The performance of the geant4 standard EM package for LHC and other applications

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The performance of the Geant4 Standard EM package for LHC and other applications

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Abstract. Current status of the Standard electro-magnetic (EM) package of the Geant4 toolkit is described. We report on the stability of results with respect to variation of production threshold and Physics List. This illustrates the trade between CPU time and precision of simulation predictions. New comparisons of the Geant4 simulation with the experimental data are shown. The CPU benchmark results are discussed.

1. Introduction

The Geant4 toolkit [1, 2] is one of important components of software for high energy physics (HEP). Geant4 has been used for BABAR simulation production since 2001, from 2004 is used as a main simulation engine for at least three LHC experiments: ATLAS, CMS and LHCb. The Standard EM package [3-6] provides simulation of ionization, bremsstrahlung and other EM interactions of particles with matter. The precision of physics models and CPU performance of the package directly effect results of the BABAR experiment [7] and coming LHC experiments [8, 9]. In view of this the efforts of the Standard EM group are focused on verification and tuning of simulation models, on providing necessary user interfaces and on optimization of CPU performance of the package. In this work we report recent progress achieved for the Standard EM package with Geant4 releases 8.3 and 9.0.

2. Recent modifications in the Standard EM package

Since Geant4 release 8.0 a new model [10] of multiple scattering (MSC) has been introduced in order to provide more precise simulation of charged particle transport in general and a sampling calorimeter response [6] in particular. Further developments were focused on improvements of the precision and CPU performance of multiple scattering and other models of the package. The optimal configuration of EM physics models and processes for different Geant4 use-cases are provided in a form of predefined Physics Lists classes distributed with Geant4 [2].

2.1. A new interface to Geant4 navigator

The information about a distance between current position of a particle and nearest geometry boundary is required for the MSC model and for the algorithm of *sub-cutoff* generation of delta-electrons (see details in subchapter 2.5). The new class *G4SafetyHelper* was designed in order to provide a unique interface between the Geant4 navigator and any part of the toolkit. This new class is capable to work as with the standard Geant4 transportation in mass geometry and with new so-called *coupled transportation*, which is required for the case of a parallel geometry. The parallel geometry assumes for the given setup a simultaneous description of detailed mass geometry and several special geometries for scoring, biasing and/or fast simulation. An advantage of *G4SafetyHelper* is in centralization of the interface and in ability to reuse information from previous calls to compute geometrical values.

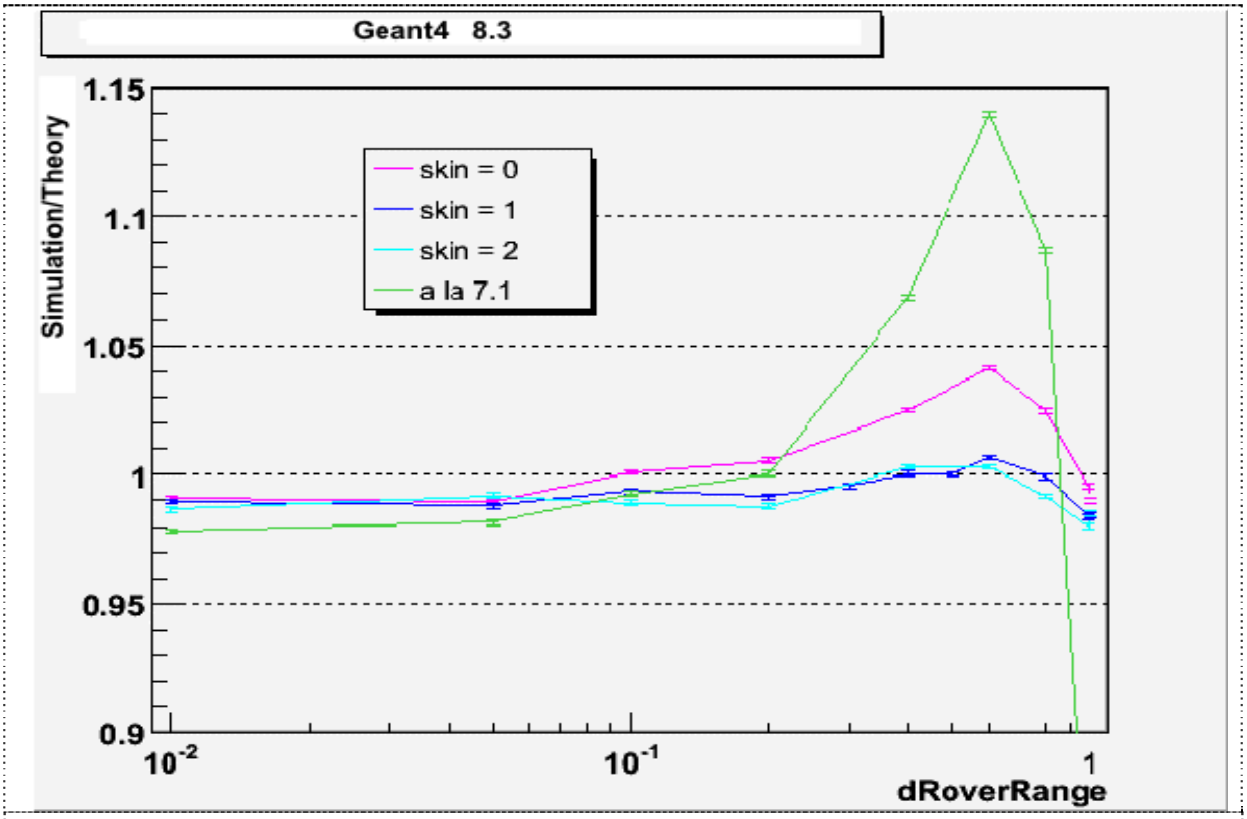

Figure 1. The ratio between predicted and simulated dose deposition as a function of tracking parameter *dRoverRange* (main step size limitation [1]). The results are obtained for 1 MeV photon beam in the cavity inside liquid water, which filled by water vapour, for different options of the multiple scattering model for Geant4 release 8.3.

2.2. Multiple scattering model upgrade

The general improvement of electron transport for HEP sampling calorimeters has been achieved with Geant4 release 8.0 [6] due to improved MSC model. However, obvious CPU penalty have been observed, so an optimization of the model was required. The MSC model was tuned [10] in order to have better CPU performance and better precision. The algorithm of MSC step limitation was upgraded and a new parameter *skin* was introduced. By default its value is zero, if *skin* is set above zero, then MSC additionally limits step size of a particle near geometry boundary. For these small steps a single scattering mode is applied for sampling of the scattering angle inside MSC model. The effect of this parameter on the simulation precision is demonstrated in figure 1, where a ratio of simulated and theoretical energy deposition in low-density material inside cavity is shown as a

function of the *dRoverRange* parameter, which provides the main Geant4 step limitation [1, 3, 6]. The value of the deviation of the result from the unit connects directly with the precision of low-energy electron transport, which contributes significantly to the simulation of a response of EM showers in HEP sampling calorimeters. For the simplified version of the MSC model similar to one of Geant4 release 7.1 (green, QGSP_EMV Physics List) the bias up to 14 % is observed. The current default MSC step limitation (magenta, used in QGSP Physics List) is accurate within 1 %. It worse notes that the default value of the dRoverRange parameter is 0.2, which means not more than 20% of kinetic energy of a particle is allowed to be lost at a step.

2.3. A new single Coulomb elastic scattering process

For simulation of Coulomb elastic scattering in thin layers and in low density materials the new process *G4CoulombScattering* has been designed and delivered with Geant4 release 9.0. This process is based on the Wentzel model [11], which is used by many MSC algorithms including the Penelope code [12]. Computation of nuclear size effect (important at high energies) is performed according to parameterization [13]. The *G4CoulombScattering* process is an alternative to the MSC process. The results for the different MSC models and this process are shown in figure 2, where Geant4 9.0 simulation predictions are compared with the data [14] of the MuScat experiment (172 MeV/c muons scattering at thin foils). All results for the central part of scattering ($\theta < 0.03$) are in agreement with the data, for the tail the option *skin = 2* seems to be the most accurate, however, other predictions agree with the data within two standard deviations. Note, that the simulation with the *G4CoulombScattering* process requires about 1000 steps in this foil instead of few for the case of the ordinary MSC process. Thus, it is practical to use *G4CoulombScattering* for special cases (low pressure gases, very thin foils), where MSC approach is not applicable. It is also useful to apply it for comparisons.

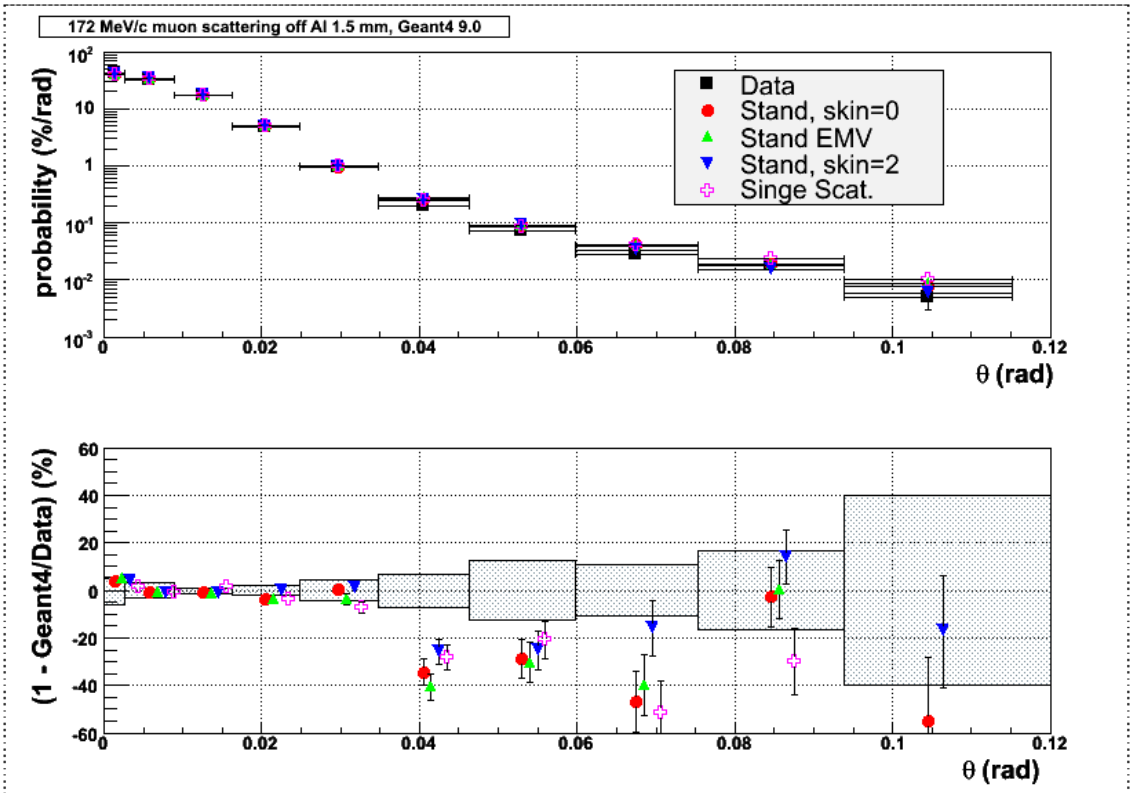

Figure 2. The projectile scattering angle distribution of 172 MeV/c muons after 1.5 mm aluminium foil: data [14] and different variants of simulation (top). The relative difference between simulation and the data in percents (bottom), hashed area shows the data errors.

2.4. Fluctuations of energy loss

The model for sampling of the fluctuations of energy loss [15] has been updated for the Geant4 release 8.3. The new parameterization of the sampling function for small steps has been introduced. The effect of this modification is demonstrated by simulation of the energy loss of 15.7 MeV electrons in thin beryllium foil for different fixed step sizes: in figure 3 the distribution for 1 um step size is biased, in figure 4 modified fluctuation model provides step size independent results.

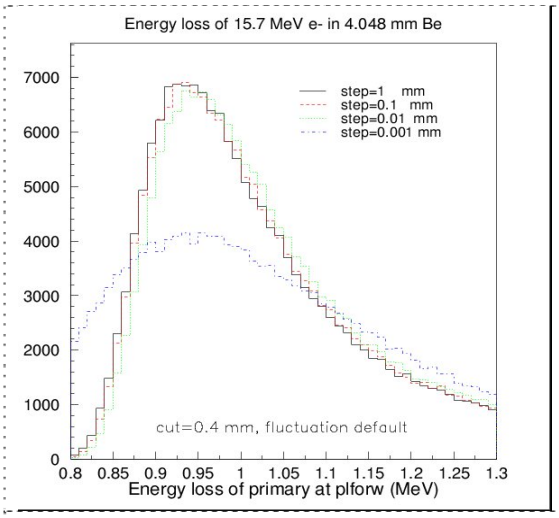

Figure 3. The energy loss of 15.7 MeV electrons in 4.048 mm beryllium foil for different fixed step size simulated with Geant4 release 8.2.

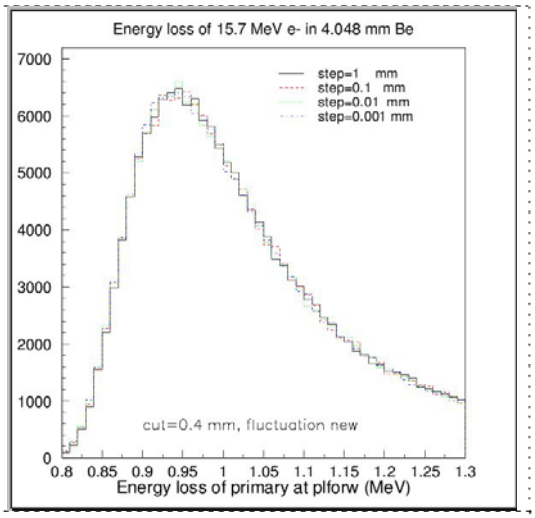

Figure 4. The energy loss of 15.7 MeV electrons in 4.048 mm beryllium foil for different fixed step size simulated with Geant4 release 8.3.

2.5. Sub-cutoff option upgrade

With the *sub-cutoff* option of the ionization process the production threshold (cut) for delta-electrons is reduced in 10 times if the distance from a point of the particle trajectory to the nearest geometry boundary is below the value of Geant4 cut in range [1]. The geometry safety information is provided by the new *G4SafetyHelper* class. This option was available in first releases of the EM package [1] but later was not supported. It has been restored with release 8.3. As a result, simulation predictions (figure 5) for sampling calorimeters with this *sub-cutoff* option (green triangles, QGSP_EMX Physics List) become practically independent on the cut in range up to value 10 mm.

2.6. EM interfaces change for Geant4 9.0 release

The review of the basic interfaces of the EM package has been performed. The following modifications were included in the EM package with Geant4 release 9.0 [16]:

- updated UI commands to define parameters for the EM package;
- updated options for MSC models;
- updated components for EM Physics Lists;
- optimization of basic EM interfaces.

The first three modifications were required in order to provide more consistent and clear initialization of parameters of the package. A new UI subdirectory */process/msc* has been added, the three types of step limitation for the MSC process were introduced:

- *Minimal* – the same as in Geant4 7.1 (used in QGSP_EMV Physics List);
- *UseSafety* – current default (used in QGSP and many other Physics List);
- *UseDistanceToBoundary* – advanced, proposed for applications without strong magnetic field.

The modifications of the basic interfaces G4VEmModel, G4VEnegryLossProcess, G4VEmProcess and G4VMultipleScattering have been performed in order to improve CPU performance of the EM package. The corresponding modifications were introduced inside all derived classes of the package. No physics algorithm change was done and validation tests show no change of the final results but visible improvement of CPU performance. This was mainly achieved by following:

- reduction of usage of virtual methods by usage of introduced inline methods;
- reduction of number of operations *new* and *delete* for vectors of secondary particles by usage of predefined at initialisation time vectors.

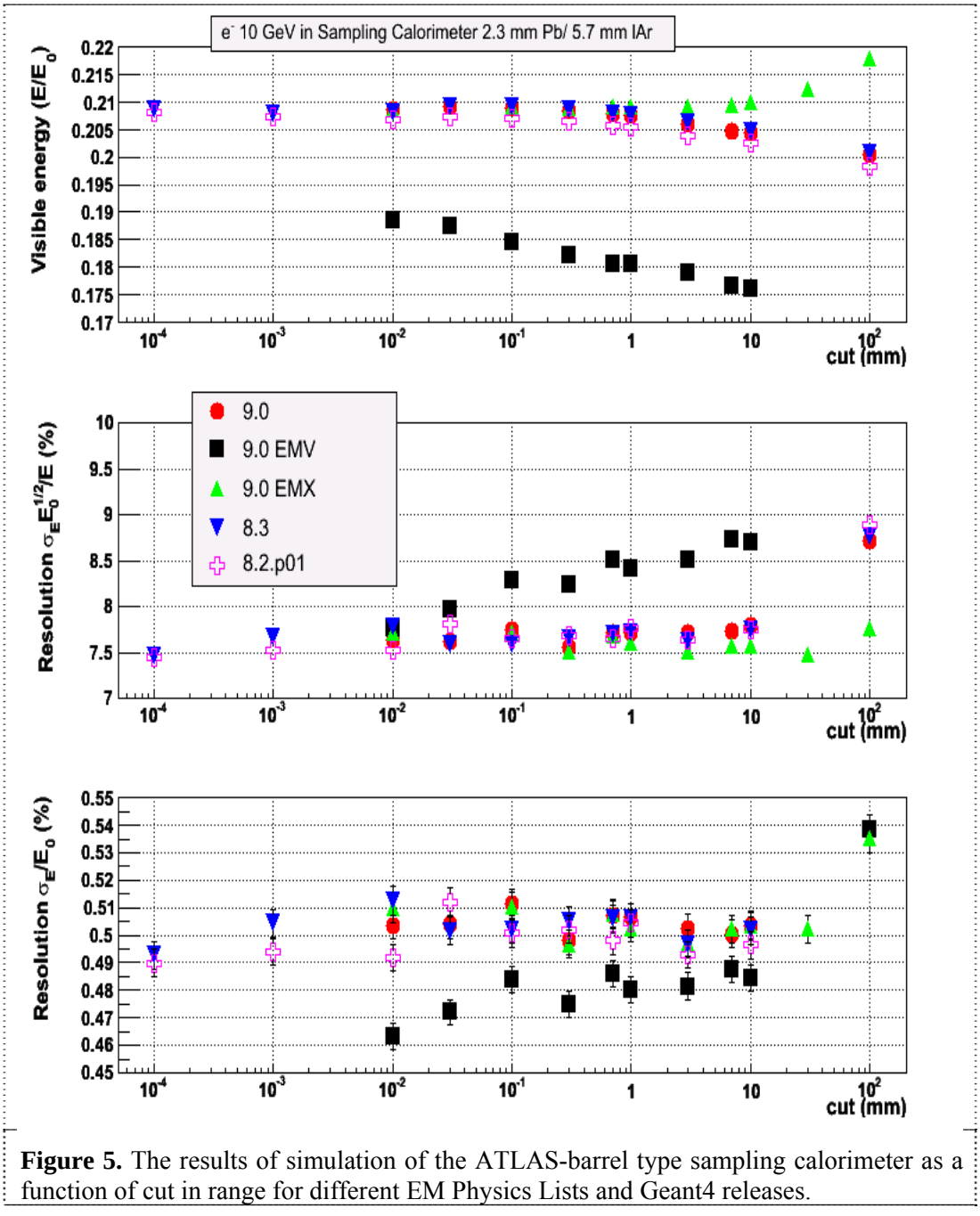

Figure 5. The results of simulation of the ATLAS-barrel type sampling calorimeter as a function of cut in range for different EM Physics Lists and Geant4 releases.

3. The evolution of the testing suite

The important component of the EM software is the testing suite [6] which is exercised on regular base and provides as comparisons between EM simulation versus experimental data (figures 2, 6-8) and regression comparisons of different Geant4 releases (figures 3-5). Recently the testing suite has been upgraded and extended, new data [14, 17-20] are utilized. The software is added to run in automatic production mode for part of tests, which migrated from PAW analysis to ROOT. The results are accessible via web.

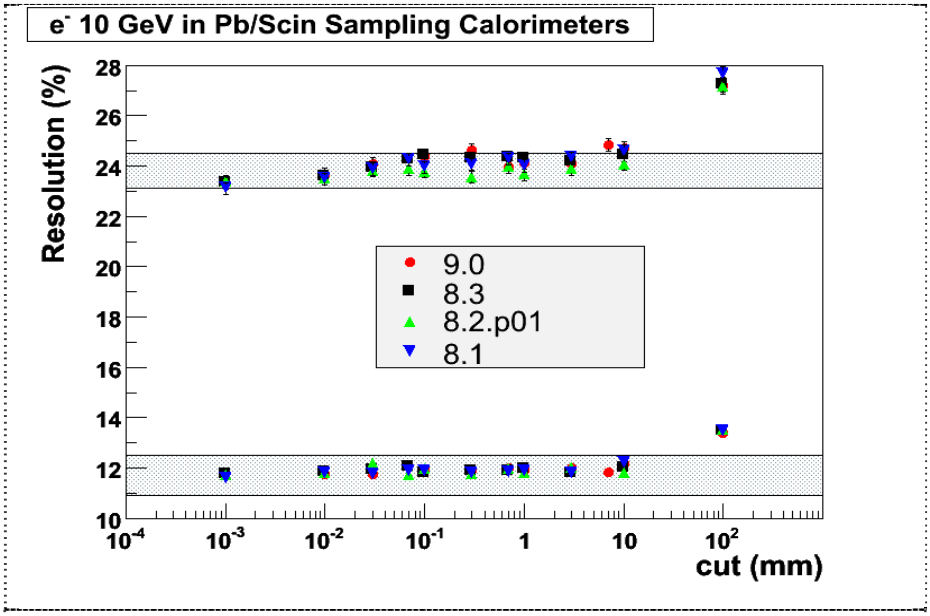

Figure 6. The resolution of two sampling calorimeters as a function of cut in range. Hashed fields show experimental errors for different calorimeter structures: upper – 10 mm lead and 2.5 mm scintillator [17], lower – 5 mm lead and 5 mm scintillator [18]. QGSP Physics List is used.

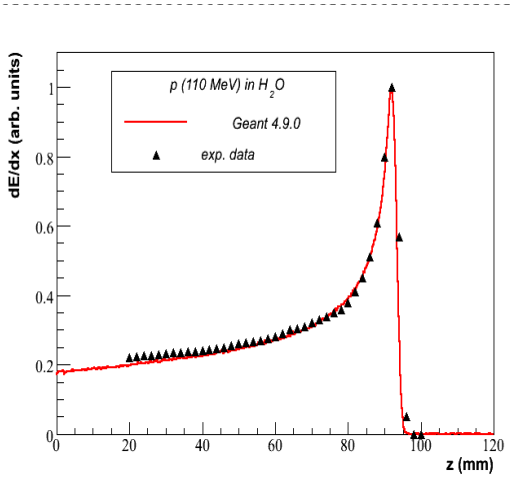

Figure 7. The comparison of the Bragg peak simulation for 110 MeV proton beam in water and the data [19]. QBBC Physics List is used, cut in range is 0.01 mm.

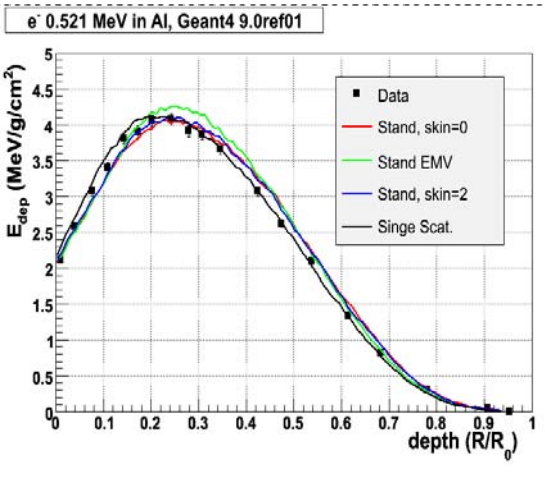

Figure 8. The simulation of energy profile of the 0.521 MeV electron beam in aluminium: points – data [21], lines – different MSC options, cut in range is 0.1 mm.

The comparisons of simulation predictions versus experimental data [17, 18] for the resolution of two different lead/scintillator sampling calorimeters are shown in figure 6. QGSP Physics List provides results which are stable and agree with the data within accuracy for wide range of cuts including the default value 0.7 mm. This confirms the fact that default cut value can be used for sampling calorimeters of LHC providing the same accuracy as lower cut values, so low cut for LHC calorimetry provides unnecessary CPU overhead.

The check of the simulated Bragg peak in water versus data [19] is being performed on regular base (figure 7). These results are important to HEP, because a significant part of energy deposition of hadronic showers is due to the hadron/ion ionization. It is also essential for non-HEP applications.

The new test [20] has been developed for the comparisons with the SANDIA laboratory data [21] to control on electron transport simulation in different materials. This is a complimentary independent validation important as to EM calorimetry and for simulation of particle detectors. In this test the profile of energy deposition of electron beam in a semi-infinite media is studied (figure 8).

4. CPU performance benchmarks

The set of benchmarks for control on CPU performance of the EM package has been created based on existing EM examples *TestEm3* and *TestEm9*:

- EM1 – CMS type calorimeter, QGSP Physics List;
- EM1_EMV – CMS type calorimeter, QGSP_EMV Physics List;
- EM2 – ATLAS barrel type calorimeter, QGSP Physics List;
- EM2_EMV - ATLAS barrel type calorimeter, QGSP_EMV Physics List;
- EM3 – ATLAS barrel type calorimeter, QGSP Physics List, cut 20 um;
- EM3_EMV - ATLAS barrel type calorimeter, QGSP_EMV Physics List, cut 20 um.

Table 1. The results of CPU benchmarking of the EM package at SLC3 Linux with Intel 2.4 GHz processor for different Geant4 releases normalized to results obtained with release 7.1p01. The shared libraries of Geant4 centrally installed at CERN are used.

Release	EM1	EM2	EM3	EM1_EMV	EM2_EMV	EM3_EMV
5.2p02	1.03	0.99	1.53			
6.2p02	0.89	0.98	0.97			
7.1p01	1.0	1.0	1.0			
8.0p01	1.33	2.24	2.26			
8.1p01	1.37	2.43	2.01	1.06	1.08	1.07
8.2p01	1.29	2.14	1.73	1.03	1.09	1.06
8.3	1.28	2.08	1.78	1.04	1.03	1.05

Table 2. The results of CPU benchmarking of the EM package at SLC4 Linux with Intel 2.8 GHz processor for different Geant4 reference tags normalized to results obtained with release 8.3 with Physics Lists QGSP_EMV. The static libraries of Geant4 locally built are used.

Release	EM1	EM2	EM3	EM1_EMV	EM2_EMV	EM3_EMV
8.3	1.33	2.30	1.84	1.0	1.0	1.0
9.0	1.21	2.05	1.65	0.92	0.93	0.94
9.0ref01	1.17	2.07	1.66	0.91	0.92	0.91

The benchmarking has been done for existing at CERN builds of Geant4 (table 1). The effect of introduction of the new MSC model with release 8.0 is clearly seen. For further benchmarking the new Linux configuration SLC4 provided for LHC start is used (table 2). The results confirm the CPU improvement with the upgrade of basic interfaces of the EM package. Other control on CPU performance is demonstrated in figure 9, where CPU time is plotted versus cut and the optimal variant of cut and Physics List can be chosen depending on required precision of simulation results.

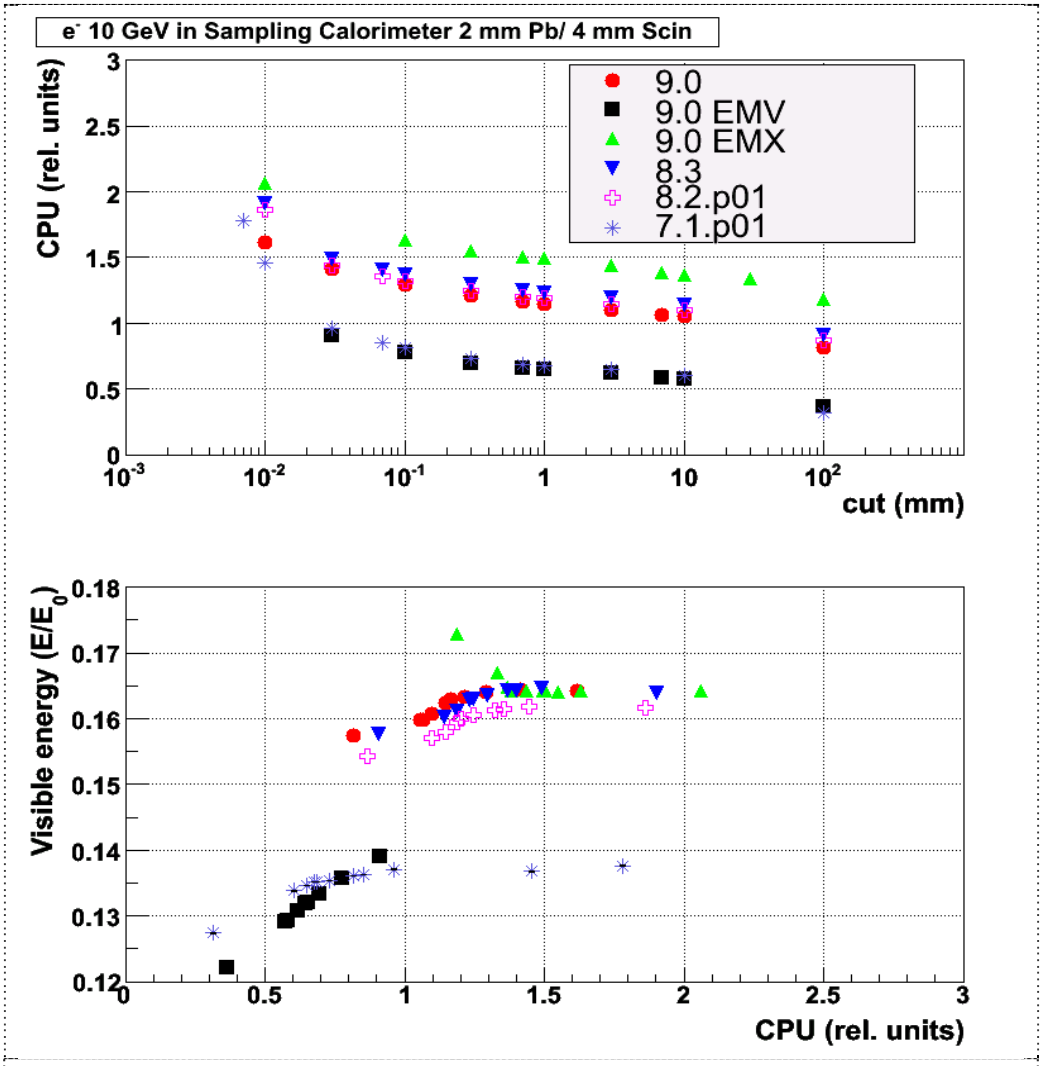

Figure 9. The CPU performance of the simulation for the LHCb type calorimeter for different versions of Geant4 and different Physics Lists: top - CPU as a function of the cut in range; bottom – visible energy as a function of required CPU. Currently the default Physics List QGSP provides the fastest simulation if 1 % accuracy of the visible energy is required.

5. Conclusions

In conclusion we emphasize that the important improvements were introduced in EM models. The performance of the EM package has been improved with Geant4 releases 8.3 and 9.0. About 10 % speedup of the simulation was achieved by efforts to optimize basic interfaces of the EM package. The testing suite for the package has been extended and the benchmarks to control CPU have been established.

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