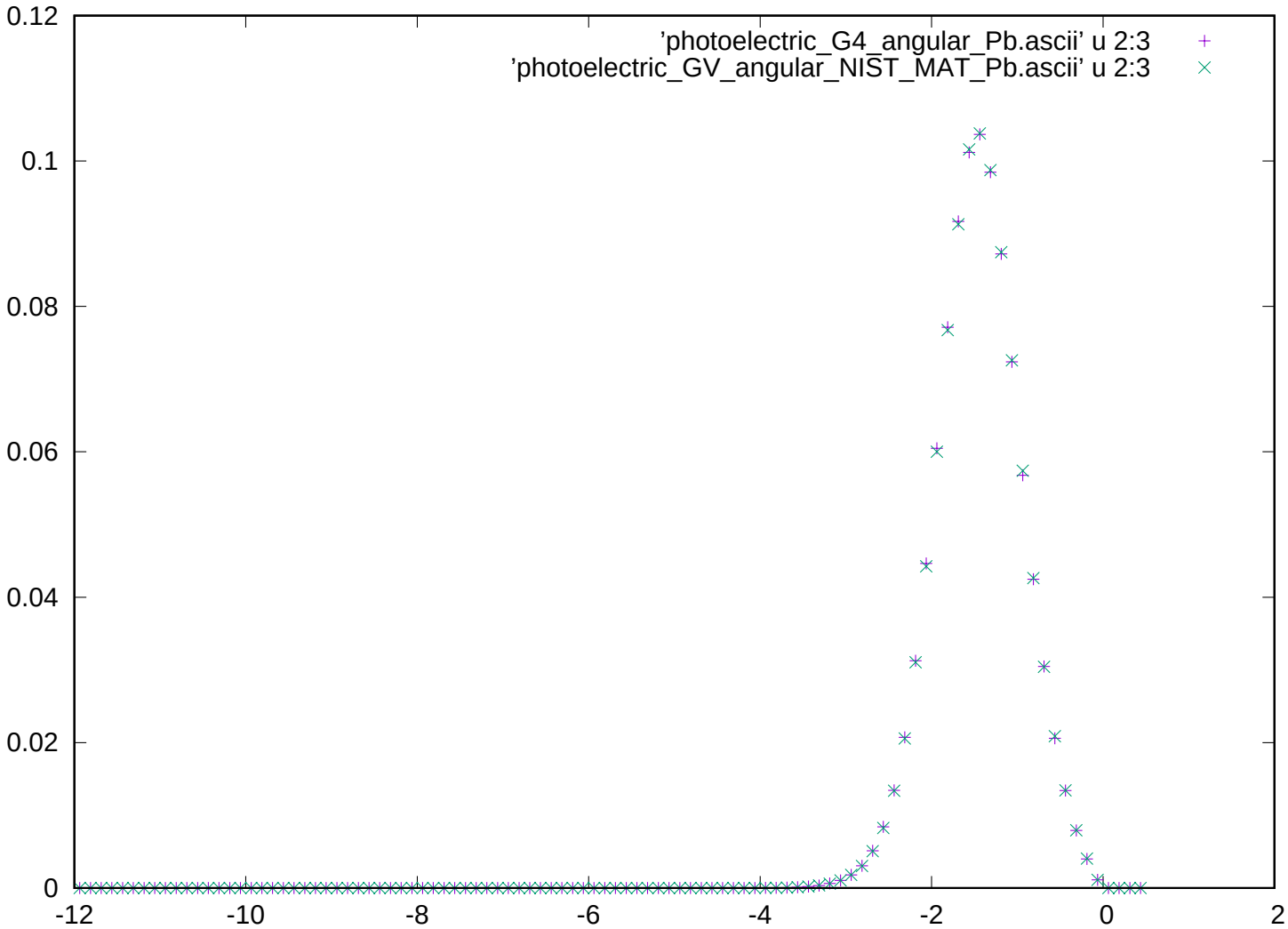
  where n_i is the number of atoms per volume of the i^{th} element of the material.
- The **mean free path**, λ, for a photon to interact via the photoelectric effect is given by:

$$\lambda(E_\gamma) = \left(\sum_i n_i \sigma(Z_i, E_\gamma) \right)^{-1} \tag{14}$$

PhotoElectric SG angular distribution



Total Photoeffect cross section correct to first order αZ

$$\sigma_\kappa = \frac{3}{2}\phi_0\alpha^4 Z^5 \frac{\beta^3(1-\beta^2)}{\left[1-(1-\beta^2)^{\frac{1}{2}}\right]^5}\left[\mathfrak{M}\left(1-\frac{\pi\alpha Z}{\beta}\right)+\pi\alpha Z\mathfrak{N}\right] \tag{15}$$

where

$$\mathfrak{M} = \frac{4}{3}+\frac{1-3(1-\beta^2)^{\frac{1}{2}}+2(1-\beta^2)}{\beta^2(1-\beta^2)^{\frac{1}{2}}}\left[1+\frac{1-\beta^2}{2\beta}ln\frac{1-\beta}{1+\beta}\right] \tag{16}$$

and

$$\mathfrak{N} = \frac{1}{\beta^3}\{-\frac{4}{15}\frac{1}{(1-\beta^2)^{\frac{1}{2}}}\}+\frac{34}{15}-\frac{63}{15}\left(1-\beta^2\right)^{\frac{1}{2}}+\frac{25}{15}\left(1-\beta^2\right)+$$

$$\frac{8}{15}\left(1-\beta^2\right)^{\frac{3}{2}}+(1-\beta^2)^{\frac{1}{2}}\left[1-3(1-\beta^2)^{\frac{1}{2}}+2(1-\beta^2)\right]\frac{1}{2\beta}ln\frac{1-\beta}{1+\beta} \tag{17}$$

Standard electromagnetic package - Geant 10.2 - Total cross-section

For each process the **total cross section** at a given energy E is obtained with a log-log interpolation.

$$\log(\sigma(E)) = \log(\sigma_1)\frac{\log(E_2) - \log(E)}{\log(E_2) - \log(E_1)} + \log(\sigma_2)\frac{\log(E) - \log(E_1)}{\log(E_2) - \log(E_1)} \quad (18)$$

where E_1 and E_2 are the closest lower and higher energy for which cross section data σ_1 and σ_2 are available **in the data libraries** respectively.

Notes

- According to G4PEFluoModel for energies $E_\gamma > 25.55 MeV$ it is assumed that the emitted photoelectron has the same direction as the incident gamma. This means that for $E_\gamma > 25.55 MeV$ $cos\theta = 1$ always.
- N.B.: Need to test/check and correct the number of bin and the number of tested energies. (with nBins=200 there aren't improvements with respect to nBins=151 which is working better than nBin=99
- Da $0.5 MeV$ in su abbiamo problemi nel riprodurre la distribuzione angolare. Update: Improved, but still need to test.

Photoelectric effect in Geant4 - low energy package

Two implementations of the p.e. effect. The Livermore and Penelope cross-sections are tabulated according to EPDL97 and EPDL89 [D.E.Cullen , 1989], respectively.

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- **G4Penelope** model is reengineered from the 2001 Penelope code.