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Geant4 models for simulation of multiple scattering

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Abstract. Recent progress in development of single and multiple scattering models within the Geant4 toolkit is presented. Different options available to users are discussed. The comparisons with the data are shown. The trade of precision versus CPU performance is discussed with the focus on LHC detectors simulation.

1. Introduction

The Geant4 toolkit [1,2] is used as the main simulation engine for many HEP applications including ATLAS, CMS and LHCb experiments prepared for LHC [3-7]. The process of multiple scattering (MSC) of charged particles is an important component of Monte Carlo transport. At high energy it defines 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 response and resolution of electromagnetic calorimeters. The default Geant4 MSC scattering model [8] has been significantly upgraded for Geant4 release 8.0 providing sampling calorimeter responses with the accuracy about 1% [9]. However, more precise simulation was achieved forcing more simulation steps of charged particles, which requires more CPU time [10].

The more detailed study of electron transport [11] shows that for the approach of the default MSC model the accuracy is limited. In order to provide alternative method of simulation new MSC model have been developed for Geant4 based on the same principles as MSC models of the Penelope [12] and EGSnrc [13] codes. For simulation of particle transport in the low-density media and as an alternative to MSC approach two single scattering models were introduced into the Geant4 toolkit. In this work the overview is presented on the status of Geant4 single and multiple scattering models.

2. Geant4 multiple scattering

Any Geant4 MSC model should provide the several basic functions for each Monte Carlo step of charged particle in a media:

- propose step limit;
- convert geometrical step length into “true” step length taking into account scatterings along the step;
- sample scattering angle and turn particle direction at the end of the step;
- sample a displacement of the end point.

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These functions are applied sequentially in the Geant4 tracking algorithm. Before any step of a particle a loop performs over all physics processes to establish step limits. There are two types of such limits:

- *random step limit* with a probability corresponding to the cross section of a process;
- *tracking step limit* providing more precise simulation.

The tracking step limit is mandatory only for the Geant4 transportation process, which stops a track at the geometry boundary between different volumes. For other processes this limit is optional but is essential to apply for achieving of a good simulation quality. For example, the process of ionisation limits step roughly by 20% of a particle range [1]. It was shown [11] that for precise simulation of electron transport small steps are required near boundaries between heavy and light materials and in Geant4 this limitation is provided by MSC models [9].

All Geant4 MSC models use two main parameters to limit the step F_R (range factor) and F_G (geometry factor), which may be modified by a user. Additional parameter $F_s = 0.3$ (safety factor) is fixed. The step limit L is combined by using the following values: particle range $R(T)$ where T is kinetic energy, inverse transport cross section $\lambda(T)$ [12, 13], geometrical safety s [10], and distance to a geometrical boundary D

$$L = \min \{ F_R \cdot \max (R, \lambda), F_s \cdot s, D / F_G \}.$$

Thus smaller value of F_R will provide stronger step limitation and correspondingly more simulation steps. As a result, the simulation will be more CPU intensive. The geometry factor is used to insure minimal number simulation steps within each volume. Described algorithm of the step limitation is complicate and multi-parametric. In order to provide users a clear alternative set of parameters a special option *G4MscStepLimitType* is used which has only three variants:

- *Minimal*, $F_R = 0.2$, F_G is ignored, used in Geant4 electromagnetic physics builder option1 (EMV option of Physics Lists);
- *UseSafety*, $F_R = 0.04$, F_G is ignored, default;
- *UseDistanceToBoundary*, $F_R = 0.04$, $F_G = 2.5$, used in electromagnetic physics builder option3 (EMY option of Physics Lists).

The type of the step limitation can be selected by choosing corresponding Physics List or can be defined via UI command interface or via *G4EmProcessOptions* helper class. The effect of different step limitation options is demonstrated in the Fig.1 for energy deposition profile of low-energy electron beam in a semi-infinite media [14]. The single scattering model provides the most precise simulation, however, requires much more CPU, because samples each elastic scattering. The fastest variant of the *Urban* MSC model (EMV) using the *Minimal* step limitation overestimates energy deposition inside Tantalum. The strictest MSC step limitation (Opt3) using *UseDistanceToBoundary* is the closest to the data.

The transformation of geometry step length to the true length is performed in all Geant4 MSC models in similar way by using the same formula as published in [12, 13]. The sampling of the scattering angle and of the displacement is different. After the sampling the same procedure is applied in all models: the value of the displacement d of the end point of the step is compared with the geometrical safety s . If $d > s$ then the direction of the displacement is kept but its absolute value is set to s to be sure that end point of the track is kept inside the same volume. After this check of safety end point of the step is shifted, as a result, the relocation of the track is performed.

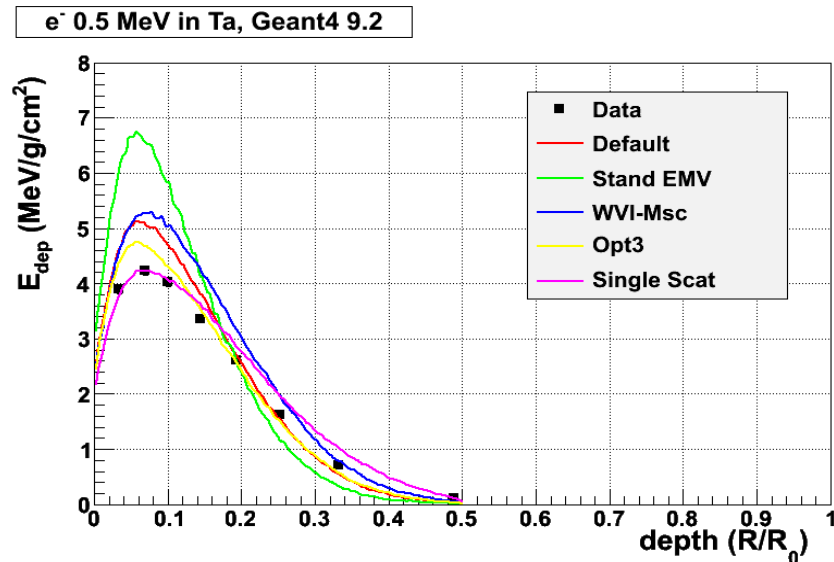


Figure 1. Radioactive dose profile of 0.5 MeV electron beam in Tantalum as a function of depth in the unit of electron range: points – data [15], curves – *Urban* MSC model with three step limitation options (red, green, yellow), *Wentzel-VI* MSC model (blue) and single scattering model (magenta).

3. Urban multiple scattering model

Urban MSC model [8] is the default model of Geant4. It is based on Lewis theory [16] and has separate parameterisations [17] of the central part of the scattering angle and of its tail. Various data on electron scattering are used for tuning of the function describing the tail of the scattering function. *Urban* MSC model is applicable to any particle type at any energy. The performance of the model is demonstrated in Fig.2, where results of simulation of sampling calorimeter of ATLAS barrel type are shown for different versions of Geant4 and different Physics List options.

These results confirm conclusions following from the analysis of MeV-electron transport in Fig.1. It is shown in Fig.2 that in the case of the EMV option of Geant4 Physics lists (black squares and magenta crest in Fig.2) the energy deposition in sensitive layers of liquid Argon is underestimated by more than 10%. Moreover, the results are very dependent on the value of the cut while with the default EM physics both the visible energy deposition and the resolution are stable for cuts below 1 mm. Thus, the same *Urban* MSC model provides different simulation accuracy by using different step limitation near the boundary between light and heavy materials. The correctness of Geant4 results with the default MSC model is independently confirmed by the analysis of the Fano theorem for the electron transport [11] and by comparisons with the published data on the sampling calorimeter response [9, 10].

It is worth to note that good stability and precision of the simulation was achieved by applying stronger step limitation, which requires more simulation steps and correspondingly more CPU. One method to improve simulation performance keeping precision is to apply production thresholds on secondary particles produced by Geant4 gamma processes (namely photoelectric effect and Compton scattering). It is implemented as EMX option of Geant4 EM physics (green triangles in Fig.2). In this case the dependence of the visible energy on the cut in range is visible above the cut value 0.1 mm, so one should be careful to select the best balance between the precision of the simulation and CPU performance.

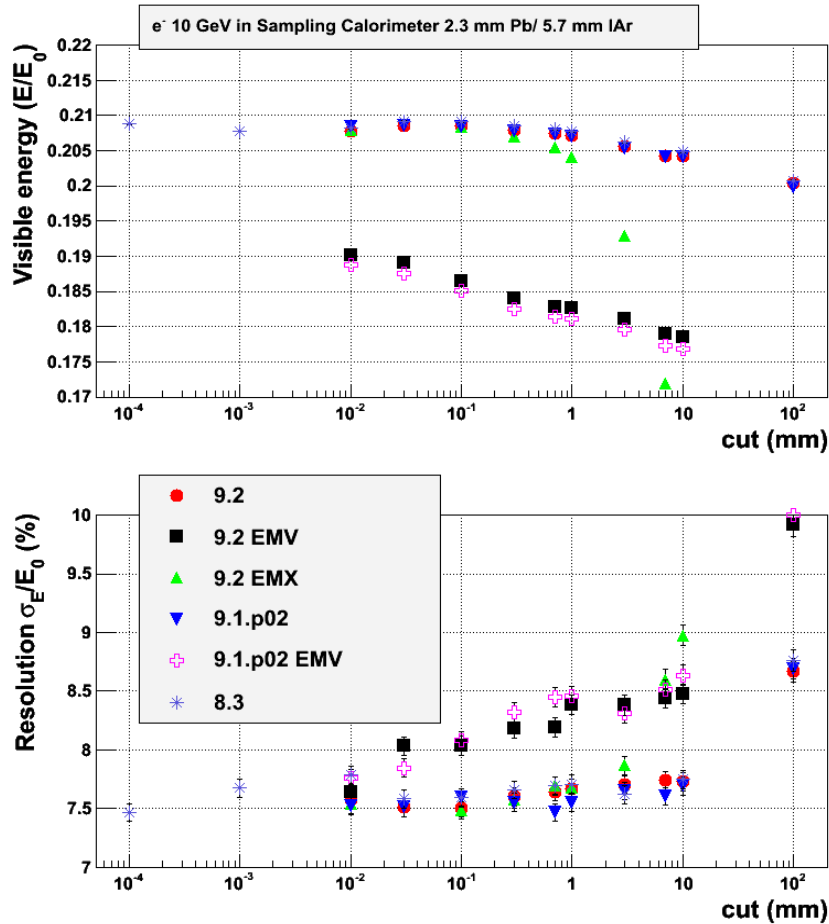


Figure 2. The simulation of 10 GeV electron beam in the sampling calorimeter of the ATLAS barrel type as a function of the Geant4 production cuts: top – response, bottom – resolution. Physics List options: default – *UseSafety* option of step limitation, EMV – *Minimal* step limitation providing biased results, EMX – *UseSafety* option of step limitation and *ApplyCuts* option (enable production thresholds for secondary particles of gamma processes).

4. Goudsmit-Saunderson multiple scattering model

In general, Urban MSC model satisfies requirements of LHC experiments but the accuracy of the Penelope [12] and EGSnrc [13] electron transport is higher [11]. This is the main motivation of the development of the new *Goudsmit-Saunderson* MSC model, which is presented for the first time in this work. The new model is currently applicable only for electrons and positrons. It is fully based on the same theory [16] as Penelope and EGSnrc. Using the ELSEPA code [17] a data base of the total and transport cross sections of electrons and positrons was generated. This data are included inside G4LEDATA structure and will be distributed with Geant4. The sampling algorithm is similar to one of EGSnrc: each step of simulation is splitted into equal two sub-steps. The sampling of the probability density function is performed according to the Goudsmit-Saunderson theory [16]. The cases of zero scattering, one scattering, and many scatterings are treated separately. The first results with the new model (Fig.3) are promising but the CPU time is about two times more than for the Urban MSC model.

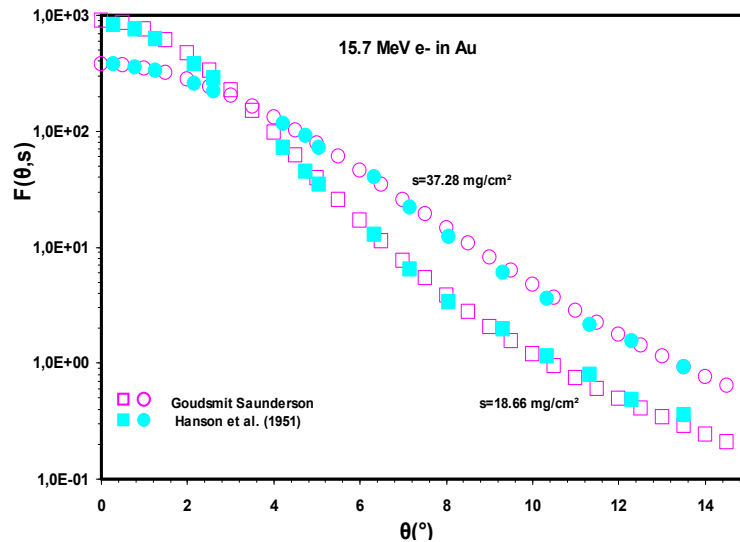


Figure 3. Simulation with the *Goudsmit-Saunderson* MSC model for the electron beam of 15.7 MeV scattering off thin Gold foils versus data [18].

5. Geant4 single scattering models

The first Geant4 single scattering model [19] has been developed in Vanderbilt University for space studies. This model is applicable to protons and ions with energies below 100 MeV/A. The new single scattering model (*CoulombScattering Model*) is based on Wentzel scattering function [20] in formulation [12] of authors of the Penelope code. To apply the model at high energies the electromagnetic form-factor of the target nucleus is introduced using parameterisation [21]. Thus, this model is applicable to all particle type and complete energy region. It can be proposed to apply this model in low density media (vacuum or gas) when MSC approach has difficulties. It also is being used for validation of MSC models. For example, the data of MuScat experiment [22] for muon scattering off 10 different foils are well reproduced by the *CoulombScattering* model. Some comparisons were shown in our previous publications [11] and the result for the polyethylene target is shown in Fig.4. The *CoulombScattering* model provides the best value of $\chi^2/n = 1.72$ for 10 targets in comparison with the *Urban* model ($\chi^2/n = 3.01$) and the new *Wentzel-VI* model ($\chi^2/n = 2.32$) which will be described below.

6. Combined single and multiple scattering model

The new approach for simulation of elastic scattering has been developed recently in Geant4. It naturally combines single and multiple scattering models. The new model (*Wentzel-VI MSC*) was designed to sample multiple soft scatterings with angles $\theta < \theta_{\max}$, where θ_{\max} is the parameter of the model with the current default value 0.2 radian. Scatterings with angles above θ_{\max} are performed by the *CoulombScattering* model. So, both MSC and single scattering processes should be included in the Physics List simultaneously. The scattering function in both models has the same shape [12]. The sampling algorithm of the *Wentzel-VI* model is different from all models described above. At each step the average scattering angle is computed and if it is above 90 degree then the simulation is performed in two steps like in the case of the Goudsmit-Saunderson model. Normally this angle is smaller and the sampling is performed only in one step. For very small steps the central part of the scattering function (average angle θ_0) is very narrow and a single scattering sampling is invoked using the restricted single scattering cross section for the interval of scattering angles $2\theta_0 < \theta < \theta_{\max}$.

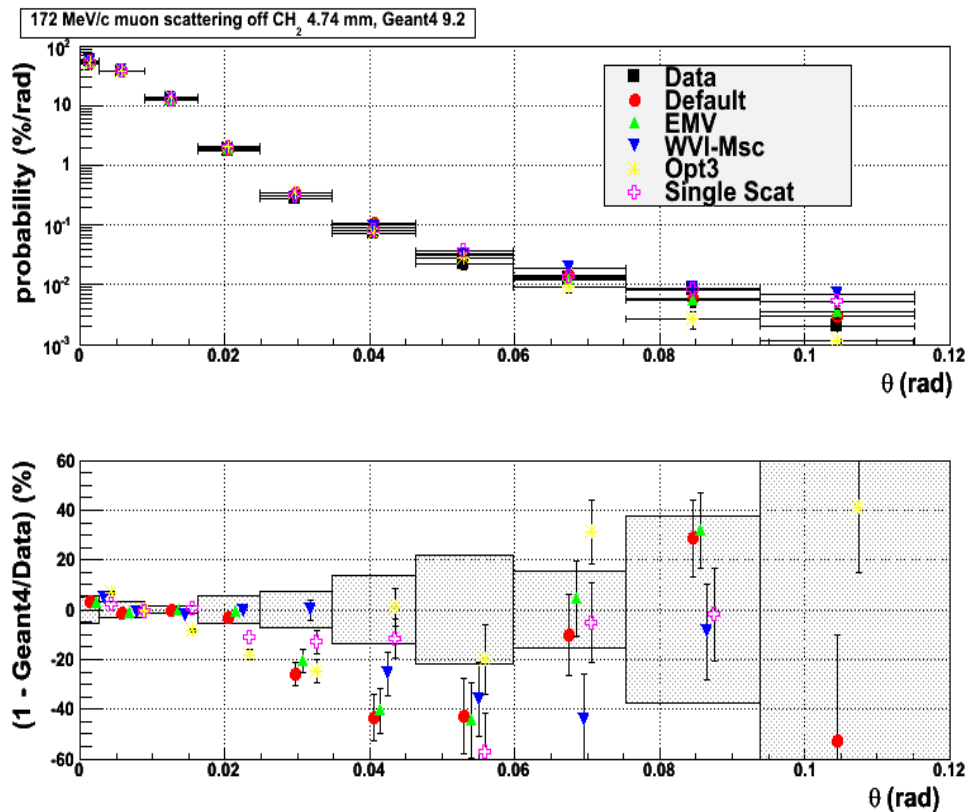


Figure 4. Geant4 simulation of μ^+ scattering off thin polyethylene target versus MuScat data [22]: top – scattering angle, bottom – relative difference of Monte Carlo and the data, hashed area shows one standard deviation. The *WentzelVI* MSC model ($\chi^2/n = 1.69$) and the single scattering model ($\chi^2/n = 1.40$) describe better the tail of the distribution than the *Urban* MSC model ($\chi^2/n = 2.14$).

The focus of this new approach is to provide precise simulation of muons and hadrons as well as nuclear recoil in hard high-energy collisions. The first results (Fig.4) show good prospects. In particular, CPU performance of the new model is competitive with one of the *Urban* MSC model.

7. Conclusions

New MSC and single scattering models are included in the Geant4 toolkit providing the variety of configurations of the Geant4 physics applicable to different use-cases. The *Urban* MSC model is used as a default, in particular, for the Monte Carlo production for LHC experiments achieving simulation precision on level of 1%. The new theory based *Goudsmit-Saunderson* MSC model is promising to have higher accuracy for electron and positrons and to be on the same level of accuracy as well established models from Penelope and EGSnrc codes.

The *Wentzel-VI* MSC and single scattering models are designed for precise simulation of muons and hadrons. The combination of these two models in Geant4 Physics List provides simulation of nuclear recoil above user defined energy threshold. Single scattering models alone can be used for validation of MSC model results and for simulation of transport in low density media, where traditional MSC approach is not valid.

Different configurations of scattering models per particle type, energy and use-case are available to users. The main goal of these developments is to provide the best accuracy of simulation with improved CPU performance.

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