The recent upgrades in the "standard" electromagnetic physics package

J. Apostolakis, V.M. Grichine, V.N. Ivanchenko, M. Maire, L. Urban

HAL Id: in2p3-00168418

http://hal.in2p3.fr/in2p3-00168418

Submitted on 28 Aug 2007

THE RECENT UPGRADES IN THE "STANDARD" ELECTROMAGNETIC PHYSICS PACKAGE

J. Apostolakis, V. M. Grichine, V. N. Ivanchenko[#], CERN, Geneva, Switzerland
M. Maire, LAPP, Annecy, France
L. Urban, MPFI, Budapest, Hungary

Abstract

The current status and the recent developments of the Geant4 "Standard" electromagnetic package (G4StEm) are presented. The design iteration of the package carried out for the last two years is completed. The internal database of elements and materials based on the NIST databases is introduced inside the Geant4 toolkit. The focus of recent activities is on an upgrade of physics models and on validation of simulation results. The significant revisions were done for multiple scattering models, ionization models and for models for transition radiation. The evolution of the verification suite is also discussed.

STANDARD EM PACKAGE

The Geant4 toolkit [1] provides general Monte Carlo simulation of particle transport and interactions. Electromagnetic (EM) interactions of photons and charged particles with matter are implemented in G4EmSt [1]-[10]. The physics models of the package were created for High Energy Physics experiments simulation but are also applicable to a wide spectrum of other applications. G4EmSt covers EM interactions of particles with energies from 1 keV up to 10 PeV. In this work the recent developments and the current status of G4StEm are described.

PHYSICS MODELS UPGRADE

A number of improvements in G4EmSt physics models have been introduced in order to provide more precision and stable results for major use-cases. Key improvements were in multiple scattering, ionization models, and models for transition radiation.

Multiple Scattering

The Geant4 model for the process of multiple scattering (MSC) [10] is based on Lewis's approach [11]. Both large and small simulation steps were allowed and step was limited only near the geometry boundaries. The model provides results, which are in good agreement with the data for hadrons and high energy electrons [7, 9]. However, a number of reports were received on the strong dependence on production cuts of results for sampling calorimeters. Moreover, the analysis [12] of the simulation of low energy electrons has been performed demonstrating that for setups with thin layers of different

materials the result continue to vary until very small cuts (~o(μm)) or very small step limits are applied.

Our studies identified that the instability of the results was due to MSC simulation of low energy electrons. To address this problem a refinement of the MSC process and model has been introduced with the following modifications:

- a correlation between scattering angle and the lateral displacement [13];
- the recalculation at each simulation step of the "safety" – the minimal distance to the geometric boundary;
- more strict step limitation near the boundary – the default value of the parameter $F_R = 0.02$;
- an extra limitation of the step size for geometrical volumes – at least 2 steps inside a volume in which a particle starts and at least 4 steps inside other volumes.

The effect of the F_R parameter is demonstrated in Fig.1 for a 1 GeV electron shower in a lead/scintillator calorimeter and in Fig.2 for an electron backscattering experiment. Note, that decreasing the F_R parameter means more simulation steps in the vicinity of a geometric boundary which requires more CPU.
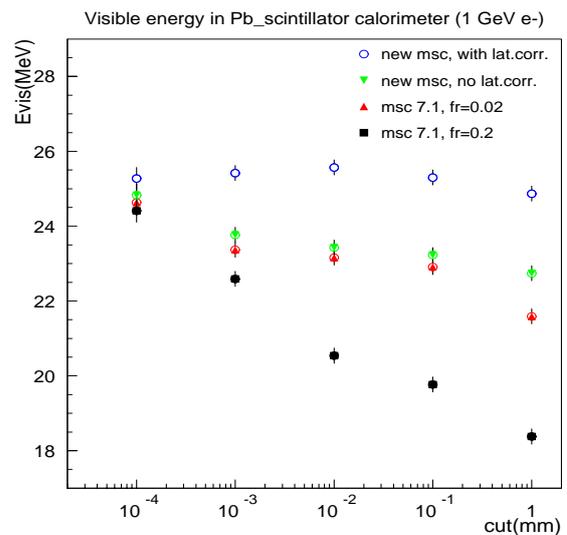

Figure 1: Visible energy in sampling calorimeter as a function of the production threshold.
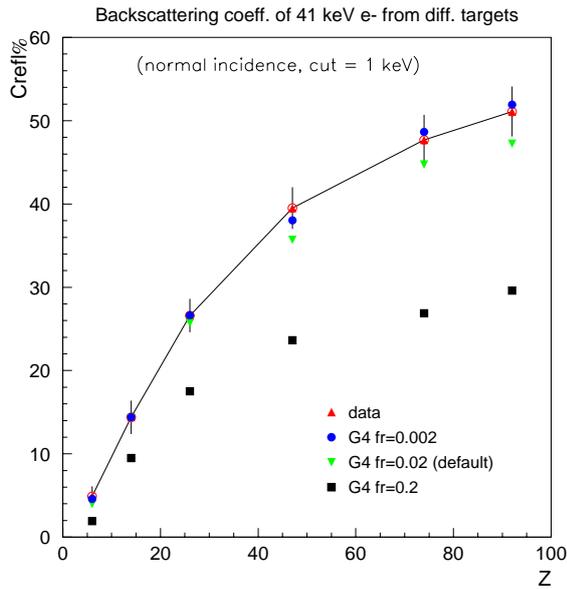
Figure 2: Electron backscattering coefficient as a function of the media atomic number, red triangle – data [14].

The safety is the distance to the nearest geometrical boundary. It is used to limit the step and the transverse displacement that MSC applies. The recalculation of the safety is required to ensure more precise value of the safety because only fast estimation is provided at each step by the Geant4 transportation. The simulation of correlation is important for low energy electrons. All together these improvements provide more precise and stable results but require more CPU. This is demonstrated in Figs.3-6 showing the simulation results for a lead/scintillator calorimeter similar to the LHCb calorimeter. Incident particles are electrons of 10 GeV, production cuts for electron and gamma are expressed in terms of the range cut [1]. The increased stability is evident with 1% accuracy up to the cut value 0.2 mm.

In previous Geant4 releases the visible energy in the calorimeter is strongly cut dependent (Fig.3). This dependence is significantly reduced in release 8.0, in which the modifications in the MSC model were introduced. As an option it is available to disable the new geometrical MSC step limitation and to establish higher value of F_R. In this case the cut dependence becomes significant again. The energy resolution of the calorimeter is less sensitive to the MSC model (Fig.4).
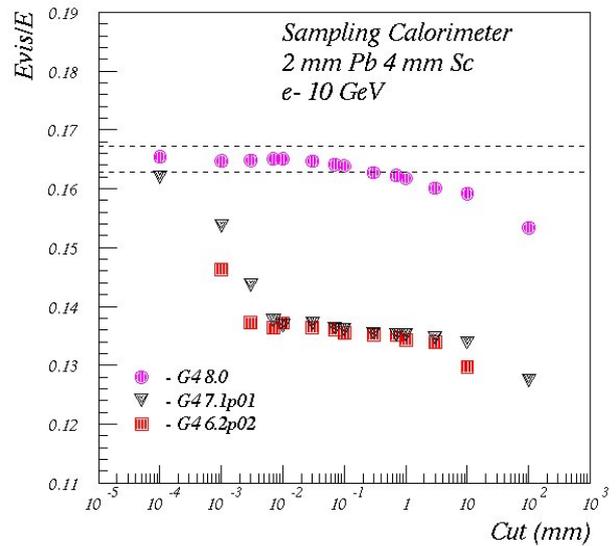

Figure 3: Visible energy deposition in sampling calorimeter as a function of the production threshold for different Geant4 releases. Dashed lines show ±1% variation around limit value. The revised MSC model of G4 8.0 shows significantly larger stability.

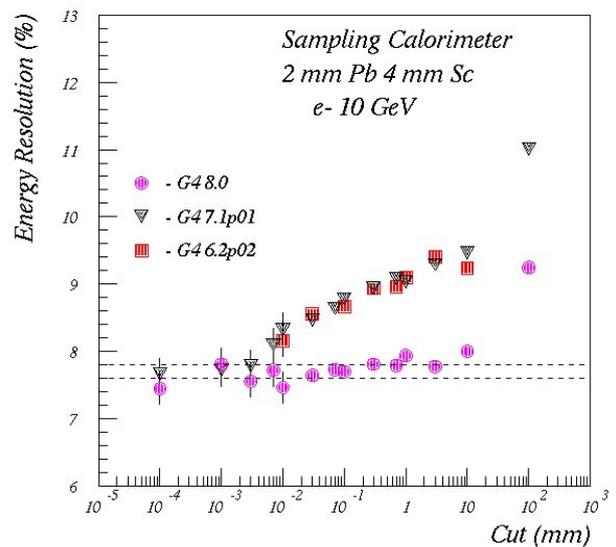
Figure 4: Energy resolution of sampling calorimeter as a function of the production threshold for different Geant4 releases. Dashed lines show ±1% variation around limit value. The revised MSC model of G4 8.0 shows significantly larger stability.
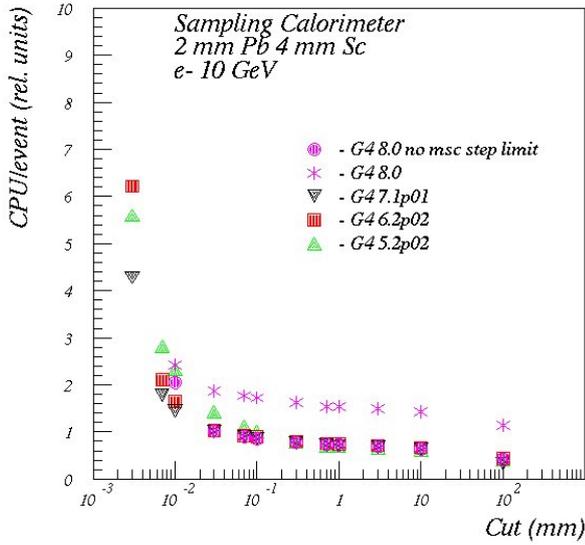
Figure 5: CPU time as a function of the production threshold for different Geant4 releases. The magenta circle corresponds to the option when MSC step limitation is switched off.
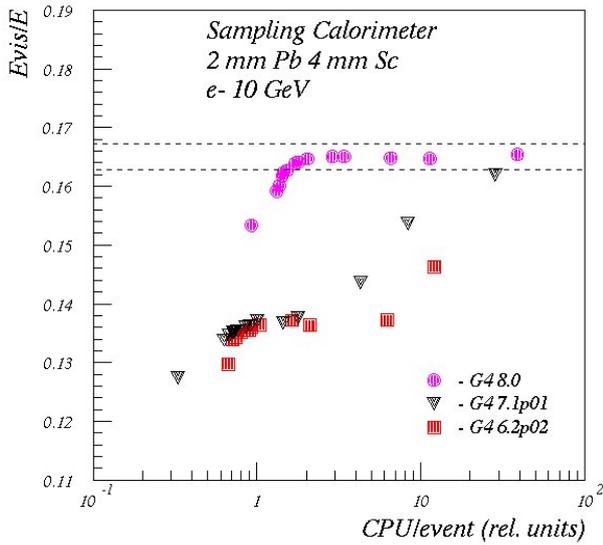

Figure 6: Visible energy deposition in sampling calorimeter versus CPU time for different Geant4 releases.

The CPU performance of the simulation has significant implication for the number of events that the LHC experiments can simulate. With the new MSC model using the same cut values, more time is required per event (Fig.5); this value, depending on cut and geometry, varies from 10 % to 100 %. With the new MSC model it is possible to use higher values of cuts to achieve the same accuracy of simulation results (Fig.6).

Ionization of Hadrons and Ions

A number of improvements based on the review [15] were provided for the simulation of ionization for hadrons and ions, which are new for G4EmSt:

- new shell correction parameterization;
- Barkas correction;
- Bloch correction;
- Mott correction;
- Nuclear stopping power.

These corrections are relatively small for hadrons and are more significant for ions. As a result, the agreement between G4 stopping powers for hadrons and ions and evaluated data [15, 16] was significantly improved. An example of the comparison is shown in Fig.7. The systematic accuracy of the data is 2-3%.

The new process *G4hhIonisation* has been designed and delivered with the release 8.0. This process provides simulation of energy loss of a very heavy exotic charged particle, which will be searched for in LHC experiments.
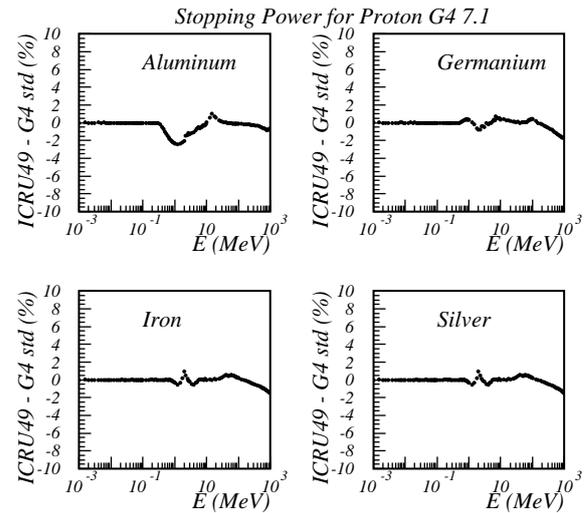

Figure 7: Results of G4EmSt proton stopping power comparison with the data of the ICRU49 report [15].

INFRASTRUCTURE UPGRADE

G4EmSt is continuously under development, in order to increase precision, performance, and arias of applicability of its components. To ensure the production quality of simulation results and to make developments easier a number of improvements are introduced inside the package itself and in the general infrastructure.

Design Iteration

Starting from Geant4 release 5.1 the design iteration for G4EmSt was performed with the following goals:

- separate management functions from physics models by providing generic abstract classes for electromagnetic physics;

- enable extensions of current models and creation of alternative models;
- provide ability to trigger special models per geometrical region;
- improve bookkeeping and maintenance.

The design iteration was completed for the Geant4 release 8.0 and current activity is focused on the extending the physics models validation and improvements. As a result of the design iteration new components and user interfaces are available:

- *G4EmProcessOptions* class enables common options to steer the package, and can be used as an alternative to the UI command interface;
- *G4EmCalculator* class provides access to the energy loss, cross section, and mean free path of EM processes;
- *G4EnergyLossForExtrapolator* class provides calculation of mean energy loss, its dispersion, and mean scattering angle to be used for event reconstruction.

Internal Database of Materials

An internal Geant4 database of isotopes, elements and materials has been created. The goal of this development was to provide a simple method to describe a media. The user can now create a new G4Material or G4Element using only the name in the database. By default an element is created with its natural isotope composition. Most of the data was obtained from the NIST databases [16]: natural isotope compositions, isotope masses, mean ionization potentials for elements and materials, material densities, and atomic composition of materials. Some extra materials frequently used by Geant4 users were also added to the database. Currently about 3500 isotopes, 108 elements, and about 300 materials are included.

Verification Suite

To provide stability of the simulation results for long-term productions, in particular for LHC experiments, a verification suite for G4EmSt has been created. It is based on the 16 EM examples distributed with Geant4. These examples are simple Geant4 applications, which demonstrate various aspects of EM physics. The following three levels of tests are carried out:

- check on cross sections and stopping powers;
- test on different physics setups from single materials to simplified calorimeters covering 120 test cases, 23 are checked as regression tests for each new G4EmSt revision;
- Large statistic tests for simplified LHC calorimeters checking with regression tests for each Geant4 reference tag and release.

During this verification the major physics observables are analysed: energy deposition, energy resolution, backscattering, forward and side leak of energy, and also the number of simulation steps, number of secondary gammas and electrons, and CPU usage. For large statistic tests the following simplified setups were designed:

- 2.3 mm Pb + 5.7 mm lAr (ATLAS Barrel);
- 2.5 cm Cu + 0.85 cm lAr (ATLAS HEC);
- 2 mm Pb + 4 mm Scintillator (LHCb);
- 5x5 matrix of $PbWO_4$ crystals (CMS).

The verification suite is equipped with scripts enable to run, store the results, analyze, and test in regression. Results shown in this work were obtained using this facility.

CONCLUSIONS

The major improvements were in simulation of multiple scattering, for sampling calorimeters demonstrate reduced dependence of results on the production thresholds. G4EmSt has been redesigned and the infrastructure of the package has been developed. The Geant4 database on elements and materials is available.

ACKNOWLEDGMENTS

REFERENCES

[1] Geant4 Collaboration (S. Agostinelli et al.), Nucl. Instr. Meth. A506 (2003) 250.
[2] K. Lassila-Perini and L. Urban, Nucl. Instr. Meth. A362 (1995) 416.
[3] J. Apostolakis et al., Nucl. Instr. Meth. A453 (2000) 597.
[4] V. M. Grichine, Phys. Lett. *B*525 (2002) 225.
[5] V. N. Ivanchenko, Nucl. Instr. Meth. A494 (2002) 514.
[6] V. N. Ivanchenko, Nucl. Instr. Meth. A525 (2004) 402.
[7] H. Burkhardt et al., "GEANT4 Standard Electromagnetic physics package", In Proceedings MC2005, Chattanooga, Tennessee, April 17-21, 2005, on CD-ROM, Americal Nuclear Society, LaGrange Park, IL (2005).
[8] J. Allison et al., IEEE Trans. Nucl. Sci, 53 (2006) 270.
[9] A. G. Bogdanov et al., IEEE Trans. Nucl. Sci, 53 (2006) 513.
[10] L. Urban, "Multiple scattering model in GEANT4", CERN-OPEN-2002-70, 2002.
[11] H. W. Lewis, Phys. Rev. 78 (1950) 526.
[12] E. Poon and F. Verhaegen, Med Physics 32 (2005) 1696.
[13] I. Kawrakow, A. F. Bielajew, Nucl. Instr. Meth. B142 (1998) 253.
[14] H. J. Hunger and L. Kuchler, "Measurements of the Electron Backscattering Coefficient for Quantitative EPMA in the Energy Range of 4 to 40 keV", Phys., Stat., Sol. (a) 56 (1979) K45.
[15] A. Allisy et al., "Stopping powers and ranges for protons and alpha particles", ICRU Report 49, 1993.
[16] http://physics.nist.gov/PhysRefData/