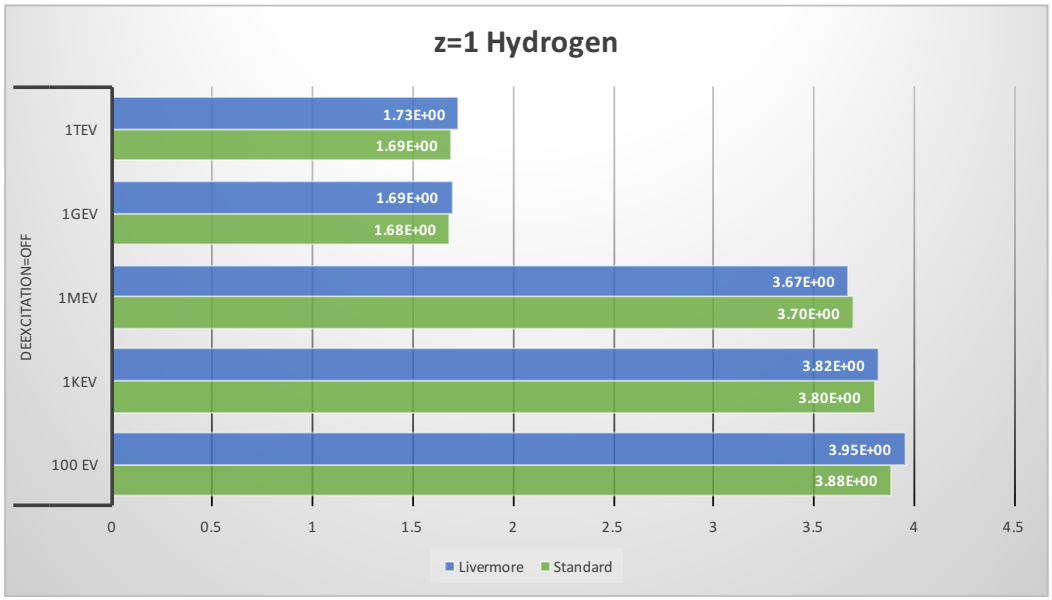
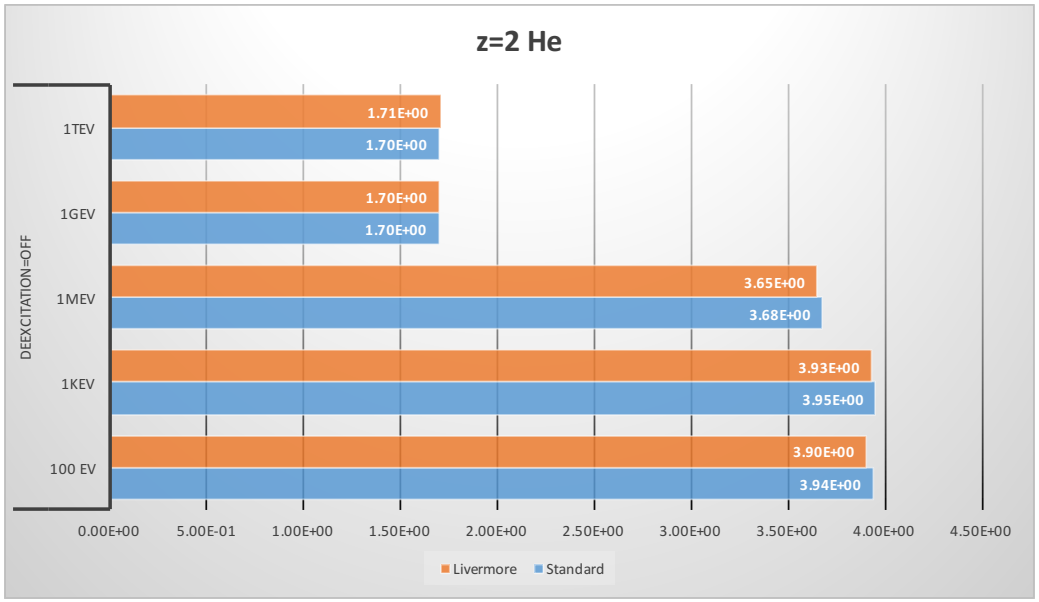
P.e. effect update

Marilena Bandieramonte
bi-weekly meeting 30-05-2017


z=1 Hydrogen
DEEXCITATION=OFF
1TEV
1GEV
1MEV
1KEV
100 EV
1.73E+00
1.69E+00
1.69E+00
1.68E+00
3.67E+00
3.70E+00
3.82E+00
3.80E+00
3.95E+00
3.88E+00
0
0.5
1
1.5
2
2.5
3
3.5
4
4.5
Livermore
Standard


z=2 He
DEEXCITATION=OFF
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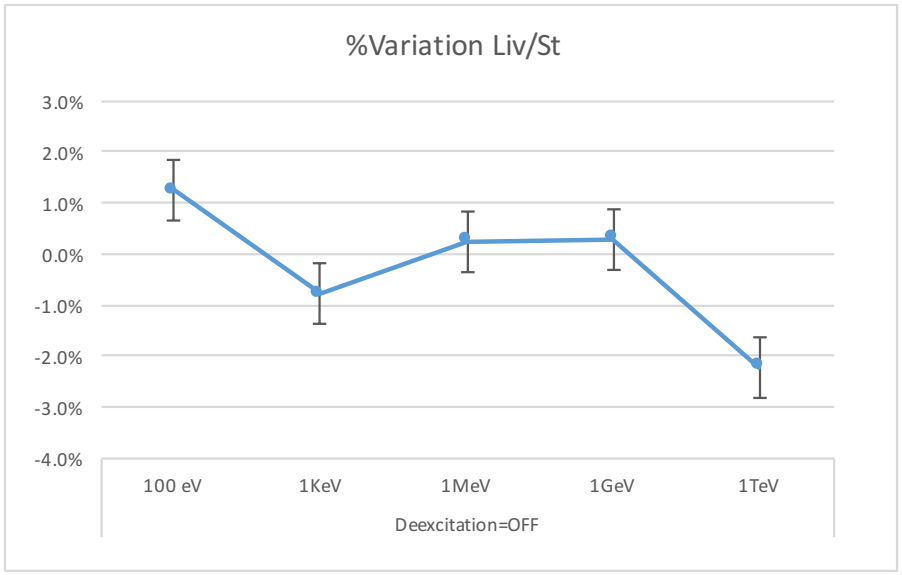
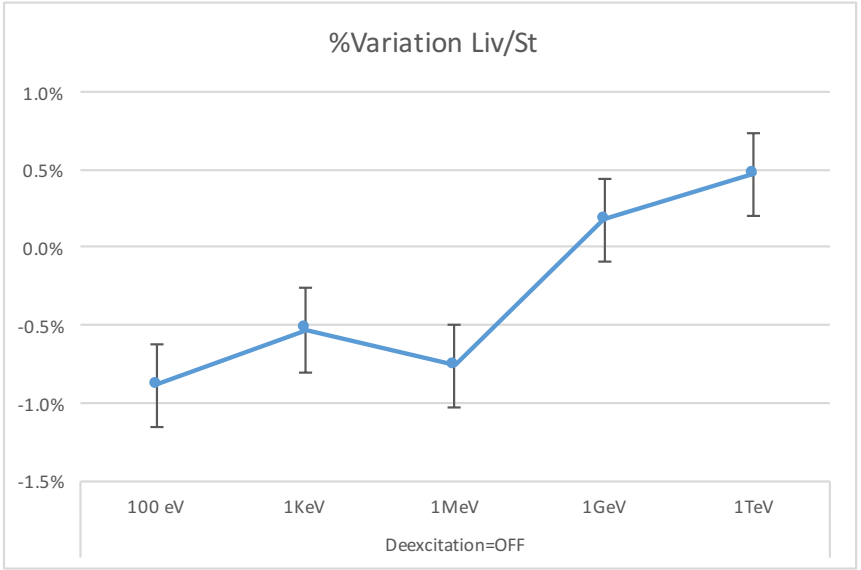
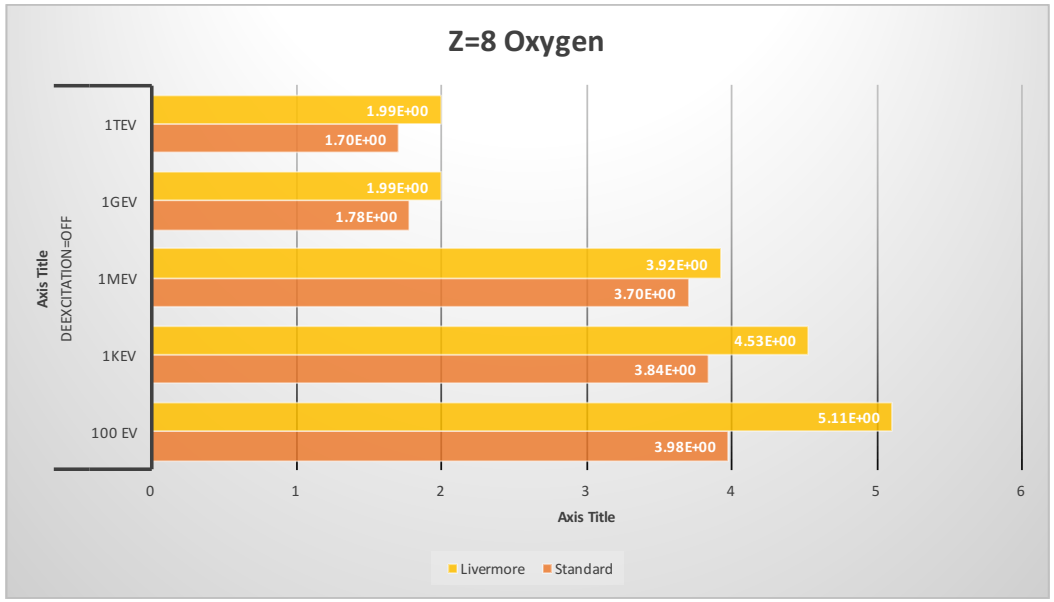
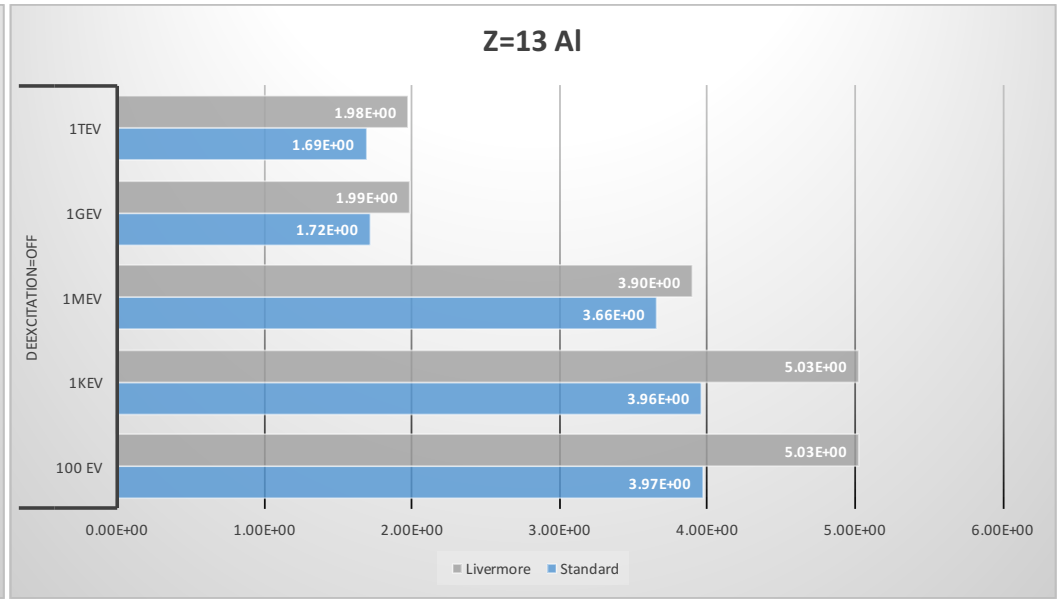
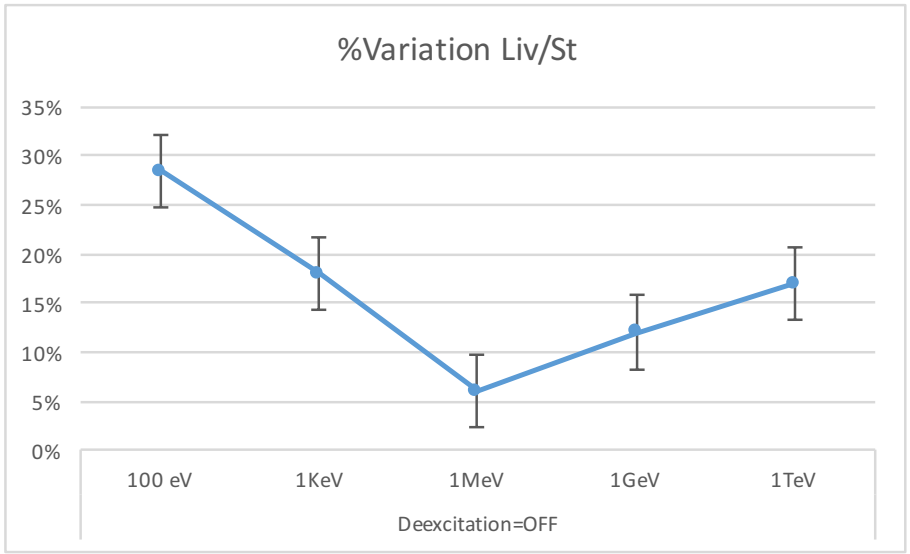
1GEV
1MEV
1KEV
100 EV
1.71E+00
1.70E+00
1.70E+00
1.70E+00
3.65E+00
3.68E+00
3.93E+00
3.95E+00
3.90E+00
3.94E+00
0.00E+00
5.00E-01
1.00E+00
1.50E+00
2.00E+00
2.50E+00
3.00E+00
3.50E+00
4.00E+00
4.50E+00
Livermore
Standard

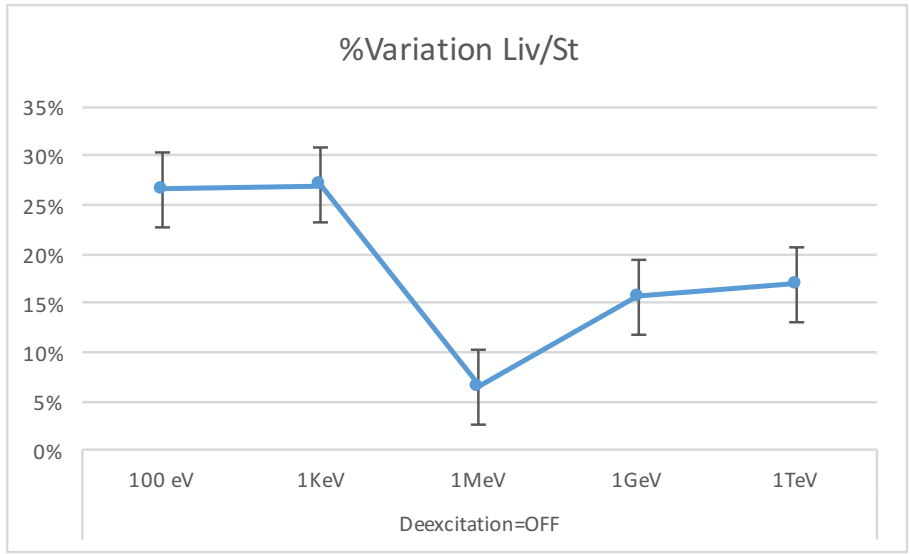

%Variation Liv/St
3.0%
2.0%
1.0%
0.0%
-1.0%
-2.0%
-3.0%
-4.0%
100 eV
1KeV
1MeV
1GeV
1TeV
Deexcitation=OFF

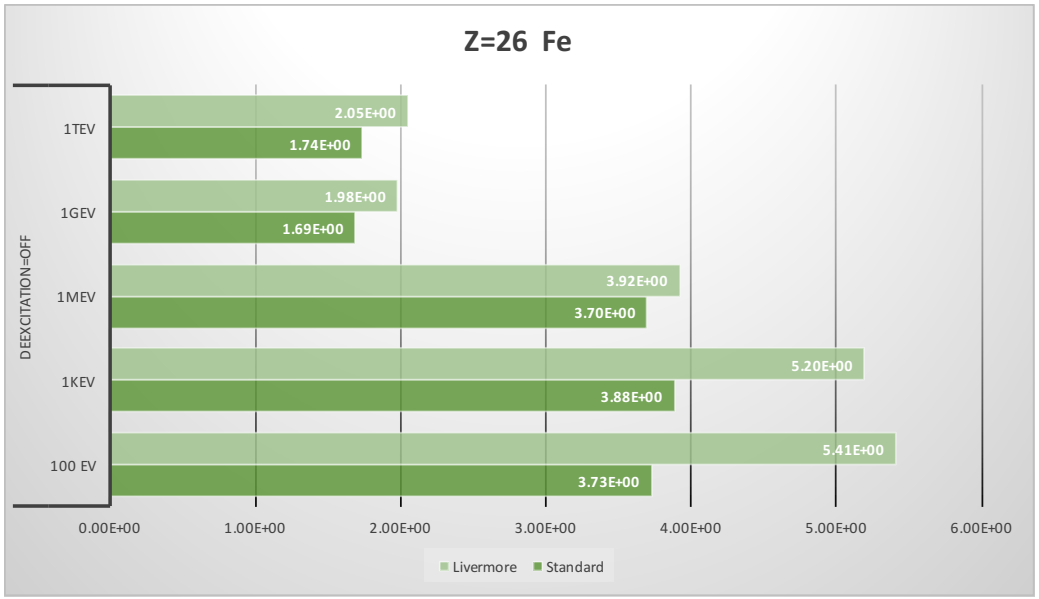

%Variation Liv/St
1.0%
0.5%
0.0%
-0.5%
-1.0%
-1.5%
100 eV
1KeV
1MeV
1GeV
1TeV
Deexcitation=OFF

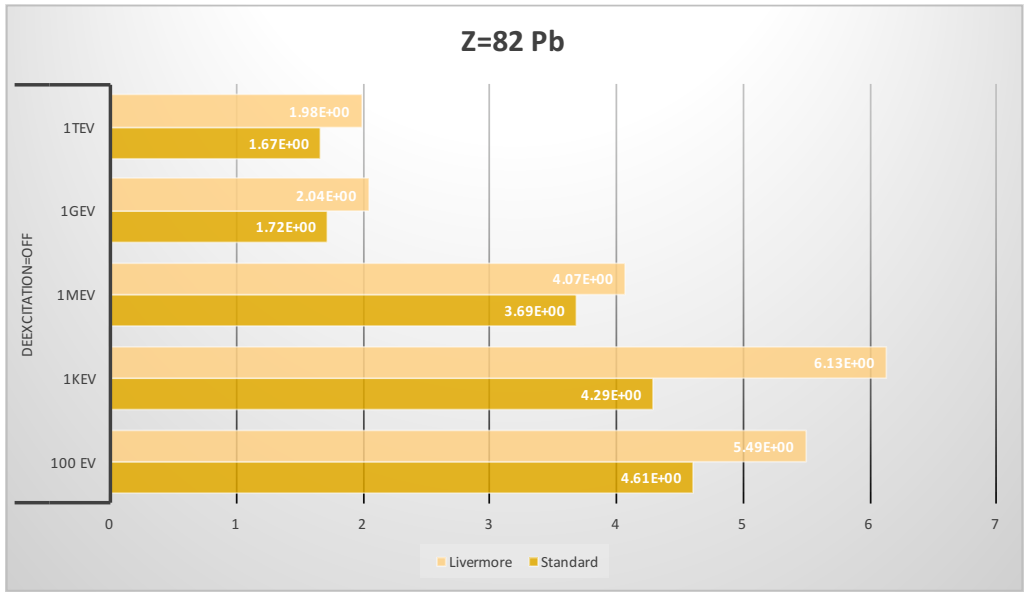

Z=8 Oxygen
1TEV
1GEV
1MEV
1KEV
100 EV
1.99E+00
1.70E+00
1.99E+00
1.78E+00
3.92E+00
3.70E+00
4.53E+00
3.84E+00
5.11E+00
3.98E+00
Axis Title
DEEXCITATION=OFF
0
1
2
3
4
5
6
Axis Title
Livermore
Standard

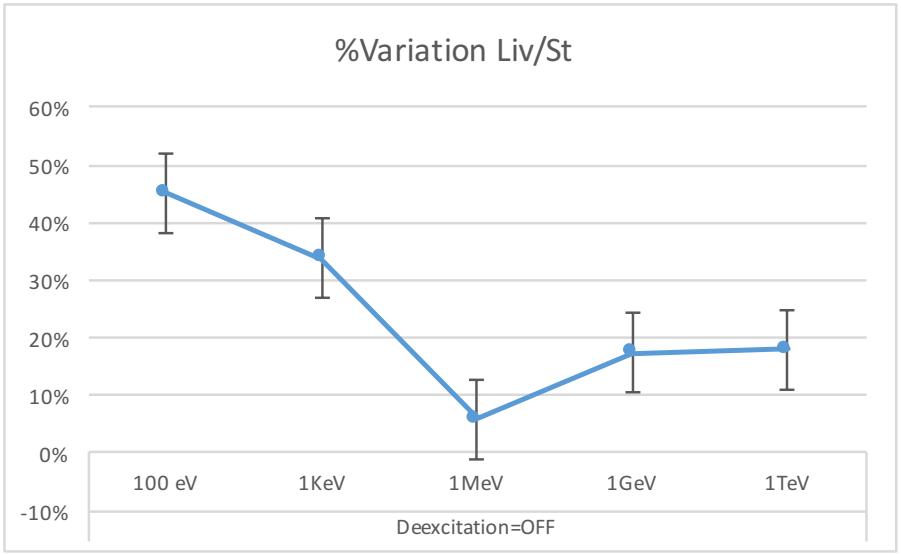

Z=13 Al
1TEV
1GEV
1MEV
1KEV
100 EV
1.98E+00
1.69E+00
1.99E+00
1.72E+00
3.90E+00
3.66E+00
5.03E+00
3.96E+00
5.03E+00
3.97E+00
DEEXCITATION=OFF
0.00E+00
1.00E+00
2.00E+00
3.00E+00
4.00E+00
5.00E+00
6.00E+00
Livermore
Standard

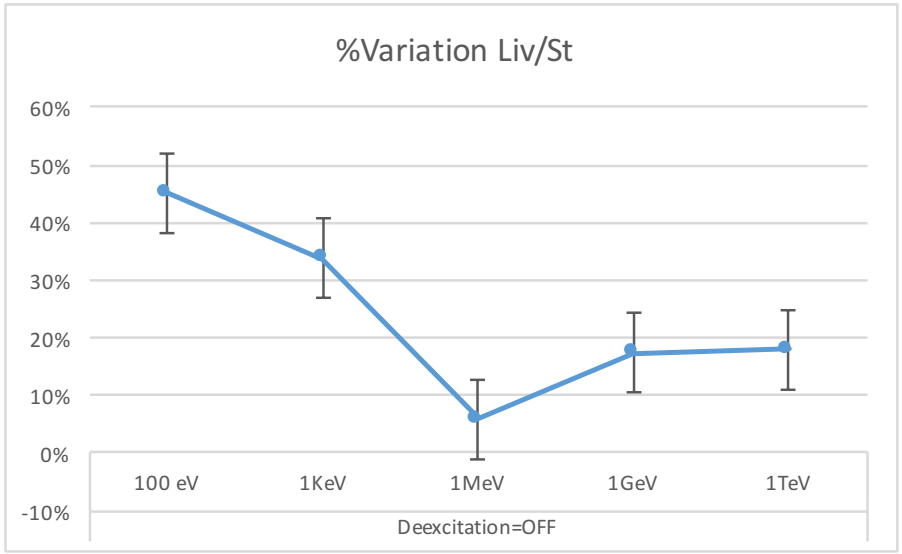

%Variation Liv/St
35%
30%
25%
20%
15%
10%
5%
0%
100 eV
1KeV
1MeV
1GeV
1TeV
Deexcitation=OFF

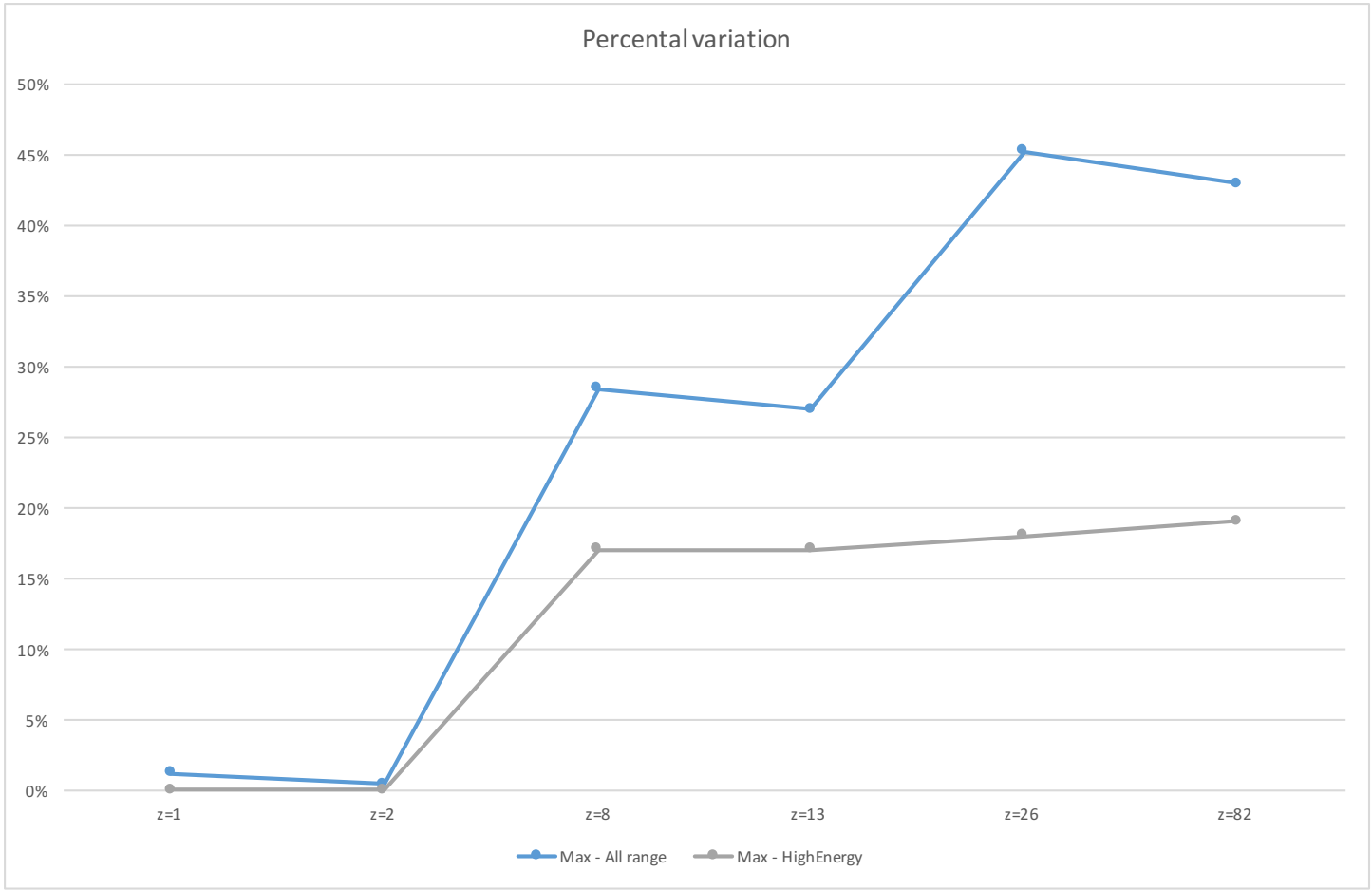

%Variation Liv/St
35%
30%
25%
20%
15%
10%
5%
0%
100 eV
1KeV
1MeV
1GeV
1TeV
Deexcitation=OFF

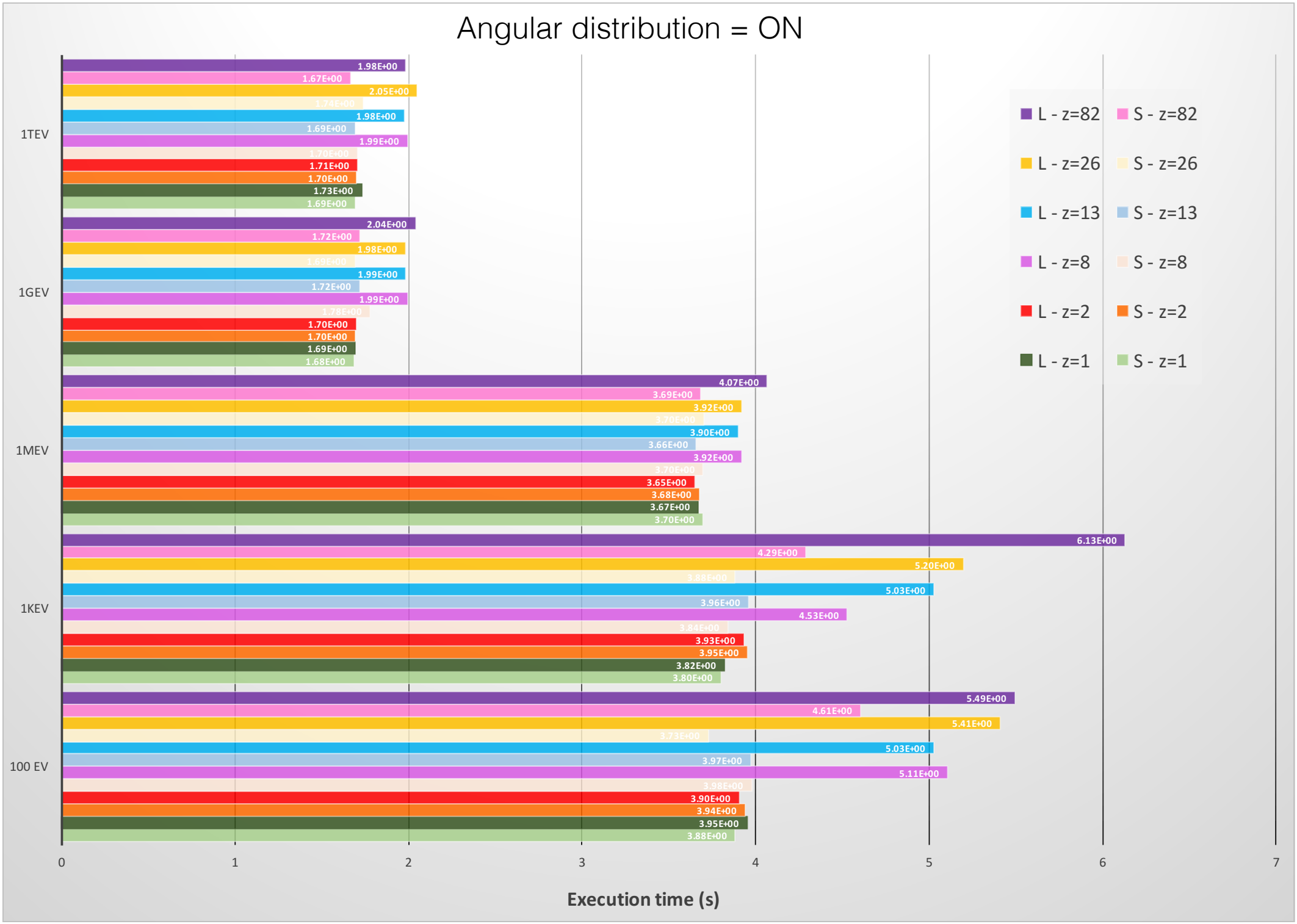

Z=26 Fe
DEEXCITATION=OFF
1TEV
1GEV
1MEV
1KEV
100 EV
2.05E+00
1.74E+00
1.98E+00
1.69E+00
3.92E+00
3.70E+00
5.20E+00
3.88E+00
5.41E+00
3.73E+00
0.00E+00
1.00E+00
2.00E+00
3.00E+00
4.00E+00
5.00E+00
6.00E+00
Livermore
Standard


Z=82 Pb
DEEXCITATION=OFF
1TEV
1GEV
1MEV
1KEV
100 EV
1.98E+00
1.67E+00
2.04E+00
1.72E+00
4.07E+00
3.69E+00
6.13E+00
4.29E+00
5.49E+00
4.61E+00
0
1
2
3
4
5
6
7
Livermore
Standard


%Variation Liv/St
60%
50%
40%
30%
20%
10%
0%
-10%
100 eV
1KeV
1MeV
1GeV
1TeV
Deexcitation=OFF


%Variation Liv/St
60%
50%
40%
30%
20%
10%
0%
-10%
100 eV
1KeV
1MeV
1GeV
1TeV
Deexcitation=OFF


Percental variation
50%
45%
40%
35%
30%
25%
20%
15%
10%
5%
0%
z=1
z=2
z=8
z=13
z=26
z=82
Max - All range
Max - HighEnergy


Angular distribution = ON
1TEV
1GEV
1MEV
1KEV
100 EV
1.98E+00
1.67E+00
2.05E+00
1.74E+00
1.98E+00
1.69E+00
1.99E+00
1.70E+00
1.71E+00
1.70E+00
1.73E+00
1.69E+00
2.04E+00
1.72E+00
1.98E+00
1.69E+00
1.99E+00
1.72E+00
1.99E+00
1.78E+00
1.70E+00
1.70E+00
1.69E+00
1.68E+00
4.07E+00
3.69E+00
3.92E+00
3.70E+00
3.90E+00
3.66E+00
3.92E+00
3.70E+00
3.65E+00
3.68E+00
3.67E+00
3.70E+00
6.13E+00
4.29E+00
5.20E+00
3.88E+00
5.03E+00
3.96E+00
4.53E+00
3.84E+00
3.93E+00
3.95E+00
3.82E+00
3.80E+00
5.49E+00
4.61E+00
5.41E+00
3.73E+00
5.03E+00
3.97E+00
5.11E+00
3.98E+00
3.90E+00
3.94E+00
3.95E+00
3.88E+00
L - z=82
S - z=82
L - z=26
S - z=26
L - z=13
S - z=13
L - z=8
S - z=8
L - z=2
S - z=2
L - z=1
S - z=1
0
1
2
3
4
5
6
7
Execution time (s)

Angular distribution sampling (Penelope2014 like)*

- 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:

$$p(\nu) = (2-\nu)[\frac{1}{A+\nu} + \frac{1}{2}\beta\gamma(\gamma-1)(\gamma-2)]\frac{\nu}{(A+\nu)^3} \tag{15}$$

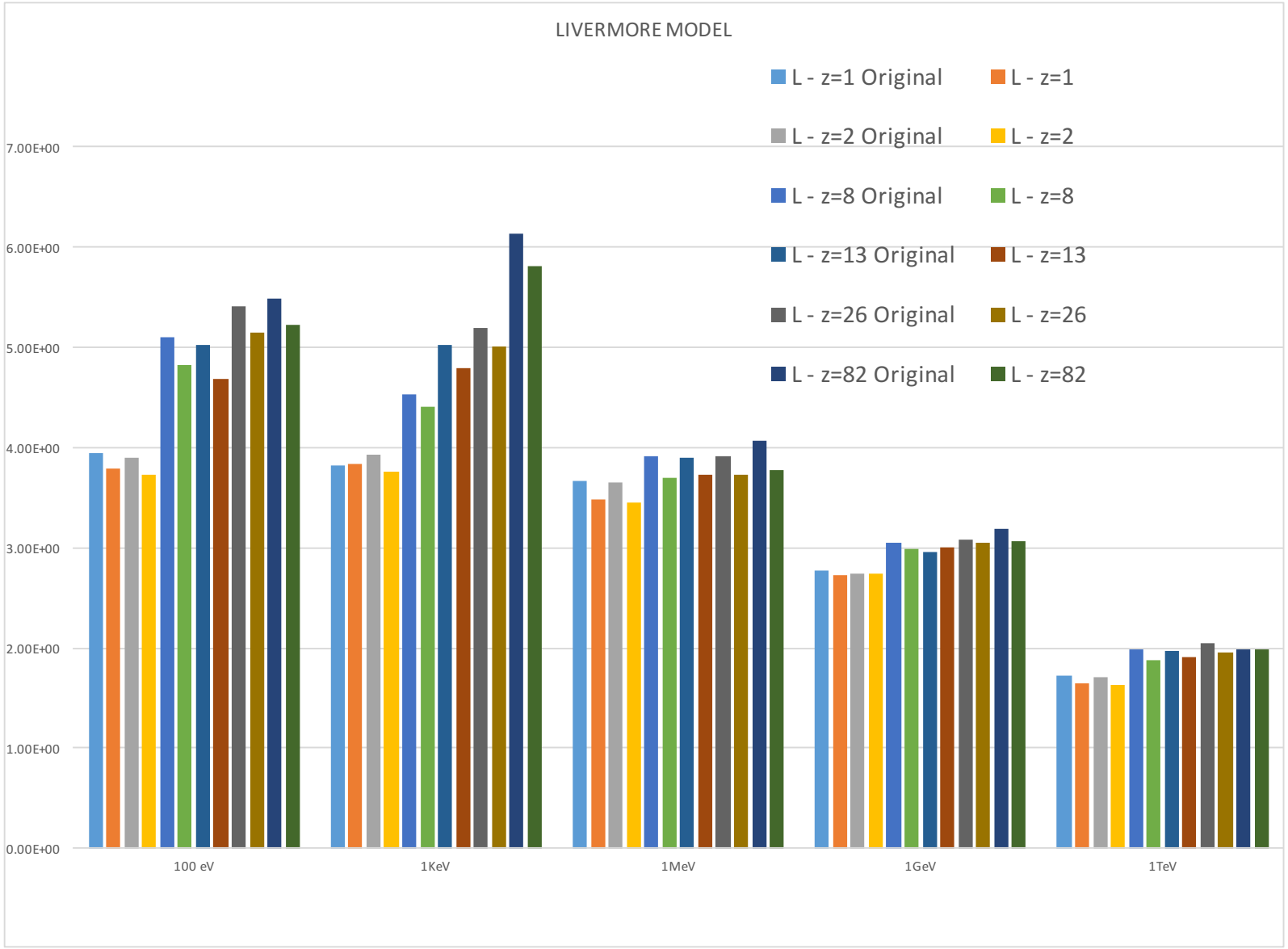
where

$$\gamma = 1 + \frac{E_e}{m_e c^2},\ A = \frac{1}{\beta} - 1 \tag{16}$$

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

*from previous presentation on p.e.:
https://indico.cern.ch/event/629729/contributions/2569301/attachments/1449139/2233786/PhotoElectricEffect_MB.pdf

Comparison between original sampling and new one (Penelope2014 like)



Achievements:

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

Using modified Livermore model (EPDL97) for p.e. as default

Results for 10.3ref04 are stable compared to 10.3ref03

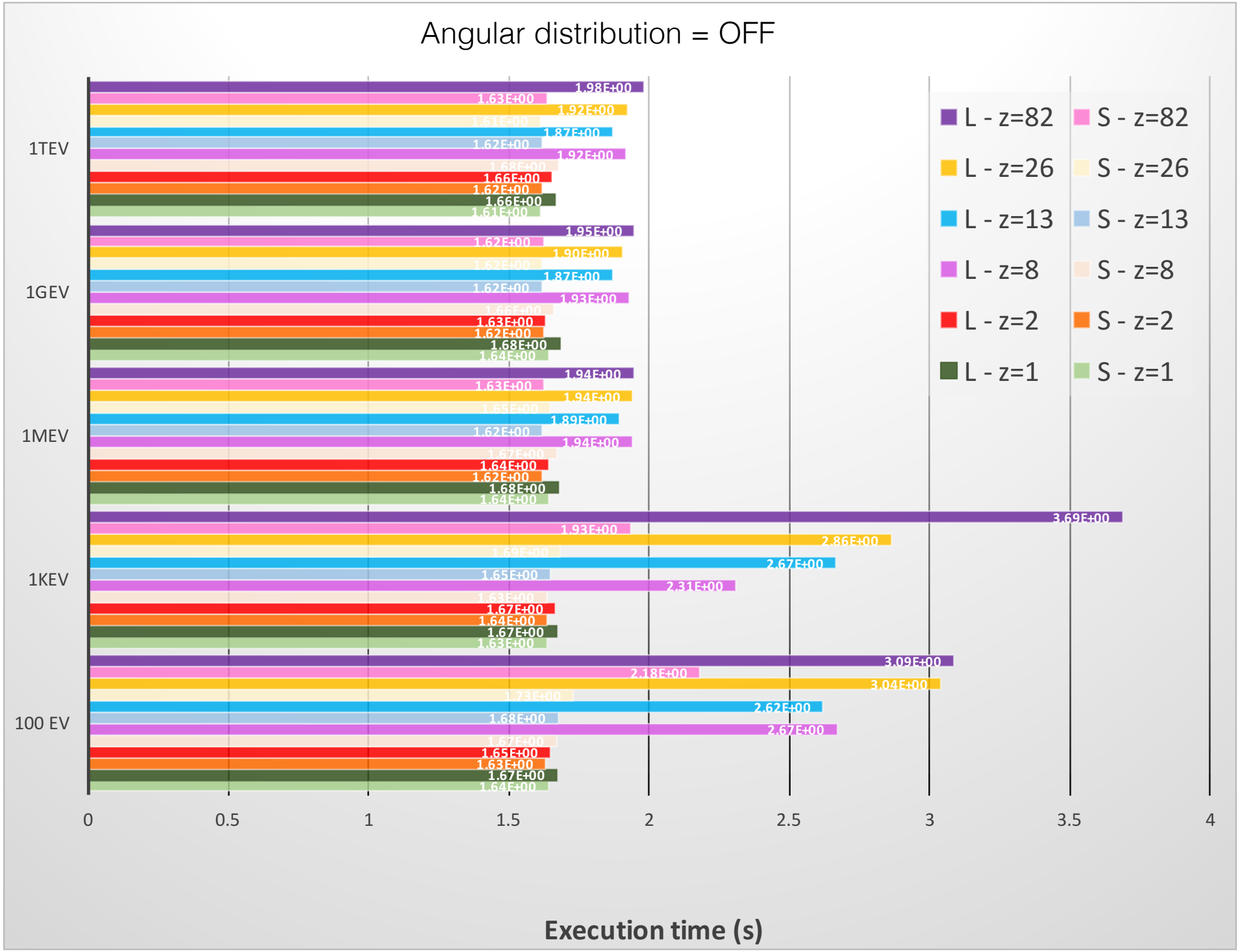
– *URL to validation results*: *https://geant4-tools.web.cern.ch/geant4-tools/emtesting/*

Conclusions on GS restructure/update:

– *No visible degradation of any result*

- Check on CPU performance
  - *Done by Soon on top of 10.3ref04*
    - https://g4cpt.fnal.gov/g4p/oss_10.3.r04em_SimplifiedCalo_01/cpu_summary.html
  - *Livermore models for Rayleigh and Photo-effect used by default*
    - *Improved quality of photon cross sections and may slightly affect shower shape*
    - *1% slowdown for Higgs sample*
    - *2% slowdown for e- showers*
  - *Can we agree with this default?*

***from V. Ivantchenko presentation @G4 meeting 2 weeks ago**


Angular distribution = OFF
1TEV
1GEV
1MEV
1KEV
100 EV
1.98E+00
1.63E+00
1.92E+00
1.61E+00
1.87E+00
1.62E+00
1.92E+00
1.68E+00
1.66E+00
1.62E+00
1.66E+00
1.61E+00
1.95E+00
1.62E+00
1.90E+00
1.62E+00
1.87E+00
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1.63E+00
1.62E+00
1.68E+00
1.64E+00
1.94E+00
1.63E+00
1.94E+00
1.65E+00
1.89E+00
1.62E+00
1.94E+00
1.67E+00
1.64E+00
1.62E+00
1.68E+00
1.64E+00
3.69E+00
1.93E+00
2.86E+00
1.69E+00
2.67E+00
1.65E+00
2.31E+00
1.63E+00
1.67E+00
1.64E+00
1.67E+00
1.63E+00
3.09E+00
2.18E+00
3.04E+00
1.73E+00
2.62E+00
1.68E+00
2.67E+00
1.67E+00
1.65E+00
1.63E+00
1.67E+00
1.64E+00
L - z=82
S - z=82
L - z=26
S - z=26
L - z=13
S - z=13
L - z=8
S - z=8
L - z=2
S - z=2
L - z=1
S - z=1
0
0.5
1
1.5
2
2.5
3
3.5
4
Execution time (s)

- Switching off the angular distribution we clearly see a **dependency on the energy** and **on the Z** of the material.

- We expected a dependency from the Z, but not from the energy (at least not so strong).

- Inspecting the code we see that there is indeed a dependency on the energy of the gamma:

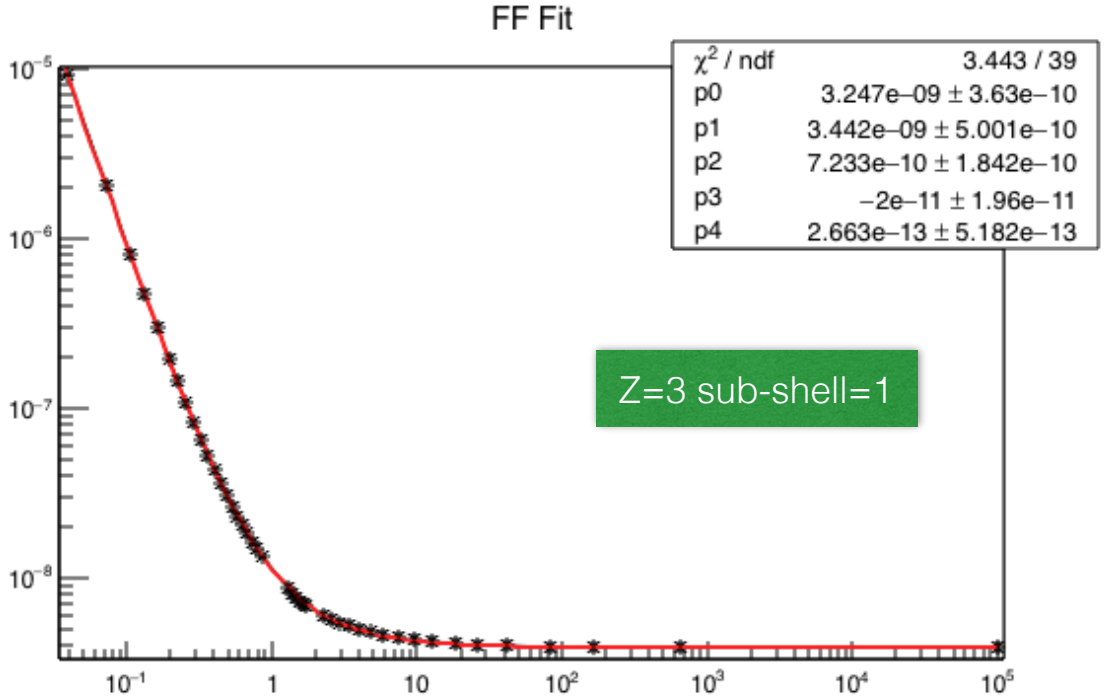
  - From threshold to 600keV (excluded): The total photoelectric and single shell cross-sections are tabulated

  - Above 600keV: EPDL97 cross sections are parameterised as follows:

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

New parameterisation with new data

- New total cross section and single shell cross section data available (livermore/ epics2014)



- Adding a parameter, with the new data the high-energies fit works well for energies>5KeV (reduced from 600KeV)

- New fit with two different energy ranges:
  - E in [5KeV-50KeV]
  - E > 50KeV
  - Constant value for E < 5 KeV -> Standard Physics or use tabulated values -> low energy model

BINDING ENERGIES data

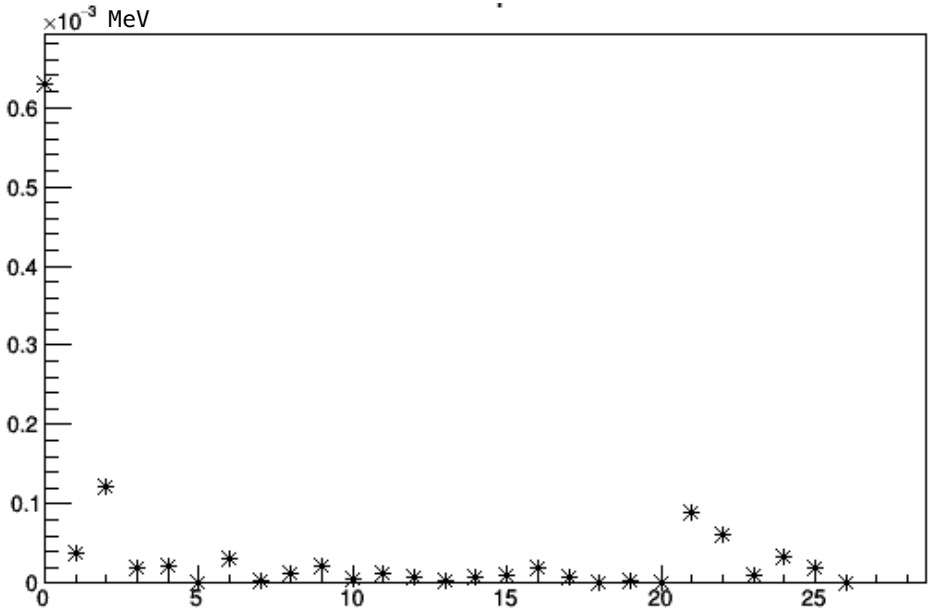
- At least **four** different sources of binding energies data in Geant4:
  - **G4AtomicShells** (used in the standard physics)
  - **G4AtomicShells_EADL** (not used for photoelectric for the moment)
  - **livermore/phot/pe-** (parametrization)
  - **fluor/binding.dat** (used for de-excitation) - same as the parametrisation ones

BINDING ENERGIES data comparison

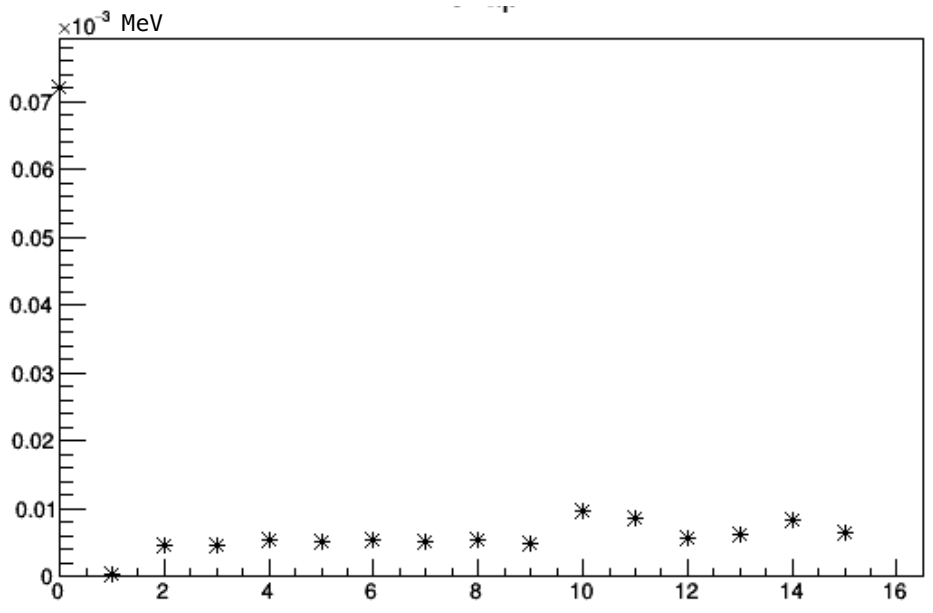
G4AtomicShells_EADL e livermore/phot/pe-
For Z<60 differences are within 35 eV. From Z=60 (mostly on k-shells) we have differences from around 50eV up to 630 eV for Z=98

G4AtomicShells and G4AtomicShells_EADL
Total differentNumShell: 38
Total n. energies that differ more than 10 eV: 19 (72 eV is one of the biggest)
G4AtomicShells_EADL has always one more shell than G4AtomicShells - and it's the right number of shells (ionisation potential taken mostly from theoretical calculations)

EADL vs livermore/phot/pe-



G4AtomicShells vs G4AtomicShells_EADL



Thanks