

REVIEW

Recent Improvements in Geant4 Electromagnetic Physics Models and Interfaces

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An overview of the electromagnetic (EM) physics of the Geant4 toolkit is presented. Two sets of EM models are available: the "Standard" initially focused on high energy physics (HEP) while the "Low-energy" was developed for medical, space and other applications. The "Standard" models provide a faster computation but are less accurate for keV energies, the "Low-energy" models are more CPU time consuming. A common interface to EM physics models has been developed allowing a natural combination of ultra-relativistic, relativistic and low-energy models for the same run providing both precision and CPU performance. Due to this migration additional capabilities become available. The new developments include relativistic models for bremsstrahlung and e+e- pair production, models of multiple and single scattering, hadron/ion ionization, microdosimetry for very low energies and also improvements in existing Geant4 models. In parallel, validation suites and benchmarks have been intensively developed.

KEYWORDS: *Geant4, bremsstrahlung, Monte Carlo, multiple scattering, energy loss*

I. Introduction

Geant4 is a general purpose toolkit^{1,2)} for Monte Carlo si-

mulation of particle transport in matter. The standard EM package of Geant4^{1,3-12)} provides simulation of EM interactions of particles in the energy interval from 1 keV to 10 PeV. It is used for Monte Carlo production for the Large Hadron

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Collider (LHC) experiments at CERN. The precision and CPU performance of the package directly affect LHC simulation results. This package also has a lot of applications in smaller size HEP experiments and in other domains like medical and space science.

The Low-energy EM package^{2,13-18)} includes an alternative set of models extending Geant4 applicability at lower energy (by default down to 100 eV):

- models based on Livermore databases EPDL¹⁹⁾ and EEDL;²⁰⁾
- Penelope²¹⁾ models implemented in C++;
- the atomic de-excitation module based on Livermore database EADL.²²⁾

This package is focused on medical and space applications and was originally developed independently of the Standard EM package. Unfortunately, this approach had some software and practical limitations which did not permit the full exploration of Geant4 capabilities. To overcome these limitations a migration of the Low-energy package to the model design⁹⁾ developed for the Standard EM package has been performed. This migration provides a boost for new model developments and validation.

In this work we describe the current status of Geant4 EM packages for the Geant4 release 9.3, selected recent developments and validation results.

II. New Geant4 EM Interfaces

1. Model Design

Geant4 physics is implemented via the general *G4VProcess* interface¹⁾ for all possible interactions: transportation, decay, EM, hadronic, optical, and others. For the EM physics processes three interfaces are implemented,⁹⁾ which inherit from *G4VProcess*:

- *G4VEnergyLossProcess*,
- *G4VEmProcess*,
- *G4VMultipleScattering*.

Each of these classes performs generic computation common to all concrete processes. For example, the first interface is used for implementation of all ionization, bremsstrahlung, and e^+e^- pair production processes. Concrete physics models inherit from the *G4VEmModel* interface. Any process may have several models specialized for the primary particle energy and geometry region²⁾ (*G4Region* object). Thus, the migration to model interface allows the combination of models from the two EM packages for the same process. Thanks to this design, an implementation of a model requires only computation of cross sections, stopping power and sampling of a final state. All management functions are performed by these virtual classes.

The consolidation of all EM sub-packages gives a boost for the development of new models, automatically resolves a number of problems²³⁾ seen in previous versions of the Low-energy package, provides new opportunities for complex simulation of high energy and low-energy effects, and allows a deeper validation of EM physics. For example, simulated particle ranges are now stable²⁴⁾ independently both of cut values and simulation conditions.

2. EM Physics Lists

Geant4 physics is encoded into Physics Lists, which are built from a collection of physics constructors. Each physics constructor implements a specific subset of particles and physics processes. A set of EM physics constructors are available (Table 1) with the Geant4 release 9.3. Each constructor includes a full list of particles and their EM interactions and can be added to any modular Physics List. The first constructor listed in Table 1 uses default parameters for all EM processes and models. The first four constructors include only processes and models from the Standard EM package. These constructors have different models and parameters for multiple Coulomb scattering (MCS) and different values of step limitation parameters for ionization⁹⁾ $\hat{\alpha}$ (default 0.2) and $\hat{n}$ (default 1 mm). Other constructors in Table 1 are built on top of the “Option3” standard physics constructor by addition of models from the Low-energy package for gamma and electrons below 1 GeV. More variants of Physics Lists are available with Geant4 extended and advanced examples.²⁵⁾

The main advantage of using these physics constructors is the fact that they are intensively validated, so these components of Physics Lists are more reliable and the accuracy of results are better predicted.

Table 1 List of EM physics constructors in Geant4 9.3

Constructor	Comments
<i>G4EmStandardPhysics</i>	Default
<i>G4EmStandardPhysics_option1</i>	minimal MCS step limitation, $\hat{\alpha}=0.8$ for $e^\pm$
<i>G4EmStandardPhysics_option2</i>	“ApplyCuts” option ⁸⁾ on, <i>G4WentzelVIModel</i> of MCS and single scattering for $\mu^\pm$
<i>G4EmStandardPhysics_option3</i>	tight MCS step limitation; increased number of bins in all tables to 220; $\hat{n}=0.1\text{mm}$ for $e^\pm$, 0.05 for $\mu^\pm$ and hadrons, 0.02 for ions; ICRU73 based ion model ²²⁾
<i>G4EmLivermorePhysics</i>	Option3, Livermore models for $\tilde{\alpha}$ and $e^\pm$
<i>G4EmLivermorePolarizedPhysics</i>	Option3, Livermore models for $\tilde{\alpha}$ and $e^\pm$, polarization for $\tilde{\alpha}$
<i>G4EmPenelopePhysics</i>	Option3, Penelope models for $\tilde{\alpha}$ and $e^\pm$
<i>G4EmDNAPhysics</i>	Option3, DNA models for low-energy interactions

3. Helper Classes

Several helper classes are available in Geant4 EM, which may be useful in various user applications:

- *G4EmCalculator* providing an interface to stopping powers, cross sections and ranges, allowing to compute these values without running a simulation;²⁶⁾
- *G4EmProcessOptions* providing an easy method to setup EM options from user Physics Lists;
- *G4EmConfigurator* providing an easy method to configure EM models per particle, energy range, and geometry region;

- *G4EmSaturation* is a class to compute Birks correction to energy loss;
- *G4ElectronIonPair* is a class to sample ionization clusters in gaseous or semiconductor detectors.

The usage of these classes is not mandatory. However, user code may be significantly simplified if these classes are employed. Geant4 extended and advanced examples demonstrate how helper classes can be applied.

4. Infrastructure Upgrade

Recently, the software for handling internal tables for stopping powers, ranges, and cross sections has been improved significantly.⁶⁾ The main goal was to improve the precision of interpolation of data points without increasing the memory used by the Geant4 application. This was achieved by the introduction of cubic spline.¹⁰⁾ In the EM design, the handling of tables is performed in generic classes described above. The benefits of the upgrade are available for all EM sub-packages and some hadronic sub-packages, which use the same methods to handle data.

An initialisation of a simple Geant4 application is very fast but for a complex geometry the size of the prepared tables is large and their filling may take a considerable amount of time. It was identified that the most significant part of the CPU time at initialisation was spent for conversion¹⁾ of Geant4 cuts in range to production thresholds in energy. The optimisation of the software for Geant4 9.3 reduces initialisation time significantly (Table 2).

Table 2 CPU time for initialisation of Geant4 EM physics (default constructor) for a setup with 289 materials

Geant4 version	AMD 32-bit	AMD 64-bit
9.2	147 s	179 s
9.3	51 s	56 s

III. Recent EM Developments

In this chapter selected developments are described, which are already available with Geant4 version 9.3 or are planned for the coming version 9.4 (December 2010).

1. Relativistic Models

A common approach for the relativistic ($E > 1$ GeV) models of bremsstrahlung and gamma conversion to e^+e^- pairs for electrons, muons, and hadrons has been developed.^{5,6,8)} Initial differential cross sections are integrated in a similar way at initialisation taking into account production thresholds (cuts). The resulting restricted cross sections and energy losses are used at run time.⁹⁾ For electron models²⁷⁾ the classical approach²⁸⁾ was implemented including the density effect suppression. The updated computation of the Landau-Pomeranchuk-Migdal (LPM) effect fits the data²⁹⁾ much better than the previous Geant4 model (Fig. 1). These new models are included in all physics constructors described in Table 1 and are used in Monte Carlo simulation productions for LHC.

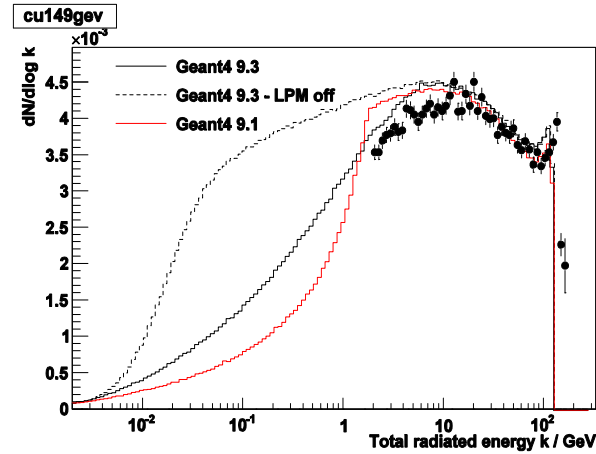


Fig. 1 Bremsstrahlung spectrum for 149 GeV electron beam on a Copper target (4% X_0): points – CERN data,²⁹⁾ histograms – Geant4 simulation results, 9.3 is in agreement with the data.

2. Multiple and Single Scattering Models

The MCS process is an important component of any Monte Carlo including Geant4.¹²⁾ At high energy it is limiting the spatial resolution of detectors. Scattering of electrons defines energy transport via geometrical boundaries directly affecting various detector responses. The default Geant4 MCS model³⁰⁾ has been upgraded³¹⁾ for Geant4 version 8.0 (December 2006) due to a problem in electron scattering.³²⁾ Later alternative models of single and multiple scattering have been added.^{11,12,33)} The main goal of these additions was to provide a choice between speed and precision specifically for different particles. Higher precision is achieved by simulation with smaller steps, which leads to an increase of the CPU time. Incorporation of corrections like spin term or nuclear form factor should be done depending on a particle type, also MCS parameters can also be optimized per particle. Thus, since Geant4 9.3 MCS processes used in EM constructors (Table 1) for electrons, muons, and hadrons are different, for each process the corresponding set of models and its parameters are defined.

To reach maximal precision the new Goudsmit- Saunderson MCS model for electrons and positrons has been developed,¹¹⁾ which is fully based on theory and reusing experience and prescriptions of PENELOPE³⁴⁾ and EGSnrc.³⁵⁾ This model provides the best results for the Fano cavity test (Fig. 2) and for other benchmarks but is significantly slower than the default model. Thus, for the newest Geant4 version 9.4beta this model is included only in Livermore and Pene-lope physics constructors.

3. New Models of Ionisation

Recently intensive developments have been carried out to improve existing models of ionisation and to design new models including ionisation of magnetic monopole¹⁰⁾ and ionisation of ions heavier than Helium¹⁸⁾ using ICRU 73 data. The last model mainly focuses on the precise simulation of the transport of ions used in radiation therapy.³⁶⁾

As the standard model for ion ionisation, the new model uses the effective charge approach,³⁷⁾ where the ion charge

state is considered in average only. But in some applications, like microdosimetry and ion beam transport in vacuum, this approach is not applicable. A set of new models have been developed (9.4 beta), which uses a dynamic ion charge instead of an effective charge. In that case the charge state should be defined by a special process of the charge exchange between an ion and the media. The demonstration of these new models will be available with Geant4 “TestEm7” extended EM and “microbeam” advanced examples.

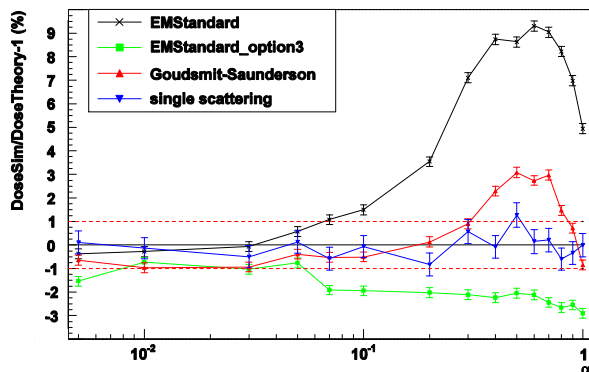


Fig. 2 Fano cavity test results³¹⁾ as a function of α (step limit parameter) for different MCS options for Geant4 9.4beta.

4. DNA Physics Model

Geant4 has been used in recent years for the simulation of experimental setups at the physics-biology frontier, including for example the design of high-resolution irradiation beam facilities at sub-micrometre size³⁸⁾ and dosimetry at the single-cell scale in realistic geometrical models of biological cells.³⁹⁾ The Geant4 toolkit is currently being extended for microdosimetry simulation capabilities in biological media in the framework of the Geant4-DNA project,^{17,40)} originally initiated by the European Space Agency (ESA) for the modelling of biological effects of ionising radiation on astronauts at the DNA scale during manned long-duration space exploration missions. The Geant4-DNA extension is a component of the Low-energy EM package. It includes discrete EM physics models applicable to electrons, protons, neutral Hydrogen, neutral Helium and its charged states (He^+ , He^{2+}) in liquid water, the main component of biological media. Geant4-DNA processes simulate explicitly all interactions on a step-by-step basis in order to reconstruct precisely track structures of ionizing particles at nanometre scale, the size of DNA molecules.

Such computations require high computing performance and they are usually used at low energies (down to a few eV) and applied to small target volumes only, such as biological cells and sub-cellular volumes. In addition, Geant4 EM condensed-random-walk processes,^{1,9)} which cover complete energy range do not simulate explicitly all interactions with such precision and are much less demanding in computing performance. Consequently, these condensed-random-walk processes could be used to simulate the radiation environment surrounding astronauts in space, taking into account high energy incoming cosmic particles and modelling their

interactions within spacecraft material, until they finally reach the target cells of interest, where Geant4-DNA discrete processes would take over.

The possibility to combine discrete and condensed processes in selected energy ranges and geometry regions is a new feature of the software design presented above. The combination of the Standard and Geant4-DNA EM models has been recently implemented in the Physics List of Geant4 “microdosimetry” advanced example, which illustrates how to perform in practice this combination of processes for a simple application case. This example proposes to simulate the irradiation of a thin liquid water slab, placed in the “world” mother volume, also filled with liquid water. Geant4-DNA processes only are activated within the slab.

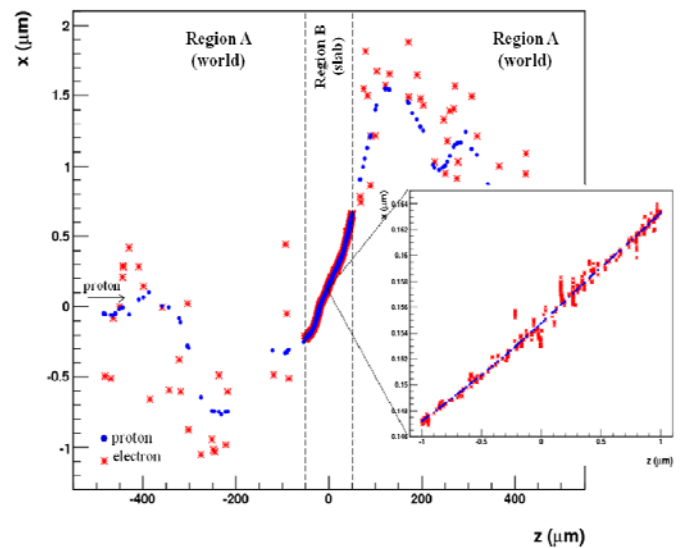


Fig. 3 Effect of combination of processes obtained with the “microdosimetry” advanced example. The 2D projected track of a 10 MeV proton in liquid water is shown. DNA processes are enabled inside a 100 μm slab. Note the scale of the vertical axis is much smaller than the scale on the horizontal axis. The inset shows a magnification of secondary tracks inside the slab.

A trajectory of a single incident 10 MeV proton on the slab is shown in Fig. 3, where two regions are used: the default *G4Region* (named “A”) and another *G4Region* (named “B”) associated to this slab. Standard EM processes are activated in *G4Region* “A”. On the contrary, proton and electron Geant4-DNA processes are activated in *G4Region* “B”. They are ionisation and excitation for both protons and electrons and elastic scattering for electrons. Because these Low-energy processes have upper applicability limit, the Standard EM processes are also activated in “B” for high energy particles, using a lower energy applicability limit of 10 MeV for protons and 1 MeV for electrons, respectively.

The incident 10 MeV proton is shot from *G4Region* “A” in the direction of the slab (Fig. 3). Inside the slab very detailed simulation of protons interactions and secondary particle transport is performed. Once the incident proton has left the water slab, it returns into *G4Region* “A” where only Standard EM processes are enabled. The possibility to combine such processes responds to a requirement of having

Geant4 Physics processes able to work at different sizes and energy scales in a single simulation application.

IV. Recent Validation Results

Validation of Geant4 EM software is a continuing task to the Geant4 EM working groups and software for validation and verification of EM packages has been developed.⁴¹⁾ Validations are performed for each modification of EM software and for each Geant4 version. Therefore software for automatic running and presenting of results has been designed. In parallel, number of specialized benchmarks was carried out recently.

The validation of the cross sections and stopping powers of Geant4 EM physics models was first done⁴²⁾ versus NIST data. In this work it was concluded that Geant4 photon cross sections agree with NIST within 3% and electron stopping powers within 5%. After the migration to common design a new validation of photon cross sections versus various databases was published²⁶⁾ which demonstrated general good agreement with the data for both the Standard and Low-energy models. Also some problems were identified mainly when databases do not agree with each other.

The validation of the electron dose deposition in semi-infinite media in different materials from Be to U has been published.^{43,44)} The primary beam energy was from 0.05 MeV to 1 MeV and primary beam angles from zero to 60 degrees. The absolute dose and longitudinal dose profile were measured. It was shown that results depend mainly on MCS model and are practically independent on ionization or bremsstrahlung. The Geant4 accuracy is about 3% for total energy deposition and is within 10% for the dose profile for majority of physics constructors. The worst precision is obtained with the Option1 constructor where simplified step limitation is used.

Another benchmark comes from medical applications of electron/gamma transport for the simulation of ionization chamber.³⁵⁾ The Fano theorem predicts with the absolute accuracy the dose deposition in a cavity filled with vapor phase of surrounding condensed material. The current results of Geant4 benchmarking⁴¹⁾ are on level of 3% for the default model and 1% for the most precise one (Fig. 2).

The recent benchmark for electron scattering of 13 MeV and 20 MeV on various thin targets was published⁴⁵⁾. The comparisons were performed⁴⁶⁾ with predictions of different Monte Carlo systems EGSnrc, PENELOPE, and Geant4. Results were in statistical agreement with the data except Geant4 predictions for low-Z targets which provides up to 10% overestimates. After this analysis Urban MCS model was tuned for all electron data excluding the data from this benchmark, which gives now satisfactory results. The tuned version of the model is available with the Geant4 version 9.3. Also the most recent version (9.4 beta) of Goudsmit-Saunders MCS model¹¹⁾ provides good results.

Another dedicated benchmark⁴⁷⁾ has been performed for EGSnrc, PENELOPE, and Geant4 using the most precise existing data for low-energy electron bremsstrahlung^{48,49)} for 10 – 30 MeV electron beams in thick targets of Be, Al, and Pb. Geant4 results are within 3 standard deviations at all energies

and angles. It is shown that the Standard EM model overestimates the photon yield compared to the Livermore model. For the total photon yield the accuracy of the data is 3%, EGSnrc results agree within 1 standard deviation, Penelope and Geant4 agree within 2 standard deviations. For the high energy the benchmarking data measured at SLAC⁵⁰⁾ and CERN²⁹⁾ are available. Only new model^{8,27)} from the Standard EM package implements LPM and density suppressions correctly (Fig. 1).

Geant4-DNA Physics models for microdosimetry in liquid water were recently quantitatively compared⁴⁰⁾ to experimental data in water collected from the literature. In particular, the agreement between Geant4-DNA total and differential cross section models and the reference data has been evaluated using the Kolmogorov–Smirnov statistical test. For this evaluation, experimental data acquired in water vapor were used as direct measurements in the liquid phase are not available. Comparisons with several international recommendations (such as the recommendations of the ICRU reports) on collision stopping powers and on stopping cross sections have also been performed.

V. Summary

Since Geant4 version 9.3 both EM packages, Standard and Low-energy, follow a common interface for processes and models. It is possible to use in the same run ultra-relativistic, relativistic, and low-energy models simultaneously for optimal precision and speed. Validation procedures for EM physics are established. The main validation results are available via EM physics web.²⁵⁾

Acknowledgments

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