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Geant4 Electromagnetic Physics for LHC Upgrade

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Geant4 Electromagnetic Physics for LHC Upgrade

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On behalf of the Geant4 electromagnetic physics working groups

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Abstract. In this work we present recent progress in Geant4 electromagnetic physics modelling, with an emphasis on the new refinements for the processes of multiple and single scattering, ionisation, high energy muon interactions, and gamma induced processes. The future LHC upgrade to 13 TeV will bring new requirements regarding the quality of electromagnetic physics simulation: energy, particle multiplicity, and statistics will be increased. The evolution of CPU performance and developments for Geant4 multi-threading connected with Geant4 electromagnetic physics sub-packages will also be discussed.

1. Introduction

Electromagnetic (EM) physics sub-packages [1]-[10] of the Geant4 Monte Carlo (MC) toolkit [11], [12] are an important component of LHC experiment simulation and other Geant4 applications. Accuracy and CPU performance of Geant4 EM affect the results of on-going analysis of LHC data. In particular, they are important for electromagnetic shower simulation essential for the analysis of $H\rightarrow\gamma\gamma$ and $Z\rightarrow ee$ decays and other reaction channels at LHC. High quality of Geant4 EM simulations were needed for successful discovery of the new boson [13], [14].

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Preparation for the new LHC run at higher energy and luminosity requires review and refinements of Geant4 EM sub-packages, which are prepared for the new Geant4 release 10.0. In this work the most important aspects of these improvements will be discussed.

2. Migration of EM sub-packages to multi-threading mode

The main goal for the new Geant4 version 10.0 is to adopt a multi-threading approach [15], and accordingly all EM Standard sub-packages have been fully adapted. This migration is essential for LHC applications. EM physics design [5] includes two main entities: physics processes and physics models. Both may keep large data structures (figure 1) such as tables of cross sections, stopping powers, and ranges. These tables are created in a master thread and shared by worker threads at run time. Processes are instantiated per thread and a process then instantiates a set of its models. During initialisation of a master thread all tables for master processes and models are built. At initialisation of worker threads pointers from data tables to the master thread are provided to each thread-local process and model. To achieve this goal of multi-threading, necessary modifications have been introduced into Geant4 material sub-library and physics table classes:

- only *const* methods are used in run time;
- all these classes are initialized before event loop;
- new interfaces are added allowing data sharing.

A drawback of this scheme is that an extension of a shared table in run time may safely be done only if a thread-synchronization mechanism is implemented (e.g. using mutex). This may cause a degradation of linearity of speedup as a function of number of threads. For this reason the shared tables cannot be modified during the event loop.

For release 10.0 a necessary change of EM interfaces for the multithreaded (MT) design was done and all processes/models used in main EM Physics Lists were migrated to this scheme. This allows the Geant4 EM Standard, Livermore, and Penelope sub-packages to be used in reference Physics Lists under the many-threads regime. Several examples are provided which demonstrate different aspects of EM simulation in MT mode. As a result Geant4 MT may be used by any LHC experiment without limitation on the number of threads.

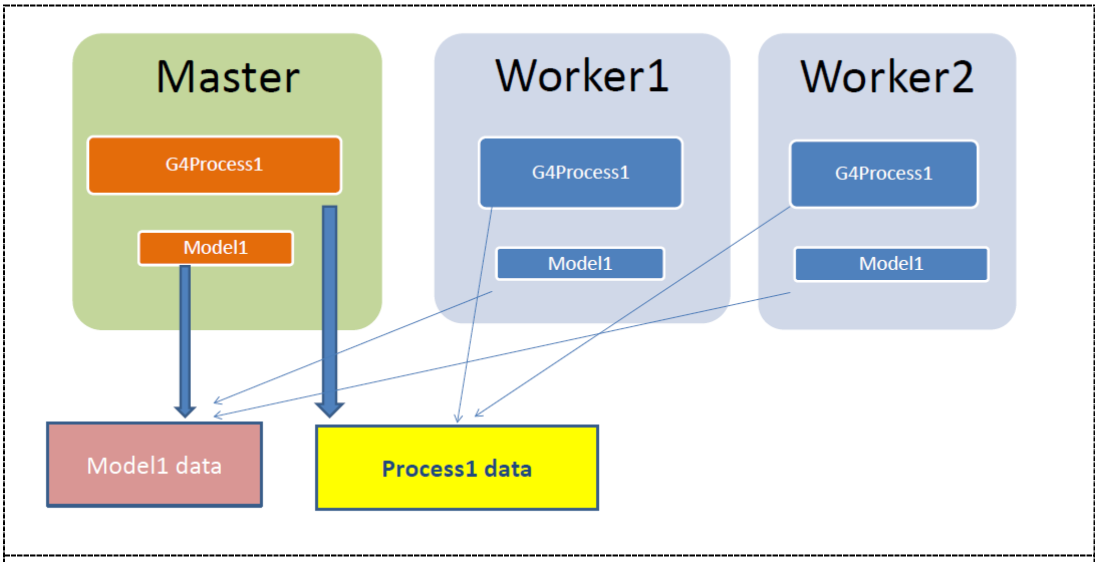

Figure 1. Relation diagram of EM processes and models in MT mode.

3. CPU performance improvements

EM physics sub-packages are CPU intensive, because ionisation, multiple scattering and other models are called at each simulation step. CPU profiling shows that *G4PhysicsVector* run time methods and standard mathematical library functions *log*, *exp*, and *pow* are the most time consuming. To improve CPU performance of EM physics a review of all sensitive parts of the code has been performed.

For Geant4 release 10.0 *G4PhysicsVector* and *G4Physics2DVector* classes were significantly updated. In particular, run time virtual methods were substituted by inline methods and all run time methods became *const*. New classes *G4Exp* and *G4Log,* extracted from the new VDT library [16], were introduced into the Geant4 kernel. The reasons for the extraction are easier maintenance of different Geant4 software platforms and simpler build configuration for Geant4 users. The accuracy of *G4Log* and *G4Exp* compared with the standard library functions is of order 10^{-15} with a significant speedup (table 1).

Another class *G4Pow* was initially created to provide look-up tables for frequently used mathematical functions of integer arguments (Z – atomic number or A – baryon number). These functions are $Z^{1/3}$, *log, exp, factorial*. Because atomic number in nature is limited the size of tables of the class is small. For the recent release *G4Pow* functionality was extended – expansions are used to get approximate function values for double arguments. The accuracy for *G4Pow::log* and *G4Pow::exp* with double arguments is not very high but better than 10^{-3}, and for $A^{1/3}$ with A > 20 and a double argument this accuracy is better than 10^{-9}. The overall speedup of Geant4 EM shower simulation due to the usage of fast mathematical functions is on a level of 5%. A similar increase of performance is expected for the Geant4 hadronic physics simulations.

Table 1. CPU time (in seconds) for mathematical functions from different libraries: standard (STD), VDT adopted for Geant4 (G4VDT), G4Pow (Geant4 internal). For each function 10^8 computations were done with randomly distributed arguments. Standard PC was used: Intel Xeon 1.6 GHz, 64 bits, gcc 4.7.2. For comparison in the last row the time for access to look-up table with pre-computed values is shown.

Function(argument)	STD	G4VDT	G4Pow
Log(double)	8.97	4.91	5.19
Exp(double)	13.93	1.95	1.34
$A^{1/3}$(double)	20.46	7.03	0.77
$Z^{1/3}$(int)	-	-	0.01

4. Gamma conversion models

Migration of Geant4 to common interfaces [10] allows a common validation for available EM models for a given physics process, independent of which sub-package a model belongs to: Standard, Livermore, Penelope, or DNA. Thanks to that, the review of EM gamma models was carried out efficiently, which allowed accurate identification of the energy range for each model. For LHC applications the most important result was obtained for the gamma conversion process, which is the main gamma cross section above a few MeV.

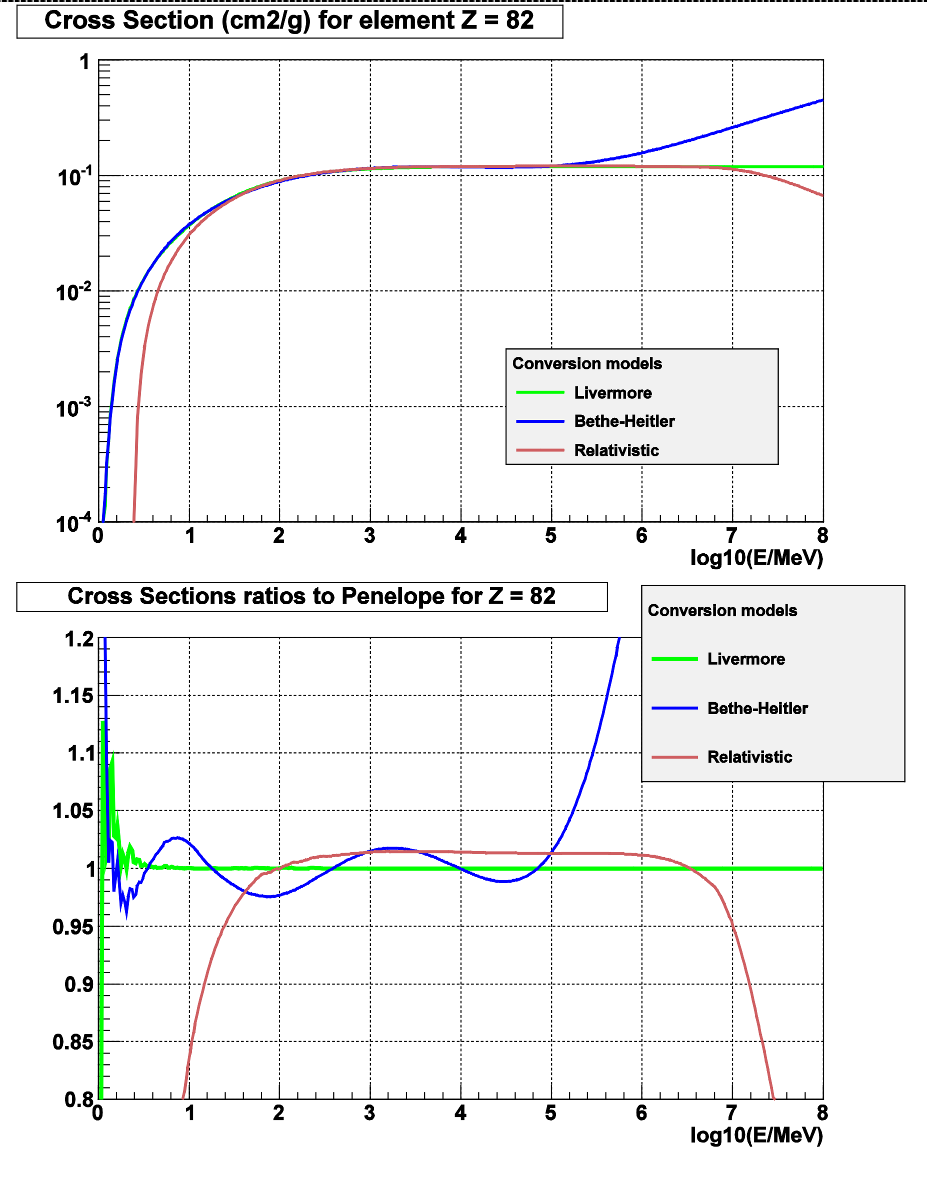

Figure 2. Gamma conversion cross section in lead as a function of gamma energy (top) and ratios of cross section to the cross section of the Penelope model (bottom).

In figure 2 the results of study of gamma conversion models are shown for the case of a lead target. In the energy interval between 100 MeV and 100 GeV all cross sections agree within 2 %. The default *G4BetheHeitlerModel* used in LHC production has a cross section which uses the Geant3 parameterisation. This parameterisation is valid below 100 GeV only, which is not sufficient for LHC applications at high energy, especially for the future 13 TeV experiment simulations. In the *G4PairProductionRelativisticModel* [4], [8] instead of parameterisation a numerical integration of the differential cross section is performed at the initialisation stage of Geant4. This model takes into account the Landau-Pomeranchuk-Migdal effect [18], which suppresses the cross section at high energy. Below 100 MeV this model becomes inaccurate because low-energy corrections are not taken into account.

Similar results and conclusions were obtained for all other targets. Since Geant4 release 9.6 the relativistic model is applied above 80 GeV in all EM Physics Lists in order to address requirements of LHC experiments. Below 80 GeV in the production Physics Lists for LHC (Opt0, Opt1, Opt2) the old Bethe-Heitler model is still used, while in other Physics Lists Livermore or Penelope models are applied.

5. Electron-positron pair production

The energy loss of high energy muons is defined not by ionisation but by the radiation process of e^+e^- pair production [1]. High energy pair production by hadrons as well as hadron bremsstrahlung should be taken into account for an accurate description of hadronic shower shape (see figure 3 in [19]). The differential cross section has a complex shape, so 2-D tabulation is required. In previous Geant4 versions, 8 points in muon/hadron energy and 1000 points in secondary energy were used. The systematic error in a sampled spectrum of produced pairs was on the level of 10% due to numerical inaccuracy of the interpolation method.

Because the muon signal is very important for the new physics search at LHC, necessary improvements were introduced in the pair production model. The number of points per energy decade was increased by a factor of four, and the upper limit of the internal table was made definable by the user. For LHC applications the highest energy was set to 10 TeV, so 16 points in energy are used in the new version of the model. Also a mechanism of sharing the same instance of class for a particle and its anti-particle has been implemented. For the Geant4 release 10.0 pair production and bremsstrahlung processes are configured for muons, charged pions, charged kaons, and also protons and anti-protons.

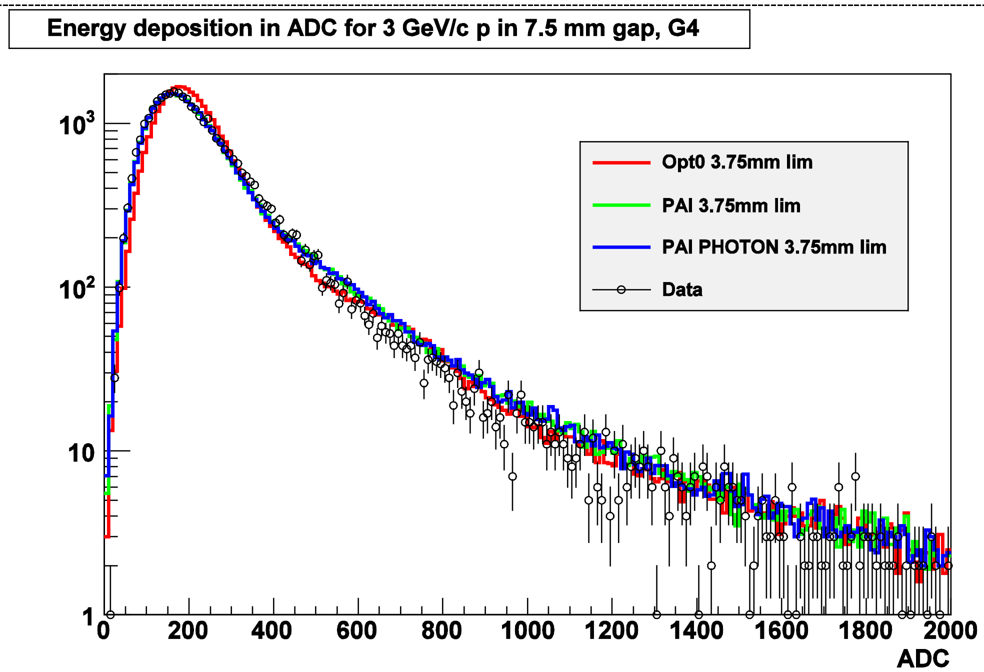

Figure 3. Proton energy deposition in gas gap in ADC counts: histogram – simulation (Opt0 means default model), open circles – data [22], [23]. Simulation was done with 1 mm cut, step limit is equal to half gap thickness 3.75 mm, beam momentum is 3 GeV/c, gas mixture Ne–CO_2–N_2; ADC scale for simulation was normalized on the PAI model peak position.

6. Sampling of energy loss fluctuations

The default Geant4 model of fluctuations of energy loss is *G4UniversalFluctuation* [20], which provides good results in general [8]. However, this model uses phenomenological parameterisations with limited ranges of applicability – for small steps the model becomes approximate and even incorrect. An alternative approach has been developed in *G4PAIModel* and *G4PAIPhotModel* [21]. PAI models are based on theory and photo-absorption cross sections which are known with a good accuracy, thus these models are accurate for any step size.

Recently Geant4 fluctuation models have been reviewed and updated. Motivations for these updates were simulation studies of new detectors for the LHC upgrade and simulation of ALICE TPC test beams, which require more accurate predictions of energy response in thin solid layers and in gases. As a result of this development, dependences of peak position and width on cut value and step limit for the default model were reduced. In figure 3 Geant4 simulations are compared with ALICE test-beam data [22], [23]. Both default and PAI models reproduce the central part and the tail of the experimental distribution. However, the PAI model is more accurate in the vicinity of the peak. Note that it is recommended to use a step limit of half the size of the sensitive area for the default model. PAI models are stable and more accurate - any cut or step limit may be used.

7. Multiple scattering models

The Urban model for multiple scattering [7] has been the Geant4 default for a long time. Recent tuning of the model provides the best accuracy for all low-energy electron benchmarks. In figure 4 the ratios of simulated to measured angular distribution widths at the 1/*e* level are shown, where the measured data from [24] includes a set of different target materials (Be, C, Al, Ti, Cu, Ta, Au). The accuracy of the measured data is about 1% and the version of the Urban model *G4UrbanMscModel* prepared for Geant4 10.0 fits all the data well.

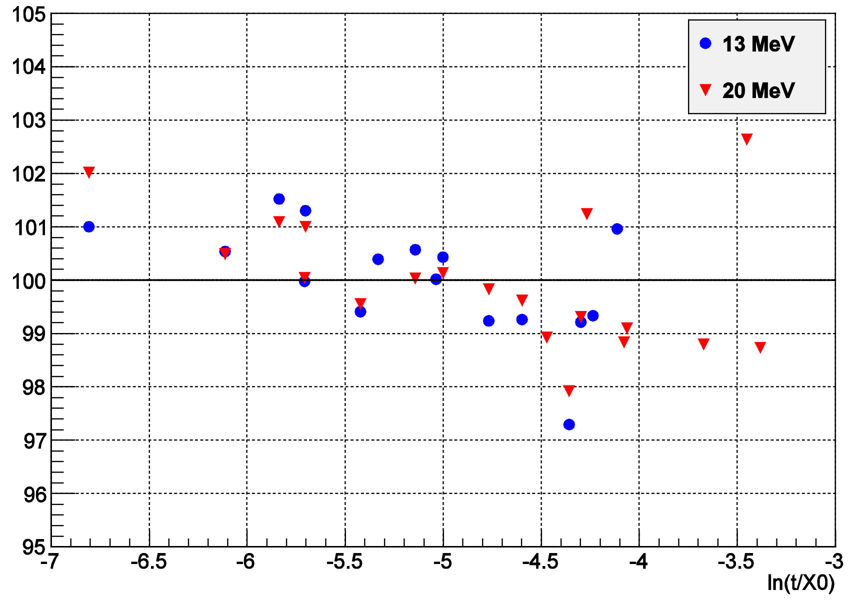

Figure 4. The ratio MC/Data for the Urban model of Geant4 10.0 for widths of the angular distributions at the 1/*e* level, vs. the logarithm of target thickness in units of radiation length. Results for all targets of electron scattering benchmark [24] are shown.

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The Urban model of multiple scattering [7] is based on several phenomenological parameterisations and is a result of a compromise between simulation speed and simulation accuracy. During recent years it was improved by tuning to available data. Thanks to the model design it was possible to provide users with the choice of different versions of the model: Urban90, Urban93, Urban95. This allowed configuring EM Physics Lists with backward compatibility, important for LHC experiments. For the release 10.0 there is no longer a need to keep these variants of the code, so only one final version *G4UrbanMscModel* is provided.

In parallel, an alternative "combined" approach of *G4WentzelVIModel* of multiple scattering and single Coulomb scattering models [7] has been developed. A number of validations demonstrate that the combined model provides more accurate simulation results than the Urban model both for low energy [7] and high energy muon data [8]. The combined model is based on theory, so applicable for wide areas of target thicknesses, densities, and energies. For simulation of LHC vertex detectors it is important that the Rutherford tail of scattering of GeV charged particles is accurately described by the single scattering model. Stability versus step size is also an important requirement for simulation of vertex reconstruction.

To understand the model capability for simulation of muon transport in a full detector, a dedicated MC benchmark was created to simulate the L3 detector [25] from the LEP collider at CERN for muons from the decay $Z\rightarrow\mu^+\mu^-$. A simplified geometry description of the L3 detector (based on real detector drawings) was created, and the simulated widths of lateral displacements of muon tracks were compared to measurements (table 2). The results clearly demonstrate that the combined model is more accurate than the Urban model, and that each new version of the Urban model is more accurate than previous ones.

Table 2. Results of simulation of high energy muon track displacement in the L3 detector for different versions of Geant4 and the multiple scattering models. Data are close to the combined model and to the most recent version of the Urban model.

Model	Geant4 version	Displacement (mm)
Urban90	9.5p02	7.726 ± 0.097
Urban93	9.5p02	7.081 ± 0.093
Urban95	9.5p02	6.464 ± 0.080
Urban96	9.6p02	6.616 ± 0.078
Urban	10.0	6.354 ± 0.077
WentzelVI+SingleScattering	10.0	6.306 ± 0.077
Data [25]	-	6.078 ± 0.028

For Geant4 9.6 a design iteration was introduced that allows combination of different multiple scattering models for different energy ranges. This allows usage of the Urban model below 100 MeV for electrons and positrons only, where this model has significant advantage in accuracy and in CPU speed. For higher energy electrons and positrons, and for all energy muons, the combined model is used.

For hadrons in the release 10.0 a new approach was used to combine G4WentzelVI model with the hadron elastic scattering model from Geant4 hadronics package, which takes into account strong interactions between the projectile hadron and a target nucleus. In order to avoid double counting, the

Coulomb single scattering model is not used. In Geant4 hadronics package there are two models: the default traditional hadronic scattering model using a parameterisation of scattering amplitude, and the "optical" model [26] taking into account interference between strong and EM amplitudes.

To verify the scattering of hadrons a new proton scattering benchmark has been developed which includes data [27] from a 172 MeV proton beam scattered off 14 different materials and many different target thicknesses. The widths of the scattering angles were measured, and an example result for the Be target is shown in figure 5. The effect of hadron elastic scattering on the characteristic angle can be seen for large target thicknesses. Agreement between MC and measurement is improved when hadron elastic scattering is enabled. The combined model is more accurate for small and large thicknesses, but for most materials the Urban model is more accurate for intermediate thicknesses. The agreement becomes better if a stronger step limitation is used. From the first results of the benchmark one can conclude that both variants of multiple scattering WentzelVI (emstandard_opt0) and Urban (emstandard_opt3) together with hadron elastic scattering provide similar results. Without any extra step limit for any target material or thickness, agreement between data and MC predictions is better than 10%.

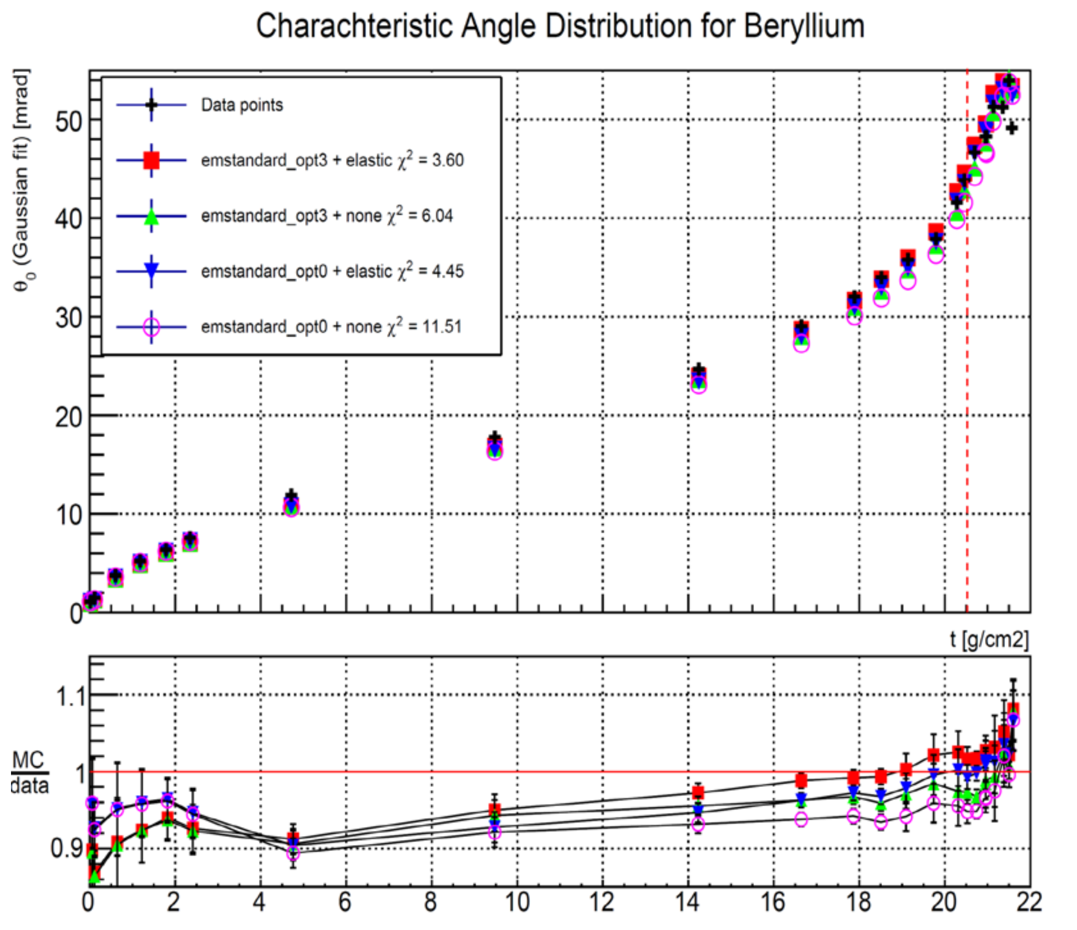

Figure 5. RMS of proton scattering angle as a function of target thickness (top) and ratio of MC result to data [27]. Combined model (standard_opt0) prediction is more accurate than that of Urban model (standard_opt3), and simulation hadron elastic scattering improves agreement with the data.

8. Calorimeter response simulation

To control the stability of Geant4 EM for LHC applications a few simplified calorimeter benchmarks were created [6] and are executed for each reference version of Geant4. In figure 6 the response and resolution of a simplified *Cu/liquidAr* (ATLAS-barrel type) sampling calorimeter are shown as a function of *cut in range* [5], [11] for different Geant4 versions and EM Physics Lists. For version 9.6p02, the predicted response is about 0.2% greater than that for version 9.4p04. No difference between 9.6 and 10.0 is expected. Note that an accurate and stable sampling calorimeter response can be obtained if a strong step limitation is applied when electrons are close to a geometry boundary between absorber and sensitive volumes. In the case of the weak step limitation (EMV type of EM physics) both response and resolution are biased.

Geant4 cuts in range are transformed into production thresholds per material at the initialisation stage of the code [5]. By default these production thresholds are applied only by energy loss processes (ionisation and bremsstrahlung). Red circles show results for the case when “ApplyCuts” option is enabled. This option establishes production thresholds to all EM processes cutting out all low-energy electrons including those which are produced by the photoelectric effect and the Compton scattering. This provides about 30% speedup of simulation for a cut of 1 mm but results in a stronger dependence of the results on cut value. Also at a cut of 1 mm, the visible energy becomes close to the value obtained with Geant4 9.4p04.

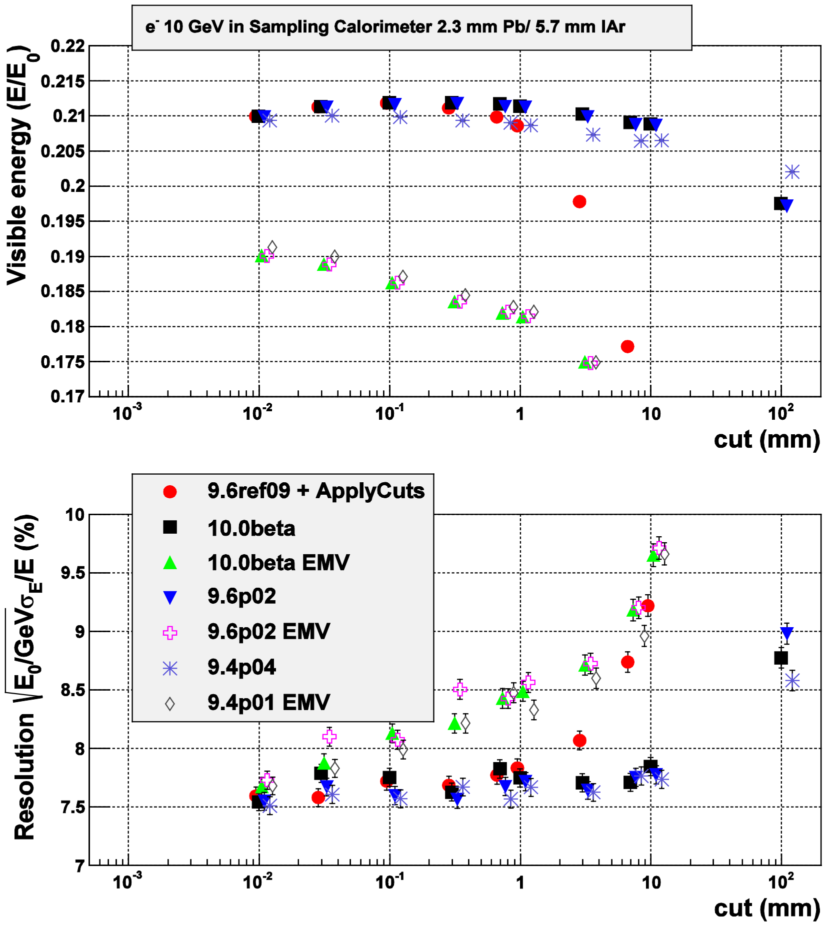

Figure 6. Results of simulation for simplified Cu/liquidAr sampling calorimeter as function of cut in range: visible energy (top), resolution (bottom). Red circles show effect of the “ApplyCuts” option.

9. Summary
Electromagnetic physics of Geant4 was successfully used for simulations of LHC experiments. Recently a consolidation of main electromagnetic models was achieved [10]. Physics performance of Geant4 EM for releases 9.6 and 10.0 is nearly the same. Some CPU speedup is expected for the version 10.0 and Geant4 EM for this version is fully multi-threading capable.

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