Progress in Geant4 Electromagnetic Physics Modelling and Validation

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On behalf of the Geant4 electromagnetic physics working groups

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Abstract. In this work we report on recent improvements in the electromagnetic (EM) physics models of Geant4 and new validations of EM physics. Improvements have been made in models of the photoelectric effect, Compton scattering, gamma conversion to electron and muon pairs, fluctuations of energy loss, multiple scattering, synchrotron radiation, and high energy positron annihilation. The results of these developments are included in the new Geant4 version 10.1 and in patches to previous versions 9.6 and 10.0 that are planned to be used for production for run-2 at LHC. The Geant4 validation suite for EM physics has been extended and new validation results are shown in this work. In particular, the effect of gamma-nuclear interactions on EM shower shape at LHC energies is discussed.

1. Introduction

The Geant4 electromagnetic physics sub-packages [1]-[10] are key components of any simulation, in particular for the simulation of LHC experiments. A small variation of EM physics may affect prediction

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accuracy and CPU performance of large scale Monte Carlo simulations for high energy physics (HEP), medicine or space science. Thus significant efforts have been spent for validation of new versions of the Geant4 toolkit. Because of synergy of EM effects for different application domains various validations are performed by groups from large LHC experiments and by groups working in space science and medical applications of Geant4. Preparation for LHC runs at higher energy and luminosity requires continuous refinements and validations of Geant4 EM sub-packages, which have been prepared for the new Geant4 release 10.1 and patches for releases 9.6 and 10.0. In this work some aspects of these improvements are discussed and validation results are shown.

2. EM infrastructure upgrades

EM sub-packages were adapted to the multi-threaded (MT) mode in the previous Geant4 (10.0) [10]. For the new version 10.1 further improvements and code optimisation for the MT mode were carried out for all EM sub-packages. Now all EM data structures are shared between threads. For steering of EM physics in the MT mode a new conception of EM parameters definition is introduced. EM parameters are subdivided into two groups:

- Static parameters shared between all EM processes;
- Parameters defined per process/particle type.

Parameters from the 1st group are kept inside a new G4EmParameters singleton class, can be modified via UI command or C++ interface, and are enabled during initialisation of a new run. Parameters from the 2nd group may be defined during construction of EM physics in order to have optimal values per particle type. It is recommended to set these parameters in EM physics constructors. Due to modification of the interface to EM parameters, all EM physics constructors from the physics_list sub-library were updated. New EM physics constructors were added and some parameters of existing constructors were changed:

- *G4EmStandardPhysics_option4* – combined standard/low-energy models, *RangeFactor* [6] for multiple scattering is set to 0.02;
- *G4EmStandardPhysicsSS* – new class uses single scattering instead of multiple scattering for all particle types;
- *G4EmStandardPhysicsWVI* – new class uses G4*WentzelVIModel* for $e^{\pm}$;
- *G4EmLowEPPhysics* – experimental physics for new low-energy models in which a new *G4LowEWentzelVIModel* multiple scattering is used for $e^{\pm}$.

3. Gamma models updates

Main Geant4 gamma processes were revised and a common approach was implemented for the Compton scattering and photo-electric effect:

- Compton cross sections are forced to be zero at the low-energy model limit;
- Photoelectric-effect cross sections are set to *const* non-zero value below first ionisation potential or below low-limit of model applicability (figure1);
- All gamma conversion cross section tables in the default EM physics configuration now have the same energy grid as in low-energy physics.

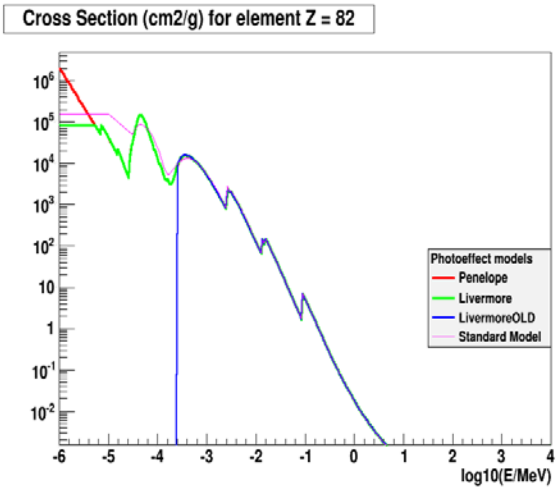

Figure 1. Cross section of photo-electric effect in silicon as a function of gamma energy for different Geant4 10.1 models. Blue line-Livermore model from Geant4 9.5.

These modifications provide prompt absorption of very low-energy gamma produced by Geant4 hadronic models in LHC simulation for all EM Physics Lists. Also the threshold cross section shape of gamma conversion is now reproduced equivalently in all EM Physics. In the current version of Geant4 the main difference between different models of gamma interactions [11] is in details of sampling of final state; cross sections of all models are very similar. Figure 2 demonstrates comparison of different Geant4 Compton scattering models versus NIST evaluated data [12]. All cross sections above 20 keV agree between each other and NIST within 2 %. Larger differences are below this energy but in that case contribution of the Compton scattering is small.

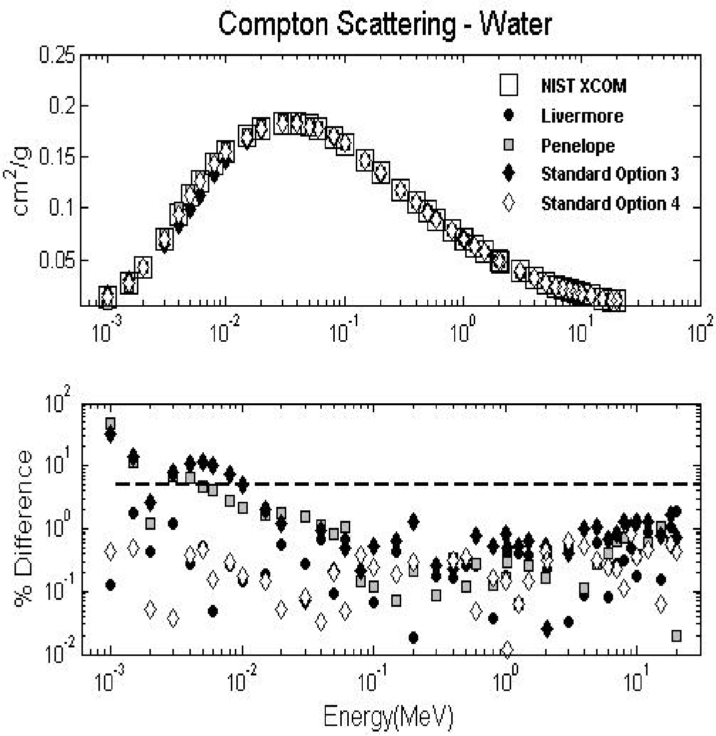

Figure 2. Energy dependence of the Compton scattering attenuation coefficient in water for different Geant4 10.1 models and NIST XCOM data [12] (top); difference between Geant4 and NIST XCOM (bottom). The dashed line is the maximum uncertainty of NIST XCOM.

4. Multiple scattering model developments

Multiple scattering model algorithms for Geant4 10.1 were not changed. Only code optimisation was introduced to improve CPU performance. Also new options were provided which can be enabled via C++ interface and new UI commands:

- /process/msc/MuHadLateralDisplacement enable/disable sampling of lateral displacement sampling for muons and hadrons, an option that may be considered for LHC simulation;
- /process/msc/DisplacementBeyondBoundary – enable/disable a new algorithm of sampling of lateral displacement when end point of a step of a charged particle is in the vicinity of or exactly on the geometry boundary.

Sampling of lateral displacement of an endpoint of a step of low-energy e± is an avoidable part of any multiple scattering algorithm [6]. For high energy hadrons in simulation of LHC experiments contribution of such displacement is small. The first option allows optimization of EM configuration for a concrete use-case in order to get faster simulation. In contrary, the second option may be used to increase accuracy of simulation. These new options are disabled by default.

5. High energy calorimeters response

After Geant4 9.6 a lot of technical modifications were introduced into EM sub-libraries due to migration to MT mode. At the same time, only some minor tunings were done for physics models. So, similar simulation predictions are expected for recent Geant4 versions. As an example, in figure 3 response and resolution of simplified Pb/liquidAr (ATLAS-barrel type) sampling calorimeter is shown as a function of *cut in range* for different Geant4 versions and EM Physics Lists. For the version 9.6p04 there is a 0.2% increased response compared to the 9.4p04 version. No difference between 9.6, 10.0, and 10.1 is observed. Accurate stable response of sampling calorimeter can be obtained with the default configuration of EM physics. Note, that in the case of weak step limitation (EMV), both response and resolution are biased.

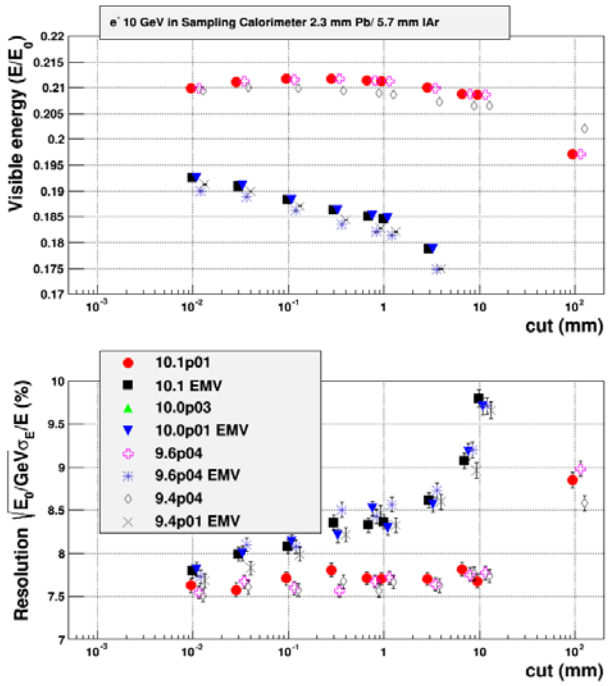

Figure 3. Response and resolution of ATLAS-barrel type simplified sampling calorimeter as a function of Geant4 cut in range. Different markers correspond to different Geant4 versions and EM physics options.

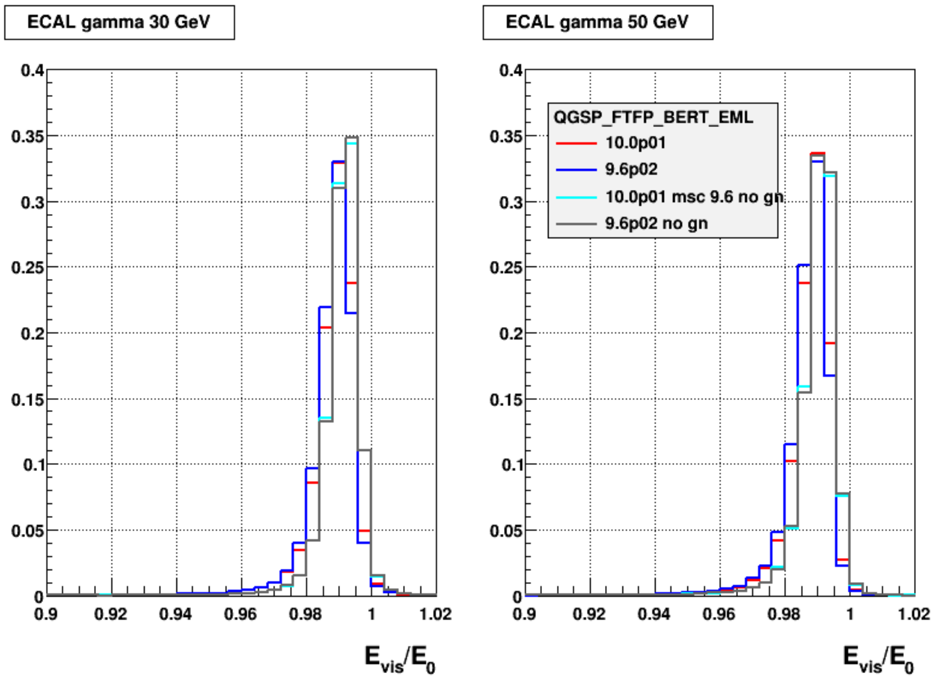

Figure 4. Response of CMS type simplified combined calorimeter (ECAL + HCAL) for 30 GeV and 50 GeV electron beams for different variants of EM physics configuration.

For CMS type crystal calorimeters an effect on EM shower from gamma-nuclear interactions was identified as a shift of peak energy deposition for 0.5%. In Geant4 10.0 these interactions are simulated with the Bertini cascade instead of the old CHIPS model and neutron yield from gamma-nuclear interaction decreases compare to Geant4 9.6. Additionally, neutron cross sections were improved. In summary these modifications provide a shift of peak position of energy deposition for 0.2%. Figure 4 illustrates this difference: red histogram (10.0p01) is shifted right from the green one (9.6p02). Changes of EM and hadronic options (TRV) have no effect, change of neutron cross sections (QBBC) provides about half of the effect.

6. High energy processes

New requirements for Geant4 come from R&D carried out for developments of a project of the Future Circular Collider (FCC). Minimisation of synchrotron radiation to detectors is the major challenge of all FCC options – ee, eh, hh (pp and ion-ion). FCC for pp 2x50 TeV with 20 Tesla magnetic field will provide 3 MW in proton synchrotron radiation with critical energy 5.4 keV compatible to B-factories. In past it was possible to simulate synchrotron radiation for electrons and positrons. Recent Geant4 version provides the *G4SynchrotronRadiation* process applicable to all types of charged particles.

An incident positron usually annihilates with an electron of a medium into two photons. If the energy of the positron is over a threshold, 43.69 GeV, the positron may annihilate into muon pairs. Annihilations to hadrons, such as to (π^+, π^-), (π^+.π^-, π^0), (K^+, K^-), (K_L, K_S), (η, γ), (π^0, γ), may also happen, with a higher energy than a threshold for each process. These rare processes are implemented inside Geant4 [2], they were verified (figure 5) and are ready to use with Geant4 10.0. They are also important for design of future linear colliders, because they provide a background to the interaction region of a linear collider. Also these processes may provide background at LHC search for new physics when high energy positron converts into muon pairs or into hadrons inside tracker providing a different signature of the event. To estimate this effect a study in a simple setup has been performed.

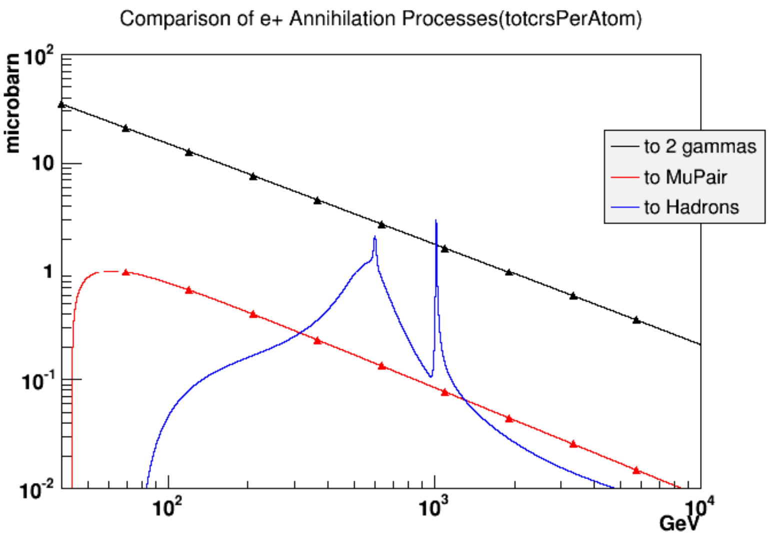

Figure 5. Validation of positron annihilation cross section per atom with electrons of media processes: lines – Geant4 cross sections; points – theoretical computations. Two gamma annihilation dominates except narrow energy region corresponding to the contribution of φ(1020) resonance.

Figure 6 shows the probability of annihilation of positrons in uniform media to muon pairs and to hadrons. On the left plot probability is computed for 1 TeV positrons as a function of atomic number, on the right – as a function of energy for the silicon target. The probabilities of these processes decrease as atomic number Z increases. In relatively light material such as silicon the probability increases above reaction threshold until it reaches plateau on level ~10^{-5}. With high luminosity run at LHC such events may occur inside trackers.

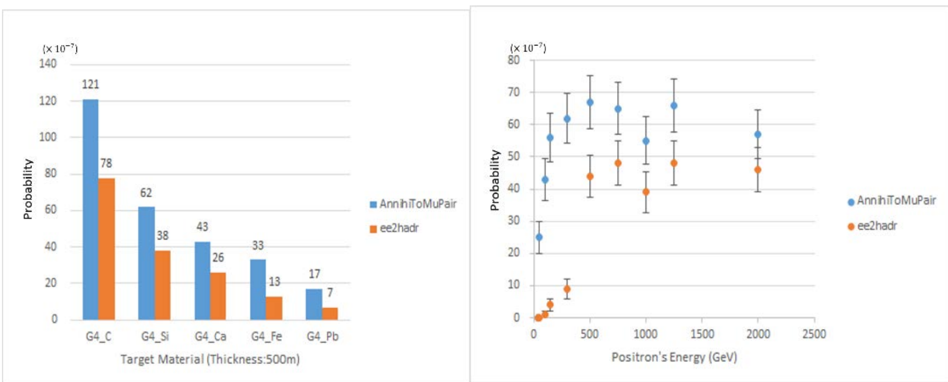

Figure 6. Probability of positron annihilation to muons (blue) and hadrons (red) as a function of atomic number for 1 TeV (left) and as a function of energy (right) in Si.

7. Validation of bremsstrahlung at low energy with thick target data

Bremsstrahlung process defines high energy EM shower shape but it may also be very relevant at lower energy, where ionization dominates, and notably in medical physics applications. The three bremsstrahlung models available in Geant4 which are applicable in the low-energy range (Standard_Option3, Livermore and Penelope) were recently compared against experimental data below 3 MeV in thick target experiments [14]. Data between 0.5 and 2.8 MeV on Al and Fe targets, which include absolute single and double differential bremsstrahlung yields, were taken from [15]. Absolute energy spectra for 70 keV electrons on Al, Ag, W and Pb targets were taken from [16]. Simulations were run using the version 9.6 of Geant4.

At the energies 0.5-2.8 MeV of [15], all Geant4 models are able to reproduce the spectral shape and the integral photon yields. The agreement for the integral yield is between 10 and 30% in the forward hemisphere, depending on bombarding energy, emission angle and target material. The agreement is less good in the backwards hemisphere, where all models systematically predict a slightly higher yield than measured. When experimental uncertainties are taken into account, all Geant4 models are found to be compatible with data. The Penelope bremsstrahlung model is in slightly better agreement with measurements than the other two models. As a general trend, the agreement between data and simulations gets improved for higher energy and lower Z.

Figure 7 shows results for the angular distribution of the bremsstrahlung yield from 0.5 MeV e^- in Al and Fe targets vs. data of [15]. At least 10^9 events were generated for each target/energy configuration. A few examples of double-differential distributions of the photon yield (in angle and energy) are displayed in [14].

All Geant4 models systematically over-estimate the integral photon yield by 70 keV electrons reported in [16], while they are able to predict the spectral shape. The agreement on the absolute yield is between 10 and 50%.

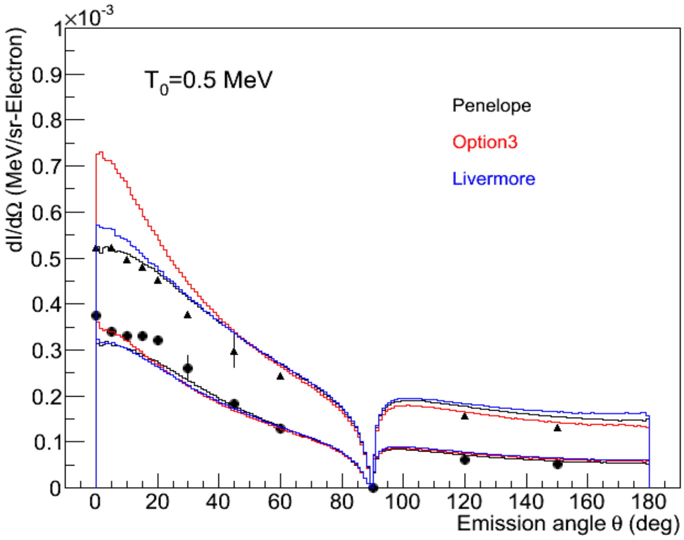

Figure 7. Angular distribution of the bremsstrahlung yield of 0.5-MeV electrons impinging on thick targets of Al (0.548 g/cm2) and Fe (0.257 g/cm2). Points are experimental data from Ref. [15] (circles - Al target, triangles - Fe target). Histograms are the predictions from the Geant4 simulation.

8. Validations of simulation of medical beams

New validation studies for different aspects of simulation of medical beams were recently reported [17]. In particular, validation of Geant4 accuracy was performed using GSI precision measurements of proton and light-ion beams in water [18]. Methods of usage of proton and carbon beams for cancer treatment have been established in recent decades in Japan. HIBMC facility provides high quality beam allowing measurement of the Bragg peak position in water with accuracy 0.1 mm. Measurements allowed the study of Bragg peak position and beam spot width. Several Geant4 Physics Lists were tested. In all cases simulation predictions reproduce the range to better than 1 mm. For Option3 EM physics, proton ranges can be reproduced to within 0.1 mm, and carbon ion ranges to within 0.3 mm at all available energies.

EM physics of Geant4 10.1 have been validated in large scale simulation (10^9 events per run) for the computation of the dose conversion coefficients, expressed in absorbed dose per air kerma free-in-air for many human organs, based on computational voxel phantoms [19]. The application was running in the MT mode with 8 or 40 threads, scoring was performed in $3 \cdot 10^7$ voxels, 30 different materials and wide spectrum of photon energies were used. For this type of application the usage of the MT mode is a critical advantage.

9. Summary

Electromagnetic physics of Geant4 was successfully used for simulations of LHC experiments. It is also widely used in medical physics and other applications. Physics performance of Geant4 EM for releases 9.6, 10.0, and 10.1 is nearly the same. The most recent version 10.1 includes full adaptation of EM sub-libraries to the MT mode.

10. References

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Acknowledgments

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