GEANT4 electromagnetic physics for Run3 and Phase2 LHC

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Abstract. For the new GEANT4 series 11.X, the electromagnetic (EM) physics sub-libraries were revised and reorganized in view of requirements for simulation of Phase-2 LHC experiments. EM physics simulation takes a significant fraction of the available CPU during massive production of Monte Carlo events for LHC experiments. We present the recent evolution of GEANT4 EM sub-libraries for the simulation of gamma, electron, and positron transport. Updates of other components of EM physics are also discussed. These developments are included in the new GEANT4 version 11.1 (December 2022). The most important modifications concern the reorganization of the initialization of EM physics and the introduction of alternative tracking software. These modifications affect the CPU efficiency of any simulation, and CPU savings depend on geometry and physics configuration for the concrete experimental setup. We will discuss several methods: gamma general process, Woodcock tracking, transportation with multiple scattering process, alternative tracking manager, and the new G4HepEm library. These developments provide a basis for the implementation of EM particle transport on co-processors and GPU. We also will present very recent updates in physics processes and in configuration of EM physics.

1 Introduction

Electromagnetic (EM) physics in GEANT4 [1–3] plays a critical role [4] in simulation of high energy physics, medical physics, space science, and other applications. Both speed and accuracy are critically important, and the code is continually updated to improve these [5, 6]. The work presented here mostly reflects updates available in GEANT4 version 11.1 (December 2022).

2 GEANT4 EM code and physics evolution

An evolution of the EM physics libraries of GEANT4 was started from GEANT4 11.0. Obsolete code was removed, and in several places the usage of common utilities replaced duplicated code. In the remaining code, uniform approaches were introduced for class initialisation and layout, access to parameters, and code formatting. The main purposes of these modifications

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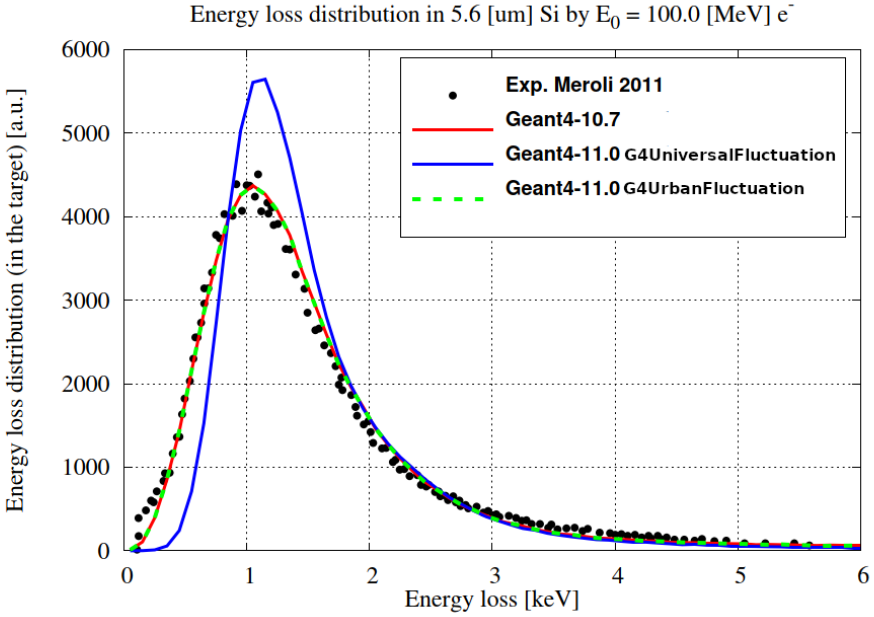

Figure 1. Energy loss distribution in 5.6 μm Si thin film by 100 MeV e^-, comparing measurements (circles) [7] to Geant4 simulations using different fluctuation models. Red line, simulations with Geant4 version 10.7. Blue line, simulations with version 11.0 and *G4UniversalFluctuation* model. Dashed green line (coincident with red line), version 11.0 and *G4UrbanFluctuation* model.

were to make the configuration of EM physics more transparent to users and to be more consistent with usage at supercomputers.

In Geant4 version 11.1, this line of work was continued but with fewer modifications to the EM code. The environment variable for EM physics that defines the path to the EM physics data is checked only once in total, for all EM classes in all threads. The path is then stored as a variable in the *G4EmParameters* class, and can be accessed by calling `G4EmParameters::GetDirLEDATA()`. This process is faster than repeatedly checking the environment variable.

An additional option to select the model of the fluctuations of the energy loss was included. For all charged particles except ions, the default model used in Geant4 10.X series was renamed to *G4UrbanFluctuation* for the 11.X series. This is the most accurate model, and is used in the EM physics lists Opt0, Opt3, Opt4, Livermore, and Penelope. For ions *G4IonFluctuations* class is used. A new fluctuation model, *G4UniversalFluctuation*, is used in physics lists Opt1 and Opt2. This model is faster than the default and, for many applications, is equally accurate. For thin films, however, the *G4UniversalFluctuation* model has reduced accuracy. Fig. 1 shows the energy loss distribution by 100 MeV e^- in a 5.6 μm thick Si layer. The *G4UrbanFluctuation* model reproduces the experimental data of Meroli et al. [7] well. The *G4UniversalFluctuation* model does not reproduce the shape of the energy deposition in this thin layer of silicon, and the mean value is biased. The list of alternative fluctuation models may be extended, and also external models of fluctuations may be used. Sampling of fluctuations may be disabled by using *G4LossFluctuationDummy*. Definition of fluctuations may also be done per geometry region in custom EM physics configurations.

The EPICS2017 dataset [8] for photons is implemented [9] and, starting with GEANT4 version 11.1, is the default for *G4EmLivermorePhysics* and *G4EmLivermorePolarizedPhysics* models. Compared to other datasets, this dataset has more data points, which enables linear (rather than logarithmic) interpolation. Due to a dataset review, these data for gamma processes have a reduced systematic uncertainty on average [9].

For proton, alpha, and ion ionization, ICRU49 [10], ICRU73 [11] and ICRU90 [12] data are used for energies below 2 MeV/amu. ICRU90 data are more detailed and more accurate, so are the first choice, but they are available only for a limited number of projectiles and for three target materials. The second choice is ICRU73 data, and for the remaining combinations of projectile and target the ICRU49 data are used.

Code developed previously [13] to simulate the quantum entanglement of MeV-scale photons from positron annihilation has been added to GEANT4. It is coded in the class *G4eplusAnnihilation* and enabled by the macro command `/process/em/QuantumEntanglement true`, and is called in the class *G4LivermorePolarizedComptonModel*.

3 Methods to speed up simulation

One approach to speed up the simulation while maintaining accuracy is to eliminate unnecessary calculations of mean free path and/or other values at simulation steps.

Firstly this was introduced in GEANT4 for the gamma transport as *G4GammaGeneralProcess* [5], and is the default since GEANT4 11.1. Prior to the introduction of this process, for each step of a gamma particle, six mean free paths were calculated, corresponding to the photoelectric effect, Compton scattering, e^+e^- pair production, $\mu^+\mu^-$ pair production, Rayleigh scattering, and the gamma-nuclear interaction. With the general process, one interaction length is calculated using precomputed tables corresponding to the total mean free path. If an interaction occurs in the step, the concrete process is sampled. This method is already used by both ATLAS [14] and CMS [15].

A method for reducing steps is to combine the multiple scattering and transportation processes into one process, which has access to both. This new *G4TransportationWithMsc* process switches internally between transportation and multiple scattering until a real, discrete interaction occurs. This produces identical physics but can show a large reduction in the number of steps by charged particles. This process is enabled with physics list *G4EmStandard_opt1* in GEANT4 11.1, and can also be enabled in other EM configurations with the macro command `/process/em/transportationWithMsc <argument>`. Passing the argument `Enabled` turns on the combined process and produces identical results to the known setup with two processes. The argument `MultipleSteps` additionally turns on the internal optimization to avoid steps limited only by multiple scattering. This more aggressive mode is expected to return statistically compatible results, but should be validated in the user application. The *G4TransportationWithMsc* method is already used in CMS simulation [15]. An important caveat is that *G4TransportationWithMsc* does not work with parallel worlds.

In some geometries, stepping between geometrical boundaries during photon transport can take a large portion of simulation time. Woodcock tracking [16] is a method of reducing steps limited by boundaries, by choosing a fictitious cross section equal to the largest cross section in the materials along the path of the photon. The effectiveness of this method strongly depends on the application. So far, the implementation is not part of the main GEANT4 repository, but it is planned to be part of the new library G4HepEm [17]. G4HepEm provides a compact and effective simulation of e^+, e^-, and γ transport. In this new library, unlike in the main GEANT4 toolkit, a pragmatic approach to perform only necessary computations during EM particle tracking is implemented. The crucial advantage is in maximum efficiency of the code. An important feature of the G4HepEm library is to be compatible with the implementation of transport on GPU accelerators.

4 Optical physics updates

Geant4 version 11.1 includes the modelling of interfaces of thin coatings as developed by Cappellugola et al. [18]. Interference phenomena and frustrated transmission beyond the limit angle are considered. This is enabled with the *CoatedDielectricDielectric* boundary process, and the user needs to specify the thickness and refractive index of the thin film. The macro coated.mac included with the OpNovice2 example demonstrates usage of this capability.

5 Summary

Simulation of electromagnetic interactions in Geant4 continues to undergo improvements in both speed and accuracy. Concrete values of CPU performance improvements are strongly dependent on the application and use case. ATLAS and CMS simulation productions have become faster using the methods described here. The Geant4 series 11.X is expected to provide a variant of EM physics that will be suitable for implementation on GPU and other accelerators.

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