Validation and verification of Geant4 standard electromagnetic physics

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Abstract. The software tools developed for the validation and verification of the standard electromagnetic physics package of Geant4 are described. The validation is being performed versus experimental data and in regression to a previous version of Geant4. Examples of validation results are presented.

1. Introduction
The standard electromagnetic (EM) physics package of Geant4 [1-4] has been developed for simulation of particle transport in matter and high energy physics (HEP) detector response [5-9]. Geant4 is the main simulation engine for the ATLAS, CMS and LHCb experiments. The requirements to the precision and stability of Monte Carlo simulation for LHC experiments are well within 1%. In order to keep under control a long-standing quality of the EM package, software suites for its validation and verification have been developed. In this work we describe main approaches for the validation and the structure of validation software.

2. Validation of the Geant4 EM physics package
Geant4 EM package includes simulation of ionisation, bremsstrahlung, photo-electric effect, Compton scattering, multiple scattering and other processes [10]. The main goal of the detailed Monte Carlo simulation of HEP experiments is to provide a realistic response of various particle detectors. LHC applications deal with particle production at 10 TeV proton-proton collisions with high energy secondary particles registered by huge experimental apparatus consisting of many sub-detectors. Even if initial particles are high energy hadrons, the response of HEP calorimeters is sensitive to EM physics simulation at energies below than 1 MeV. Low-energy secondary particles (gamma, electrons, positrons and others) contribute to responses of majority of HEP detector systems providing as main signal and background. Thus, validation of the EM physics package for LHC applications should be done for all particle types and for the complete energy range from 1 keV to the maximum energy of the experiment. It is necessary to control energy loss, ranges, straggling, cross sections and other physics quantities. The validation sequence includes following types of tests:

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• developer unit tests and tests versus specific data;
• low and medium statistic tests with control on basic numbers;
• high statistic regression tests with comparison to data and to results of the previous version of Geant4;
• user validation.

The testing suite for the EM physics has been developed for many years [4, 10, 11]. It is mostly based on official Geant4 code examples distributed together with the toolkit. Thus, allowing any user to repeat validation performed by the Geant4 EM working group. Additionally few special tests are created for the validation of essential experiments or use-cases. The testing suite (Figure 1) includes a data-base of experimental data, a set of Geant4 applications and the additional software, which is needed to perform data conversion from a publication format to the testing suite format, storage of results, regression analysis and publishing of validation results in the web [10].

![General scheme of validation software](image)

**Figure 1.** Geant4 EM physics validation.

3. Basic medium statistic tests of EM physics
The core part of the testing suite is a set of medium statistic tests (Table 1), which are run on regular basis by the Geant4 EM physics group after any modification of the EM package. The results are stored in the database for each Geant4 reference version. The same tests are executed by the Geant4 system testing team on all supported software platforms in nightly mode [12]. The selection of initial conditions of these tests was based on following requirements:

- all EM processes and models should be tested;
- all important use-cases should be tested;
- the reference output of physics quantities should be provided for all tests;
- required CPU is limited (< 15 minutes);
- statistical comparisons between simulation results and the data should be performed whenever it is possible;
- statistical comparisons with regression to the previous reference version of the software should be performed whenever it is possible.

The results is qualified as “accepted” if no warning or errors appears during execution and obtained results of all tests are in statistical agreement with the reference values within allowed deviations.
Table 1. Basic medium statistic tests

| Test        | Particle | Energy  | Cut (mm) | Target   | Purpose                        |
|-------------|----------|---------|----------|----------|-------------------------------|
| TestEm0     | e⁻       | 500 keV | 1        | Ge       | Cross sections                |
| TestEm1     | e⁻       | 10 MeV  | 1        | Al       | Cross section                 |
| TestEm2     | e⁻       | 100 MeV | 1        | PbWO₄    | Shower shape                  |
| TestEm3     | e⁻       | 100 MeV | 1        | Pb/lqAr  | Sampling calorimeter          |
| TestEm4     | γ        | 100 MeV | 1        | C₆H₆     | Gamma processes               |
| TestEm5     | π        | 5 GeV   | 0.007    | Si       | Multiple scattering           |
|             | e⁻       | 15.7 MeV| 0.01     | Au       |                                |
|             | μ⁺       | 96.2 MeV| 0.01     | Polyethylene |                                |
|             | μ⁻       | 100 GeV | 1        | Fe       |                                |
|             | p        | 174 GeV | 1        | Al       |                                |
| TestEm6     | γ        | 100 TeV | 1        | Fe       | Rare high energy processes    |
|             | e⁺       | 1 TeV   | 1        | Fe       |                                |
|             | pbar     | 1 GeV   | 1        | Fe       |                                |
| TestEm7     | P        | 160 MeV |          | Water    | Ranges and Bragg peak for hadrons and ions |
|             | ¹²C      | 3.5 GeV |          | Water    |                                |
|             | K⁺       | 100 MeV | 1        | Cu       |                                |
|             | ³He      | 0.265 keV|         | Vacuum   |                                |
|             | ⁴He      | 100 MeV |          | Water    |                                |
| TestEm8     | P        | 200 GeV | 1        | Xe+CH₄+C₃H₈ | PAI ionisation model       |
| TestEm9     | e⁻       | 1 GeV   | 0.3      | CsI      | Crystal calorimeter            |
| TestEm10    | e⁻       | 2 GeV   | 1        | Xe+CO₂ gas | Transition radiation          |
| TestEm11    | e⁻       | 500 keV | 1        | Si       |                                |
| TestEm12    | e⁻       | 4 MeV   | 0.001    | Water    |                                |
| TestEm13    | γ        | 100 keV | 1        | Water    |                                |
|             | e⁻       | 100 MeV |          | Water    |                                |
| TestEm14    | γ        | 100 keV | 1        | Water    |                                |
|             | e⁻       | 100 MeV |          | Water    |                                |
| TestEm15    | e⁻       | 5 MeV   | 1        | Water    |                                |
|             |          | 100 keV |          | Water    |                                |
| TestEm16    | e⁻       | 10 GeV  | 1        | Vacuum   |                                |
| TestEm17    | μ⁺       | 10 TeV  | 1        | Fe       |                                |
|             | π⁺       | 10 TeV  | 1        | Fe       |                                |
|             | p        | 10 MeV  | 1        | Water    |                                |
| GammaTherapy| e⁻       | 50 MeV  | 0.1      | Water, Be, W |                                |
| fanoCavity  | γ        | 1.25 MeV| 10⁴      | Water, water-vap |                                |
| fanoCavity2 | e⁻       | 1 MeV   | 10⁴      | Water, water-vap |                                |
| Pol01       | γ        | 10 MeV  | 0.1      | Fe       |                                |
| Monopole    | Monopole | 100 GeV | 0.7      | Si       |                                |
Table 2. High statistic testing suite for EM physics.

| Test                    | Particle | Energy | Setup             | Target          | Purpose                                                                 |
|-------------------------|----------|--------|-------------------|-----------------|-------------------------------------------------------------------------|
| Sampling calorimeter    | e⁻       | 10 GeV | ATLAS barrel      | Pb/liquidAr     | Cut and energy dependences of calorimeter response and resolution       |
|                         |          | 10-120 GeV | ATLAS HEC, LHCb, ZEUS | Cu/liquidAr, Pb/Scint. |                                                                         |
| Crystal calorimeter     | e⁻       | 10 GeV | CMS ECAL          | PbWO₄           | Cut dependences of calorimeter response, resolution and transverse energy profile |
|                         |          |        |                   | Pb/Scint.       |                                                                         |
| Combined calorimeter    | e⁻, γ    | 1-300 GeV | CMS ECAL + HCAL  | PbWO₄, Fe, Cu, Scint. | Cut and energy dependences of calorimeter response, resolution and shower shape |
| Energy deposition profile | e⁻       | 0.3-1.0 MeV | Semi-infinite media | Al, Mo, Ta, TaAl, AlAuAl | Low-energy electron transport                                             |
| Fano theorem            | γ        | 1 MeV  | Cavity filled by vapour gas | Water          | Low-energy electron and gamma transport                                 |
| Electron scattering     | e⁻       | 1-16 MeV | Thin targets      | Al, Au          | Multiple scattering                                                     |
| Muon scattering         | µ⁺       | 96.2 MeV | Thin targets      | liquidH, Li, Be, C, CH₂, Al, Fe | Multiple scattering                                                     |
| (MuScat data)           |          |        |                   |                 |                                                                         |
| Bragg peak              | p, He, C | 100-400 MeV | Uniform media     | Water           | Ranges, straggling, scattering                                           |
| High energy muon        | µ⁺       | 100 GeV | Uniform media     | Fe              | Energy loss, straggling, scattering                                      |
| penetration             |          |        |                   |                 |                                                                         |

4. High statistic tests of EM physics

The high statistic tests (Table 2) are executed for each public release of Geant4 or after any major modification of the EM package. Typically, two weeks of wall clock time are needed for the execution at CERN lxbatch and IN2P3 computer centre. The regular runs for validation of proton and ion physics for medical applications were performed also in KEK.

The high statistic tests are focused on the main HEP detectors, first of all on various HEP calorimeters. The reason is in usage of Monte Carlo simulation for calibration of LHC calorimeters, defining a scale of a calorimeter response for hadronic showers. The requirements to the stability of these responses are very strict (down to 10⁻³), because any change of EM scale of a calorimeter will require its recalibration for the data analysis, which is a very time consuming job. The resulting energy scale of the experiment depends on accuracy of the simulation, thus final results (like the mass of a possibly discovered new particle) are affected by the precision of the EM interaction simulation.

For the validation of the Geant4 EM package simplified structures of calorimeters are used, which are similar to real HEP calorimeters [4, 10]. As an example, in Figure 2 the simulation results are shown for the Lead/Scintillator calorimeter structure of LHCb-type. These results are used to control the stability of the EM simulation for different Geant4 versions and production cuts. The verification versus the data (Figure 3) is being performed for the classical Lead/Scintillator sampling calorimeter setups used in ZEUS test-beam studies [13, 14]. These two structures have sampling fractions different by a factor 2, calorimeter geometry and materials are taken from the publications. The results are obtained without any tuning of Geant4 simulation. They demonstrate stability between Geant4 versions and the precision versus the data.
As it was mentioned above, the accuracy of the low-energy electron transport directly affects the accuracy of the simulation of high energy calorimeters. Two special tests have been developed focusing on validation of low-energy electron transport:

- the energy deposition profile of MeV electron beams in extended media [15] versus Sandia calorimetric data;
- the test of the Fano theorem [16] - energy deposition in a cavity of a media filled by gas.

The results for low-energy electron transport are very sensitive to the accuracy of a multiple scattering model. One can see in Figures 2-3 that EMV Physics List provides biased results, because electron transport between high density material and low density material require more number of steps. The same conclusion can be made from Figure 4, where Geant4 simulation is compared with the Sandia data.

The accuracy of a multiple scattering model may affect the resolution of vertex and muon detectors. The dedicated tests for medium and high energy scattering results are also part of the validation suite.
Large user communities perform their own validations of Geant4 software and make conclusions on the quality of the EM package. In particular, test-beam analyses for LHC experiments are reported on a regular basis (see for example [7-9]). The feedback is taken into account by the EM working group.

5. Conclusions
The validation suite for Geant4 EM physics has been established. The developed software allows performing regular validation in the development phase and intensive validation in the phase of Geant4 release. The practice of recent Geant4 releases demonstrates that LHC calorimeters and other detectors simulation results are stable and were predicted in advance by the EM working group. Changes and evolutions of the results are under control. As a rule, user feedback confirms predictions obtained with the EM testing suite. However, the suite is not covering all aspects of EM physics and some issues are reported by Geant4 users. Thus, further development of the suite is required and extensions are planned by Geant4 EM working group, first of all, by adding more experimental data and more use-cases for validation. The structure of the testing software allows easy additions.

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Figure 4. Geant4 simulation of the depth dose profile of 0.5 MeV electron beam in Molybdenum: points – Sandia data [17], curves – different Geant4 options for electron scattering. Single scattering model (magenta) reproduce the data, Option3 of EM physics (yellow) uses the most strong step limitation, fastest variant EMV (green) uses the most weak step limitation.

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