Geant4 electromagnetic physics for high statistic simulation of LHC experiments

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Abstract.
An overview of the current status of electromagnetic physics (EM) of the Geant4 toolkit is presented. Recent improvements are focused on the performance of large scale production for LHC and on the precision of simulation results over a wide energy range. Significant efforts have been made to improve the accuracy without compromising of CPU speed for EM particle transport. New biasing options have been introduced, which are applicable to any EM process. These include algorithms to enhance and suppress processes, force interactions or splitting of secondary particles. It is shown that the performance of the EM sub-package is improved. We will report extensions of the testing suite allowing high statistics validation of EM physics. It includes validation of multiple scattering, bremsstrahlung and other models. Cross checks between standard and low-energy EM models have been performed using evaluated data libraries and reference benchmark results.

1. Introduction

Geant4 is a toolkit for Monte Carlo simulation of the transportation and interaction of particles in matter [1, 2]. It is applicable for a wide variety of applications including high energy physics, space and medical science. It is used for the large scale simulation production for experiments at the LHC, like ATLAS [3], CMS [4], and LHCb [5], and many other experiments. The Geant4 EM Standard physics sub-packages [6–10] are important components of the toolkit. The stability and accuracy of the simulation results for large scale simulation production is a major requirement for Geant4.

In this report we summarize results of recent developments for Standard EM Geant4 models and new validations results. Significant efforts have been made to improve the description of EM shower shapes in order to describe details of $H \to \gamma\gamma$ signal [11, 12] and other reactions. The Bremsstrahlung process and multiple scattering description were reviewed and improved, having been identified as key components in defining EM shower shapes. LHC detector responses for high energy projectile particles are sensitive to precision of simulation of electron and gamma transport in MeV energy region. Therefore a significant validation and benchmarking are being carried out for medium and low-energy electrons and gamma. For these validation studies experimental data are used as well as comparison with other Geant4 models of low-energy EM the sub-packages Livermore and Penelope, which have been recently adapted to the common interface with the Standard EM sub-packages [13]. Also comparisons are performed with published results of EGSnrc and Penelope codes. For high scale simulation production CPU performance and memory management are important characteristics of the toolkit and we discuss results of monitoring of Geant4 electromagnetic physics performance.

2. New Geant4 Bremsstrahlung Models

In the last few years substantial efforts have been made to improve the description of the bremsstrahlung process in Geant4. With Geant4 version 9.2 a relativistic model [14] with an improved treatment of the Landau-Pomeranchuk-Migdal (LPM) effect has been provided, resulting in an better description of energy spectrum of high-energy electrons above 1 GeV. Version 9.5 introduced a data driven model which covers the energy range from 1 keV to 10 GeV. A new parametrized model is subject of current research, with the aim to become an alternative in the intermediate energy range (1 MeV to 10 GeV). These models are discussed in more detail in the following.

2.1. The Seltzer-Berger Model

The Monte Carlo description of the bremsstrahlung processes is dominated by the single-differential cross section $d\sigma/dk$, where k is the energy of the emitted photon. It can be written as a sum of a contribution of bremsstrahlung produced in the field of the screened atomic nucleus $d\sigma_n/dk$, and the part $Z\, d\sigma_e/dk$ corresponding to bremsstrahlung produced in the field of the Z atomic electrons,

$$\frac{d\sigma}{dk} = \frac{d\sigma_n}{dk} + Z\frac{d\sigma_e}{dk}\,. \tag{1}$$

The differential cross section depends on the energy k of the emitted photon, the kinetic energy T_1 of the incident electron and the atomic number Z of the target atom. The total cross section and the restricted energy loss can be obtained by integration of the differential cross section [9].

Seltzer and Berger have published extensive tables for the differential cross section $d\sigma_n/dk$ and $d\sigma_e/dk$ [16, 17], covering electron energies from 1 keV up to 10 GeV, substantially extending previous publications [18]. The results are in good agreement with experimental data, and provided also the basis of bremsstrahlung implementations in many Monte Carlo programs (e.g. Penelope, EGS). The estimated uncertainties for $d\sigma/dk$ are:

- 3% to 5% in the high energy region ($T_1 \geq 50\,\mathrm{MeV}$),
- 5% to 10% in the intermediate energy region ($2 \geq T_1 \leq 50\,\mathrm{MeV}$),
- and 10% at low energies region compared with Pratt results. ($T_1 \leq 2\,\mathrm{MeV}$).

Recently a new model has been introduced within the Standard EM sub-package, `G4SeltzerBergerModel`, based on an interpolation of the original Seltzer-Berger data table. The total cross section and the restricted energy loss are obtained by numerical integration performed at initialisation stage of Geant4. This guarantees consistent description independent

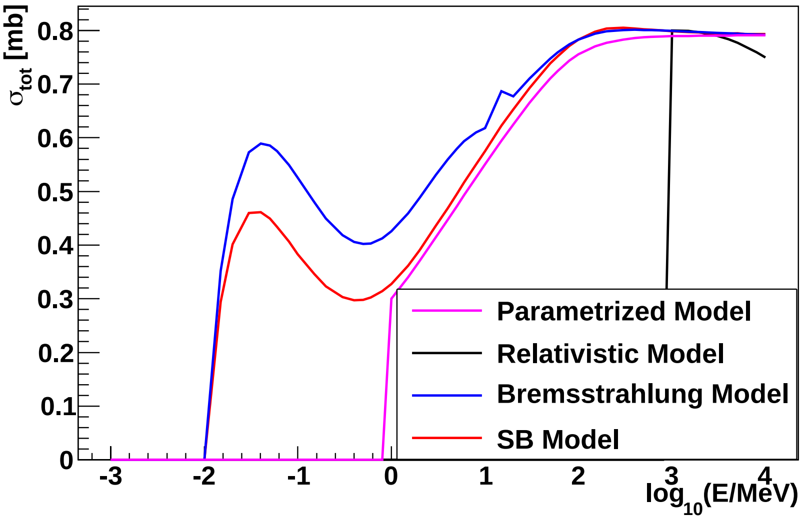


Figure 1. Total cross section comparison between models for $Z = 29$: Parametrized Bremsstrahlung Model, Relativistic Model, Bremsstrahlung Model (Geant4 9.4) and Seltzer-Berger Model. The discontinuities in the Parametrized Model and the Relativistic Model at 1 Mev and 1 GeV, respectively, mark the validity range of these models. The small kink visible in the old bremsstrahlung model is due to the non-smooth transition between two parameterizations for high and for low gamma energies.

of the energy cutoff. The current version uses an interpolation in tables for 31 available electron energy points versus 14 photon energy points, and for atomic number Z ranging from 1 to 99. It is the default bremsstrahlung model in Geant4 version 9.5.

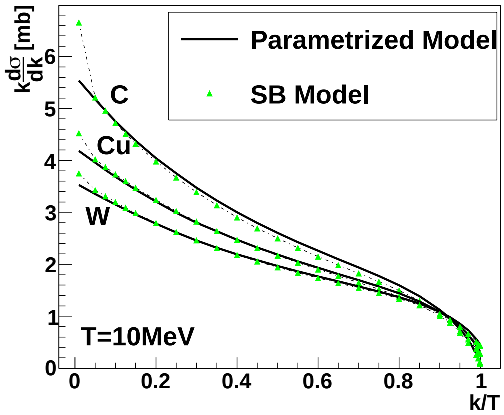
Figure 1 shows a comparison of the total bremsstrahlung cross sections with the previous implementation, and with the relativistic model. The differential cross section is depicted in Fig. 2 and exhibits similarly good agreement between the models and with the original Seltzer-Berger data table. Further improvements to the `G4SeltzerBergerModel` include the use of an extended version of the Setlzer-Berger data tables (52 points in electron energies and 31 in photon energies), which is currently under investigation.

2.2. Parametrized Bremsstrahlung Model

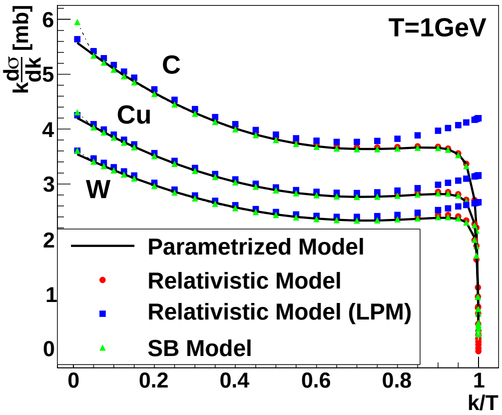
Until Geant4 version 9.4, the standard bremsstrahlung model was based on independent parameterisations for the total cross section, energy loss dE/dx, and differential cross section [19]. In the current research a single parameterization of the differential cross section $d\sigma/dk$ has been introduced. The total cross section and the energy loss functions are calculated by numerical integration at initialisation of Geant4 in the same way as it is done in the Seltzer-Berger model. The proposed parameterisation is based by the Bethe-Heitler cross section [19]

$$\frac{d\sigma}{dk} = \frac{c}{k}[(1 - ax)F_1(\delta) + bx^2 F_2(\delta)] \tag{2}$$

where $x = k/T$ with k and T being the photon and electron energy, respectively. $F_1(\delta)$ and $F_2(\delta)$ are the Thomas-Fermi screening functions [20], while a, b and c are the parameters to be fitted. The best parameters are determined for all elements ($Z = 1 - 92$) by an iterative optimization procedure. The reference data are provided by the extended Seltzer-Berger tables, and the minimization is performed using Minut2 package provided with the ROOT framework. Figure 2 shows a comparison between the differential cross section of the parametrized bremsstrahlung model with other models and the Seltzer-Berger data. The parametrized bremsstrahlung model provides good agreement with other models for electron energies from 1 MeV to 10 GeV, and for atomic numbers from $Z = 4$ (constrained by the Thomas-Fermi screening functions [20]) to $Z = 92$. It is in good description of the Seltzer-Berger data points and it has a good transition to the relativistic model, see figure 2-(c).



(a)



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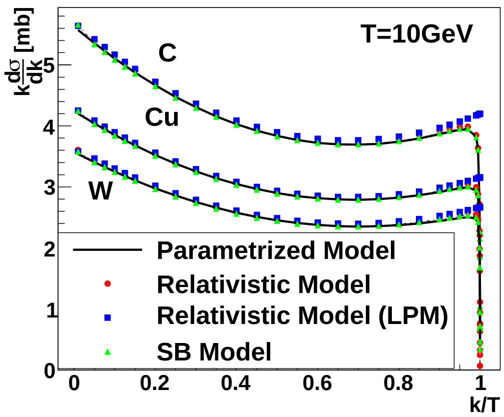

(c)

Figure 2. Plots (Relativistic Model, LPM effect activation, Seltzer-Berger Model and Parametrization Model) for $Z = 6, 29, 74$ and T=10 MeV, 1 GeV and 10 GeV, respectively.

2.3. The Relativistic Model

For relativistic electron energies the Bethe-Heitler cross section with the complete screening approximation provides a good description of the differential bremsstrahlung cross section. It provides the basis of the `G4eBremsstrahlungRelModel`, which was first introduced in Geant4 version 9.2 [14]. In contrast to the Seltzer-Berger model and the parametrized model as introduced above, it allows the incorporation of Landau-Pomeranchuk-Migdal effect (LPM) [15]. Special emphasis was put to a consistent combination of the LPM effect with Ter-Mikaelian effect (polarization effect), both limiting the number of low energy photons. Comparison with

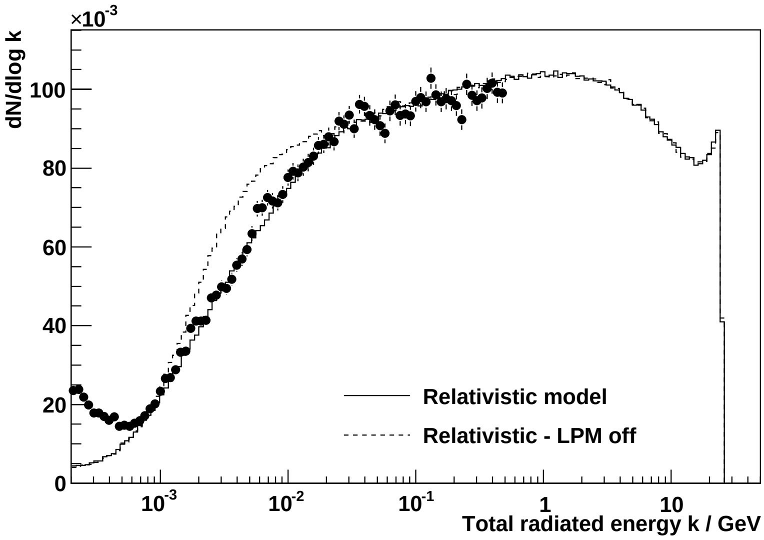

Figure 3. Relativistic model vs experimental data for 25 GeV electron on Aluminum [21].

experimental data shows good agreement. Figure 3 simulation results for a 25 GeV electron beam on a thin Aluminum foil, together with data from the E-146 experiment [21] at the Stanford Linear Accelerator (SLAC). Low-energy data shape shows some increase which according to authors is connected with experimental background from other processes and not bremsstrahlung itself. The relativistic model is currently being improved to include Thomas-Fermi screening functions. This allows the application of the model to the intermediate screening regime, and increases the range of applicability to lower energies allowing more smooth transition to low-energy models described above.

3. Electron multiple scattering model update

The process of multiple scattering (MSC) of charged particles is a key component of Monte Carlo transport. At high energy it defines the deviation of charged particles from ideal tracks, limiting the spatial resolution of detectors. Scattering of low-energy electrons defines energy flow via volume boundaries, directly affecting all application domains including transmission through shielding and transmission of energy from absorbers to sensitive elements of the setup. The Geant4 toolkit offers several models of multiple scattering [22]. The production model is developed by L.Urban and it is used in Geant4 by default. Because of high sensitivity of simulation results on MSC model for high statistics Monte Carlo production for LHC experiments, any modification of the Urban model algorithm is provided in a separate C++ class. This approach allows to configure backward compatible Physics Lists with new versions of Geant4. In particular, `G4UrbanMscModel95` provided better agreement with the scattering data [23] for electrons (Fig.4) than previous version of the model `G4UrbanMscModel93`. The list of upgrades introduced in this model include:

- new tuning of tail of scattering function;
- added sampling of correlations between scattering angle and lateral displacement for a step;
- added sampling of end of step position along particle direction.

This new variant of MSC model is the default for version 9.5 of Geant4.

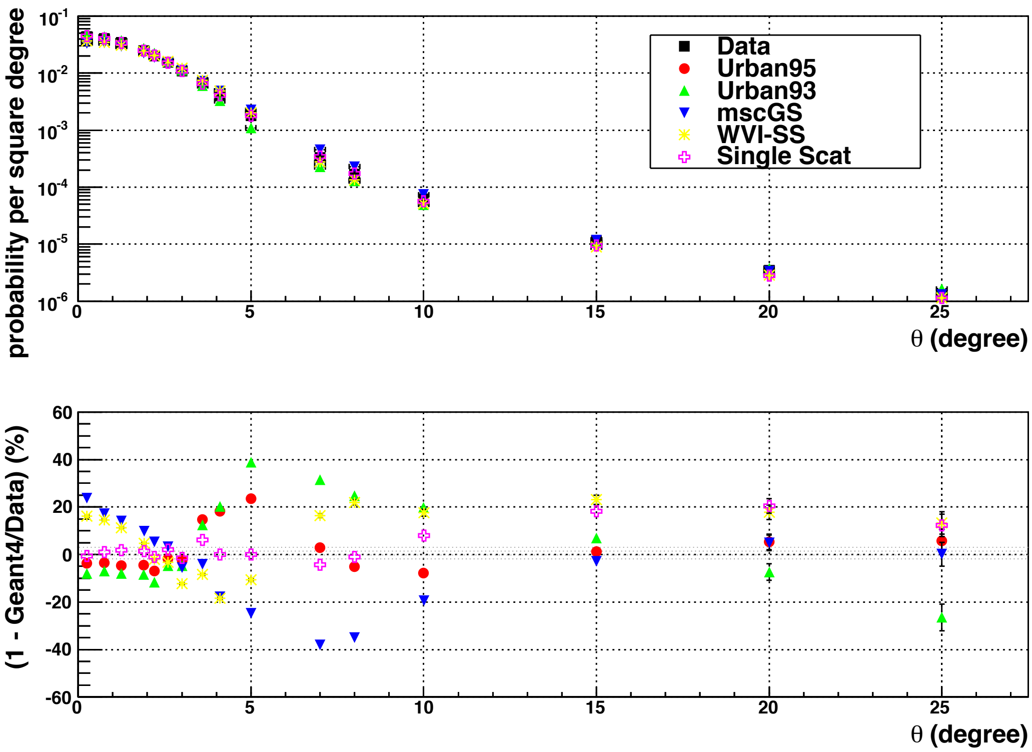

Figure 4. Comparison of different Geant4 MSC model predictions and experimental data [23] for 15.7 MeV electrons scattering off 9.68 um Gold foil: angular distribution (top); Monte Carlo over data (bottom). Urban model 95 and the single scattering model provides overall better agreement with the data.

4. Penelope models upgrade

The Penelope models implemented originally in Geant4 were based on the version 2001 of the Penelope code [24, 25]. Recently the sub-package have been progressively updated to the version 2008 [26]. The full set of upgraded models is available since the release 9.5.beta of Geant4 (June 2011). The G4Penelope v2001 models are still present in Geant4 9.5 for backwards compatibility and to allow for a through validation of the new v2008 models. They will be removed from Geant4 in the release 9.6.

The new models provide improved physics performance with respect to the v2001 models. A clear difference is observed for Rayleigh scattering and for bremsstrahlung. The Rayleigh scattering model in G4Penelope v2008 model features:

- tabulated cross sections in place of analytical parametrization, thus improving the agreement with experimental data, which was relatively poor at low energy [27];
- a revised management of the sampling of the final state, which is more stable and efficient.

The bremsstrahlung model in Penelope v2008 greatly improves the double differential (energy-angle) cross section profiles in thin targets, which showed an unphysical shape at large transferred energy for small angles. Apart from these physics improvements, which are coming from the developments of the Penelope code, a special attention was paid to the specific implementation of the physics models in Geant4. In particular, care was taken to improve the CPU performances and to reduce the memory usage by the models.

5. Low energy extension of ionisation models

Geant4 photo-absorption ionisation (PAI) model [28] was extended in low energy region using a parametrized correction in the spirit of the Thomas-Fermi atomic model. The correction parameter was selected as a function of the target atomic number. The Geant4 ionisation models were compared with experimental data for the mean energy loss (dE/dx). The Moller-Bhahba standard model was improved in the low energy region. The models show good agreement with the experimental data for the electron energy interval $0.01 - 10\,\mathrm{MeV}$.

The PAI differential ionisation cross section is modified with additional factor like a simplified Fermi-Teller correction in the spirit of the Thomas-Fermi atomic model. The factor reads

$$\left\{1 - \exp\left[-\frac{v}{a(Z)v_o}\right]\right\},$$

where v is the projectile particle velocity, v_o is the Bohr velocity ($v_0 = \alpha c$, where α is the fine structure constant and c is the speed of light in vacuum). The correction factor $a(Z)$ is a function of the target atomic number Z. The correction improves the description of dE/dx in the energy interval below the ionisation minimum and allows a user to describe the ionisation energy loss down to $\sim$ 100 eV for electrons and $\sim$ 100 keV for protons. For very low energies, when $v \ll v_o$, the correction is proportional to the square root of the projectile kinetic energy. This type of correction is used in some Geant4 ionisation models (Bhabha) directly in the formula of dE/dx.

Validation of Geant4 ionisation models have been done against experimental data of electron ionisation for Al, Au, Cu and Si from the compilation [29]. The data for liquid water, hydrogen, nitrogen, oxygen and carbon dioxide were obtained from compilation [30]. Typical results for Geant4 9.5 is shown in Fig. 5. Geant4 models PAI, Moller-Bhabha, Livermore, Penelope, and new Penelope08 all are in a good agreement with each other above 1 keV and with the data. Below predictions are different and each model has its own low-energy limit. The same trend is observed also for ionisation losses of electrons in other media and protons in gases. The PAI model may be recommended for simulation of gaseous detectors or thin silicon layers when accurate treatment of low-energy delta-electrons is needed. The default electron ionisation model Moller-Bhabha also can be applied down to 100 eV in majority of materials.

6. Extension of EM interfaces and new models

Recently Geant4 software interfaces for electromagnetic physics processes were unified between all electromagnetic sub-packages including Standard, Livermore, Penelope and DNA [13]. As a result, combined Physics Lists collecting a desired set of models from different sub-packages can be built per particle type and energy range. The Standard models are used above 1 GeV in all cases; for low-energies a selection should be made to provide the needed accuracy in a concrete Geant4 application efficiently. A correction is applied to high energy models in order to provide continues shape of cross sections, energy loss, and ranges if two or more models are used. The unification of Geant4 interfaces for electromagnetic physics was completed when a common approach for simulation of atomic de-excitation had been developed [31]. This was achieved by introduction of a new abstract `G4VAtomDeexcitation` interface and its first concrete implementation, `G4UAtomicDeexcitation`. With this new interface the atomic de-excitation module can be activated for any electromagnetic or other physics model of Geant4. Both UI and C++ interfaces are provided with Geant4 9.5 allowing activation of de-excitation on top of any PhysicsList for whole geometry or specifically per *G4Region*.

To utilize new capabilities a new photo-electric effect model with fluorescence (class `G4PEEffectFluoModel`, uses the SANDIA table) have been introduced into EM standard sub-package. The deexitation model provides simulation of K- and L-shells emission after photo-electric absorption. Geant4 photo-electric models were tested versus the reference database EPLD97 (Fig. 6). All models provide in average an accuracy better than 5% in the photon

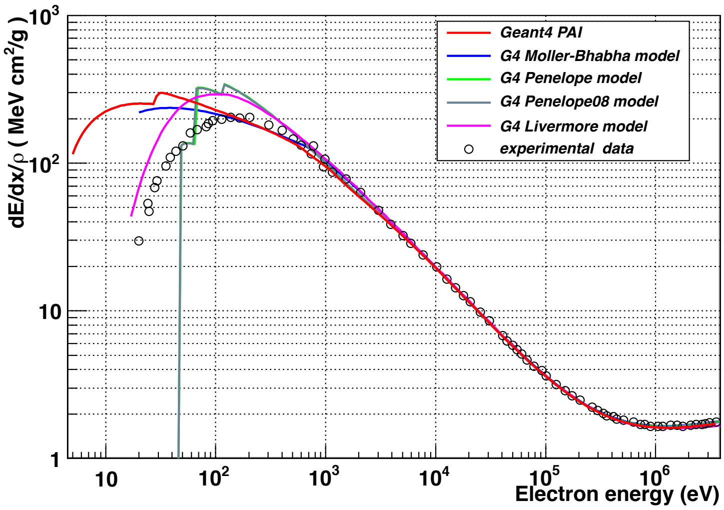

Figure 5. Electron mean energy loss in CO_2 vs. electron energy: points are data [30], solid lines - different Geant4 models. Moller-Bhabha and PAI model follow the date down to 100 eV. Below 200 eV Penelope and Livermore models show effects caused by the treatment of atomic shell effects.

Table 1. The relative CPU time of sampling for photo-electric effect at the photon energy 0.02 MeV for different models.

Photo-electric model	performance (s)
standard	1
standard with fluorescence	1.1
PENELOPE	8.5
PENELOPE08	3.9
Livermore	9.0

energy range $0.01 - 10$ MeV. The new standard model shows similar CPU performance than the old standard model, the cross section of the new model is indistinguishable from the old one. Both are the fastest models compared to Livermore and Penelope models (Table 1). The new model is a default for production Physics Lists since Geant4 version 9.5.

A new abstract interface to generate angular distribution has been introduced in EM infrastructure allowing to configure different angular generators for the same EM model. This may be applied to models where sampling of energy of a secondary particle can be factorized out of sampling of particle angle. In particular, such models are photo-electric effect, Rayleigh scattering and bremsstrahlung. A new angular generator applicable for bremsstrahlung `G4DipBustGenerator` has been introduced, which is based on the standard dipole angular distribution in primary electron rest frame [32]. It is providing very fast sampling of gamma direction (Table 2). The quality of results are compatible with the default generator `G4ModifiedTsai`, which include parameterization of Tsai distribution [20] developed in GEANT3. Alternative generators `G4Generator2BS` and `G4Generator2BN` [33] are available in the low-energy sub-package. The new dipole model is in a good agreement with the Penelope model (Fig. 7). Both have a long tail at large angles which is absent in the Tsai generator.

Table 2. The relative time of sampling of gamma angle for 15 MeV e$^-$ in 36 mm thick Al.

Bremsstrahlung (angular model)	performance
emstandard (dipole)	1
emstandard (BS)	1.011
emstandard (Tsai, default)	1.039
G4-PENELOPE	4.556
G4-Livermore (Tsai)	3.589

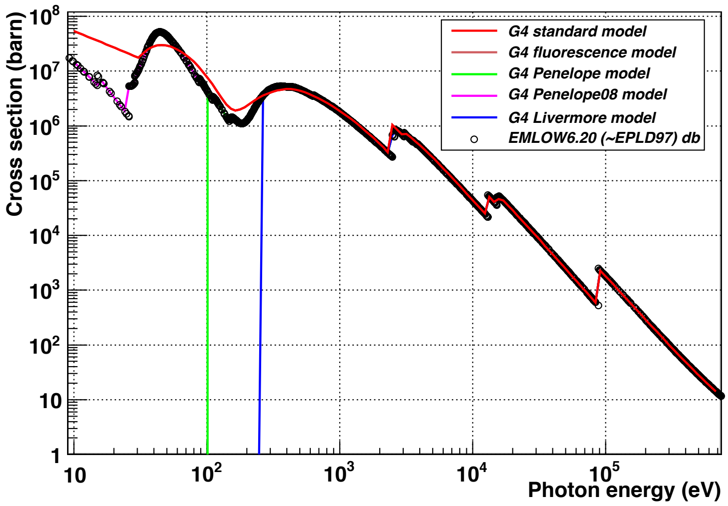

Figure 6. Photoelectric cross section in Lead vs. photon energy: points are evaluated data, solid lines - Geant4 models. Penelope08 has no energy limit, the new standard model has less precision below 250 eV. Livermore and Penelope have energy limits of 250 eV and 100 eV, respectively.

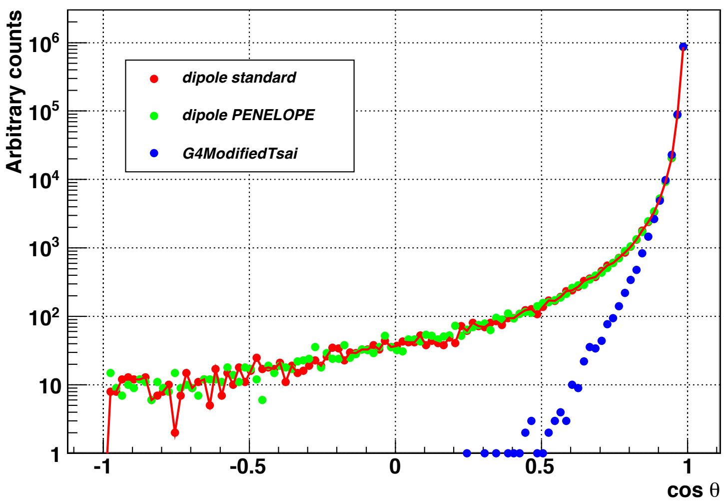

Figure 7. Bremsstrahlung angular distribution of 10 MeV electrons off Aluminum target.

7. Biasing options for EM physics

With Geant4 9.5 a new biasing framework for EM physics processes have been introduced. This is based on the std EM model design [9] and thus also applicable to low-energy physics processes and models, thanks to unification of EM interfaces. In this design all management functions are performed by generic classes and are working independently of any concrete physics model. All biasing options are available via UI or C++ interface and may be applied to any Physics List. The following EM biasing options are available:

- cross section biasing per process;
- forced interaction per process and per `G4Region`;
- splitting of secondary particles (bremsstrahlung splitting);
- Russian roulette method.

The first option provides the possibility of changing of any electromagnetic cross section by a defined factor. This option allows studies of the accuracy of electron shielding simulation due to the uncertainty in EM cross sections. Also it may be applied to rare processes. A weight factor can be used to artificially enhance a process, but it should be taken into account that the method has limitations: in the current implementation from Geant4 9.5 no cross section/weight correction is computed.

The second option allowing studies of effects provided by a particular physics process, for example, photo-electric effect of primary gamma in a shielding material. This is implemented in a way that only primary particle interaction is forced. The particle type and forced interaction process are selected via UI command. The selected process is forced to happen inside a `G4Region` defined by the same UI command. The implementation ensure that only first interaction is forced, all secondary interactions of the primary particle are not forced.

Splitting (in particular, bremsstrahlung splitting) means the creation of a defined number of copies of secondary particles inside a `G4Region` of interest. This method allows enhancing of the gamma flux from bremsstrahlung after a shielding material. For example, 0.1 MeV primary electrons are absorbed by 2 mm Aluminum shielding but some bremsstrahlung gamma may penetrate through. For traditional simulation a huge statistics is needed to quantify this effect. Using bremsstrahlung splitting the estimation of the gamma flux may be done using much lower statistics. This option is also activated via UI command or C++ interface which specifies process, `G4Region`, splitting factor and energy limit of splitted secondaries. In the implementation for Geant4 9.5 secondary particles are cloned – and not resampled. This simplified variant of splitting requires upper energy limit for secondaries to avoid large fluctuations in final spectra.

The Russian roulette method can be considered as the inverse of the splitting method: With some probability secondary particles are killed and not propagated. If a particle is propagated it got an enhanced weight. This method is likely more important for fast simulation of electromagnetic showers but may be useful for some shielding simulations. The same interface as for the splitting is used but in contrary to the splitting the factor should be below unity.

8. Validation results

Geant4 EM physics is validated on a regular basis using an extended validation suite [34]. For each new Geant4 version the full set of available tests are executed. The validation is performed against publish data and/or versus previous versions of Geant4. The regression tests for a simple calorimeter setups allowing to predict stability or some drift of the calorimeter response. In Fig. 8 results for the response and resolution of the ATLAS barrel type calorimeter are shown. The detector response was increased by about 0.5 % with Geant4 version 9.4 mainly due to modification of MSC model for electrons. The relative width of the response is larger by about 1 % with Geant4 version 9.5 due to usage of the Seltzer-Berger model.

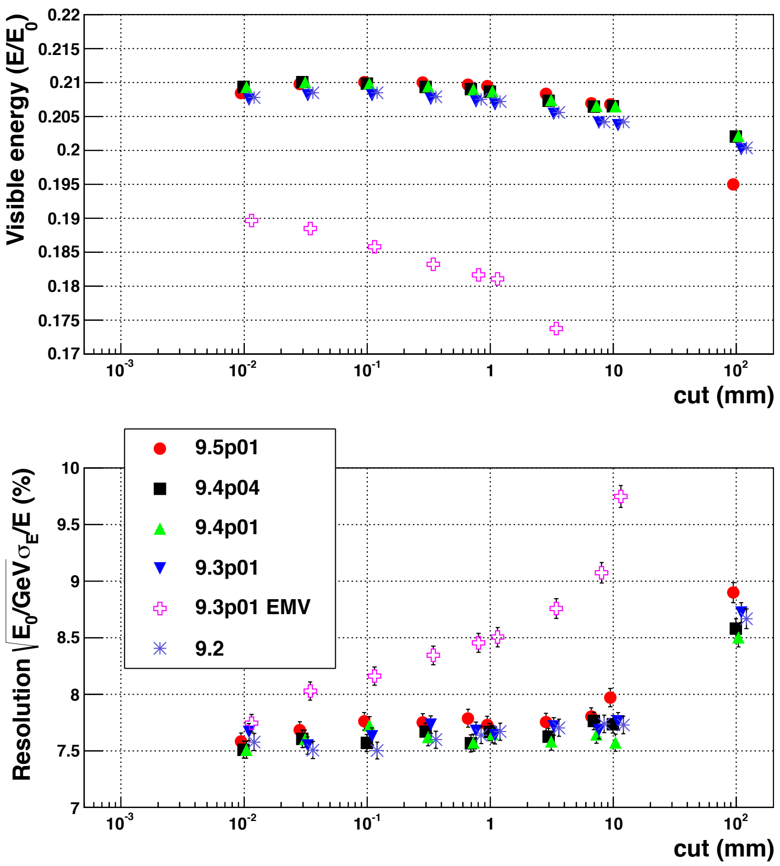

Figure 8. Visible energy and resolution for a 10 GeV electron response in a simplified sampling calorimeter with 2.3 mm Lead and 5.7 mm liquid Argon as a function of cut in range for different Geant4 versions. With the exception of the fast EM physics (EMV), all versions of Geant4 yield stable response over a wide range of cut parameters.

Experimental data [35, 36] for electron bremsstrahlung off Aluminum foil are used for benchmarking of the standard EM models, Livermore and Penelope modes of Geant4, and the published results of the PENELOPE code [37]. The bremsstrahlung intensity spectrum produced by 2.8 MeV electrons was evaluated at the angle of 15 ° after Aluminum target 6.41 mm thick (Fig. 9). The experiment [38] with 15 MeV electrons off 36.1 mm thick Aluminum target was evaluated in terms of bremsstrahlung spectrum to compare the Geant4 model predictions at 10 ° (Fig. 10). In this case the published results of EGS4 simulation [38] are compared with Geant4 models and the data. These results demonstrate that current models, including the new Seltzer-Berger model sub-package, reproduce the data with good accuracy. In contrast, the standard bremsstrahlung model of Geant4 9.4 was not able to describe data of the same benchmark at 2.8 and 1 MeV.

An electron scattering benchmark [39] has been developed to perform detailed comparisons between Geant4 scattering simulation and data [40]. Several different multiple scattering Geant4 models were used to generate distribution for scattering of 13 and 20 MeV electrons in thin foils. The characteristic scattering angle, defined as the angle at which the scattered intensity fell to $1/e$ of its value on the central peak, was extracted from the simulated data by fitting a Gaussian

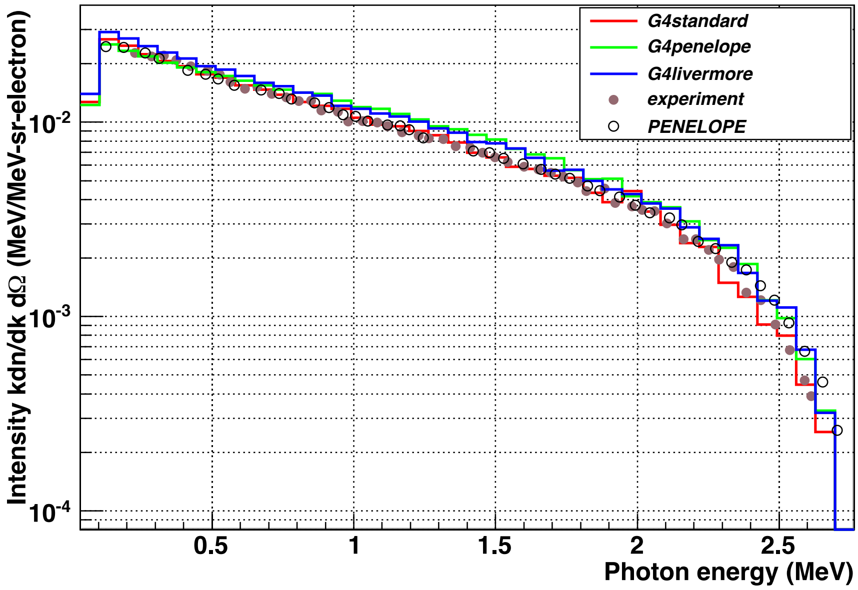

Figure 9. Bremsstrahlung intensity spectrum for a 2.8 MeV electron beam off 6.41 mm Aluminum target evaluated at the angle of 15°: solid points – data [37], opened points – PENELOPE published result, histograms – Geant4 models.

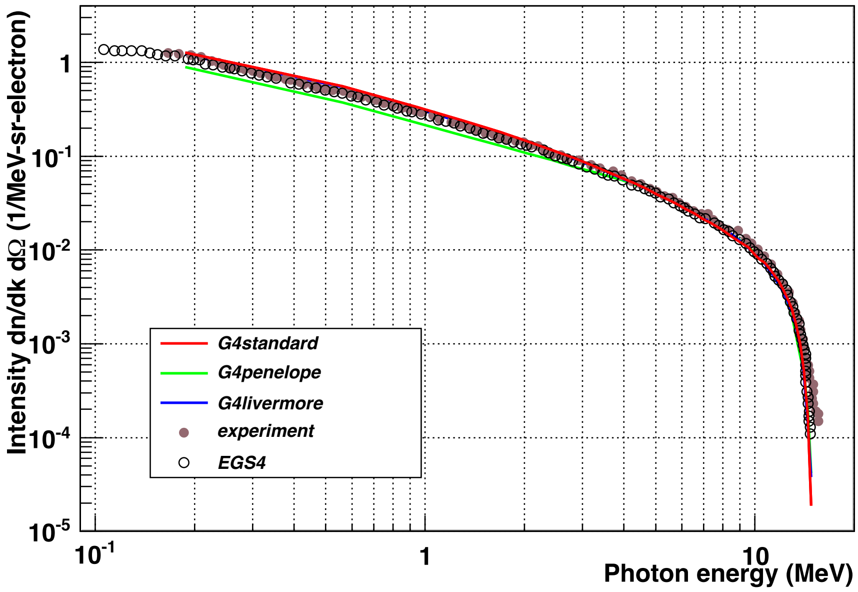

Figure 10. Bremsstrahlung intensity spectrum for a 15 MeV electron beam off 36.1 mm Aluminum target evaluated at the angle of 10°: solid points – data [38], opened points – EGS4 published result, histograms – Geant4 models.

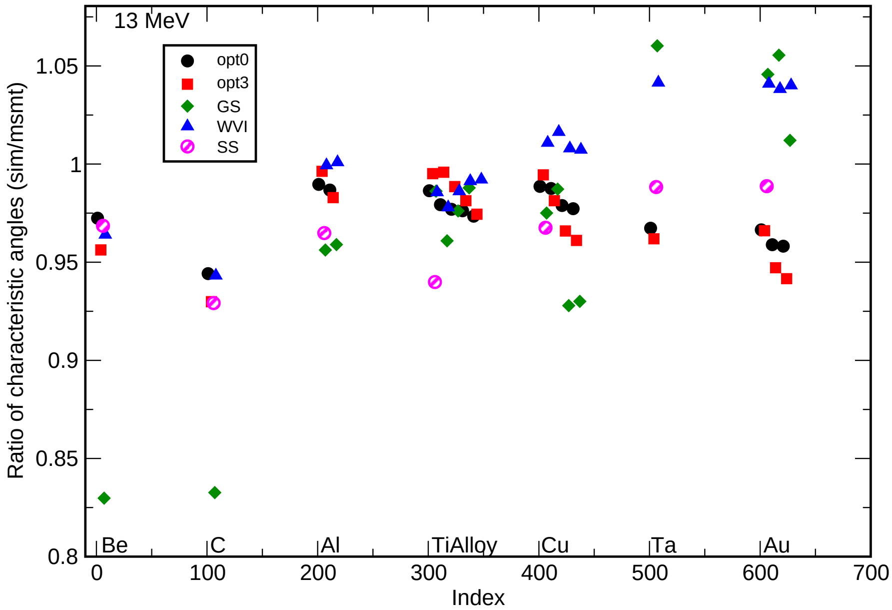

Figure 11. Ratio of simulated to measured characteristic scattering angles for 13 MeV electrons on different target materials and for different MSC models: Urban model, default EM Physics List (opt0), Urban model, high-precision EM Physics List (opt3), Goudsmit-Saunderson MSC model (GS), Wentzel-VI (WVI) and Single Scattering (SS) models.

to the central portion of the curve. The ratio of simulated to measured characteristic angles at 13 MeV is shown in Fig. 11. Agreement with measured values was within 7%, except for the Goudsmit-Saunderson model at low atomic numbers. The simulated values tended to be smaller than measured, aside from the Wentzel-VI and Goudsmit-Saunderson algorithms at high atomic number. Results at 20 MeV are similar.

9. Conclusions

In summary we would like to emphasize that EM sub-packages of Geant4 provide stable results for high statistics Monte Carlo production for LHC experiments, but at the same time are continuously improved. Extensions allowing to apply EM models down in energy from 1 keV to 100 eV which is important for simulation of gaseous and micro detector responses. New models of bremsstrahlung provide very good description of available experimental data from 1 MeV to 300 GeV. The results of the testing suite confirms better agreement of Geant4 9.5 results with various benchmarking data.

10. Acknowledgments

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