

GEANT4 and its validation

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GEANT4 is an object-oriented toolkit for simulating the passage of particles through matter. At the very heart of GEANT4 there is a wide set of complementary, and sometimes alternative, physics models which describe the basic interaction of particles with matter. After a review of the main characteristics of the toolkit and a status report of the current activities, the results of a series of detailed tests for the quantitative validation of the electromagnetic models of GEANT4 are presented. Such precision tests demonstrate the reliability of the physics models provided in GEANT4 and are hence particularly relevant for critical applications of simulation models.

1. Introduction

GEANT4 is an object-oriented (OO) toolkit for the simulation of the interaction of particles with matter [1]. The physics processes it provides (hadronic, electromagnetic and optical) cover a comprehensive set of particles and materials over a wide range of energy. Besides the physics, it also offers a complete set of functionality, like tracking, visualisation and geometry description. GEANT4 has been developed by a large worldwide Collaboration and created exploiting a rigorous software engineering and OO approach. The GEANT4 kit, that can be publicly downloaded from the web [2], includes the C++ source code, an extensive documentation and several tutorial examples, showing complete applications of GEANT4 to realistic experimental set-ups. The toolkit can be installed on several supported platforms (Linux, SUN, Windows). It does not require any commercial software, though it can be interfaced with some for specific applications, and it relies on free software only (e.g.

CLHEP libraries). Moreover, it can be interfaced with several visualisation tools, like DAWN [3] and VRML.

Physics is managed in GEANT4 through a set of abstract interfaces. This solution, which is related to the OO approach, makes tracking independent from physics and allows to treat in a uniform way both the electromagnetic and hadronic processes, as they all share the same set of abstract interfaces. A key point in GEANT4 is the clear distinction between the physics processes and the models that are used to describe them. This offers the possibility to have multiple independent models (alternative or complementary) for the same physics process. The users have hence the complete freedom to choose in their own codes those models that best match their needs (i.e. energy range, precision vs. CPU time). The physics in GEANT4 is an open system, in the sense that the users can easily create and use their own customised models.

Thanks to the flexibility of GEANT4 and the availability of dedicated physics models (e.g. for

low energy), the toolkit is widely used from different experimental communities, ranging from HEP and accelerator physics to astroparticle physics, astrophysics and medical physics. The requirements from the users concerning extensions of the physics models or other capabilities are continuously collected, tracked and updated.

2. The activities in progress

The current activities of GEANT4 are particularly focused on the improvement and the extension of the physics content.

The main upgrade of the last year in the electromagnetic physics package, which can handle the electromagnetic interactions of leptons, γ rays, optical photons, hadrons and ions, is the implementation of the cut-per-region approach: from version 5.2 it is possible to set different thresholds for the production of the secondaries (e^+ , e^- and γ) in different regions of the detector. This capability is particularly useful when the precision required for the Monte Carlo tracking is different in different parts of the experimental setup (e.g. vertex detectors and calorimeters). The GEANT4 electromagnetic package provides both high-energy physics models (from 1 keV up to 100 TeV), that are fundamental for accelerator and cosmic rays experiments, and specific low-energy models (down to 250 eV), that include atomic and shell effects and are hence appropriate for space science, medical and astroparticle physics applications. The most recent developments in the standard (= high energy) electromagnetic package have been the improvements of the models for the multiple scattering, for the μ interactions (ionisation and pair production) and for the scintillation and transition radiation. Moreover, a re-design of the software has been performed in order to allow multi-model approach for the standard electromagnetic processes starting from version 6.0.

The Low Energy Electromagnetic (LowE) package provided in GEANT4 includes specific low-energy models (down to 250 eV) for the description of the electromagnetic interactions of electrons, γ -rays, protons, antiprotons and ions. At least two alternative and independent set of mod-

els are presently available for the processes of the lowE package. A complete set of dedicated and original low-energy electromagnetic models has been obtained by re-engineering the Penelope code [4] in GEANT4. Penelope (PENetration and ENERGY LOSS of Positrons and Electrons) is a FORTRAN77 Monte Carlo code for the simulation of electromagnetic showers which can handle electrons, γ -rays and positrons. The flexibility in the extension and in the implementation of new models is the direct result of the use of OO-technology, as all processes do obey to the same abstract interfaces. The other lines of development in the lowE package are related to the angular distribution of the bremsstrahlung photons, for which 3 independent and dedicated low energy generators ($E < 500$ keV) are available, and to the PIXE (particle-induced x-ray emission). The first implementation of a new data-driven approach for PIXE in the energy range from 5 keV to 500 MeV and atomic number between 6 and 92 will be released in the forthcoming 6.2 version of GEANT4. The GEANT4 hadronic package handles the hadronic interactions of hadrons and ions, as well as the interactions of leptons and photons with nuclei. In recent times several models, both data-driven and theory-driven, were implemented or improved (binary cascade, Bertini cascade, low energy interactions of strange particles and antiparticles, elastic scattering recoils, etc). The databases for photon evaporation, radioactive decay and π cross sections were extended and a lot of minor improvements were also performed. Moreover, a set of educated guess physics lists [2] for hadronic physics and for different specific applications (calorimetry, dosimetry, air showers, etc.) is presently available through the GEANT4 website

Though the main developments lines are focused on the physics models, a large activity is also carried out on the kernel and on the other tools of GEANT4, in order to improve the performance and the robustness. In particular, the Run Manager was recently re-designed to allow a better modularisation and to accommodate the cut-per-region approach. Several improvements were performed in the Geometry and Visualisation packages (e.g. addition of G4Division, possibility to

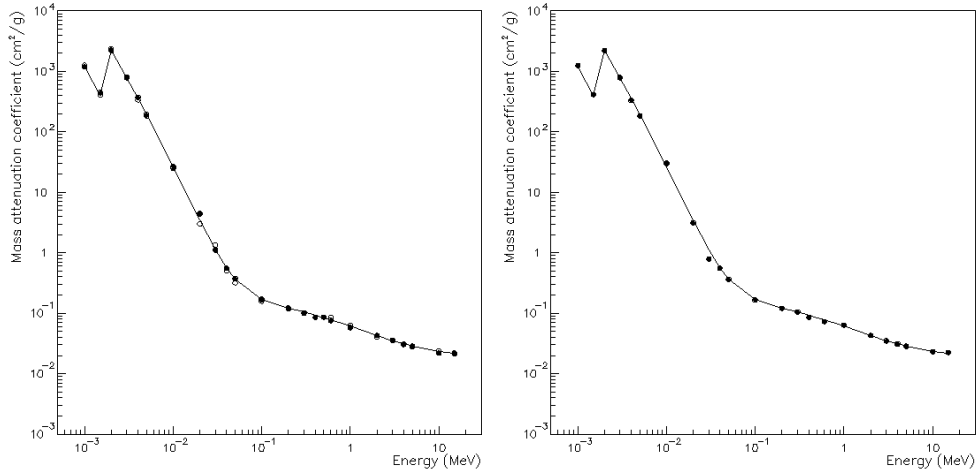


Figure 1. Mass attenuation coefficient vs. energy for γ rays in Al from GEANT4 simulations, superimposed with reference data (solid line) from the NIST database. Left: Low Energy (\bullet) and Standard (\circ) models; Right: Penelope models. A χ^2 test has been used to quantify the agreement of the simulated and the experimental distributions: the p -values are 0.08 for reference data vs. GEANT4 simulation with Standard models, 0.87 for data vs. LowE models and 0.63 for data vs. Penelope models.

visualise boolean solids). In addition, new techniques for event biasing have been implemented and the performances for the tracking of charged particles in electromagnetic fields have been enhanced.

Finally, a new project has been recently launched for a GEANT4 Physics Book, with the main aim to provide a solid and comprehensive reference on all the physics models included in GEANT4, focusing in particular on their validation.

3. Validation

A systematic and extensive validation of the whole physics content of the toolkit is clearly fundamental in order to guarantee the reliability of the GEANT4-based simulations. Two different levels of validation can be distinguished, testing respectively

1. microscopic quantities of the various elementary processes, as cross sections, angular/energy distributions, attenuation coefficients,

stopping powers, CSDA ranges, etc.;

2. macroscopic quantities coming from use cases, i.e. from the simulation of complete experimental set-ups.

At each of the two testing levels, the results of the GEANT4 simulations are compared with established and authoritative reference data (wherever they exist), taken possibly from open and recognized databases (NIST, ICRU, etc.) or from publications on refereed journals. The agreement between the simulations and the reference data must be tested in a quantitative way, making use of suitable statistical tools [5].

3.1. Microscopic analysis

The complete validation of the GEANT4 models requires specific tests on several microscopic quantities, as the integral cross section, the angular/energy distribution or the multiplicity of the final state, the attenuation coefficient, the stopping power, etc. Of course, the validation must

be performed, for each single model, in systematic way and for a wide range of energies and materials. On the other hand, this huge amount of work, which is heavily CPU-demanding and time-consuming, requires a flexible automatic system, both for the submission of the simulation jobs and for the comparison with reference data [5].

The analysis is currently focused on the electromagnetic physics: the 3 sets of models (standard, lowE and Penelope) describing the interactions of photons, electrons and positrons have been extensively tested and validated against experimental data provided by NIST [6].

Fig. 1 shows for instance the mass attenuation coefficient versus energy for γ rays in aluminum in the energy range 1 keV – 100 MeV. The results coming from the simulations with the GEANT4 Standard, Low Energy and Penelope photon models have been compared with reference data from NIST; the agreement of distributions has also been quantitatively evaluated using χ^2 -based statistical tests.

Similarly, Fig. 2 shows the angular distribution of 15.7 MeV electrons transmitted through a thin slab of gold (18.66 mg/cm²) and Fig. 3 the backscattering coefficient for electrons versus the atomic number. Also in these cases, there is a good agreement between the simulations and the data.

A similar work is currently in progress for the validation of the electromagnetic models for protons, α particles and ions. A further step will then involve the systematic quantitative validation of the hadronic physics models.

3.2. Macroscopic analysis

The validation at the macroscopic level consists on the simulation of complete detector setups and on the comparison of the results with the corresponding experimental data. In this case the models contained in the physics list act together and it is possible to test at the same time also the geometry and the tracking of GEANT4. The validation at macroscopic level needs more care with respect to the microscopic one because, for instance, it is sometimes necessary to disentangle in the simulation the effects of physics from those of geometry or detector response. On the

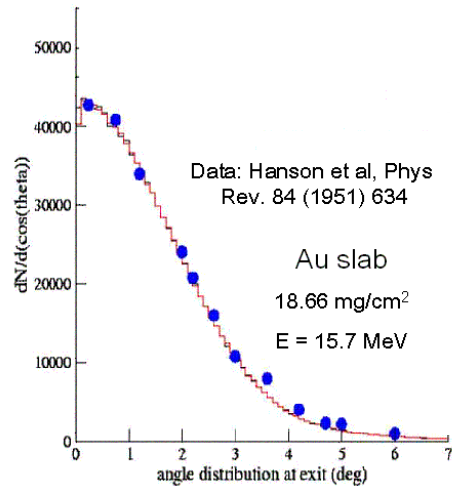


Figure 2. Angular distribution of electrons with energy 15.7 MeV transmitted through a gold slab of thickness 18.66 mg/cm². The distributions coming from the GEANT4 simulation (histogram) are superimposed with the reference data (●).

other hand, in most cases one also has to understand and evaluate the systematic errors of the reference data. The realistic and accurate simulation of a complex experiment requires the detailed knowledge of the detector, so macroscopic validation tests must be carried on in a close collaboration of GEANT4 developers and research groups. It is certainly of great importance to take into account experiments and detectors referring to different scientific communities (accelerator physics, astroparticle physics, space science, medical physics), in order to verify the reliability and suitability of the GEANT4 models in different energy ranges and experimental areas. A few of the many available examples of these applications are described below.

In the context of accelerator physics, GEANT4 has been used to simulate the electron response in the ATLAS calorimeters and the results have been compared with the corresponding test-beam data. It turns out (see Fig. 4) that GEANT4 can simulate very well (better than the old GEANT3

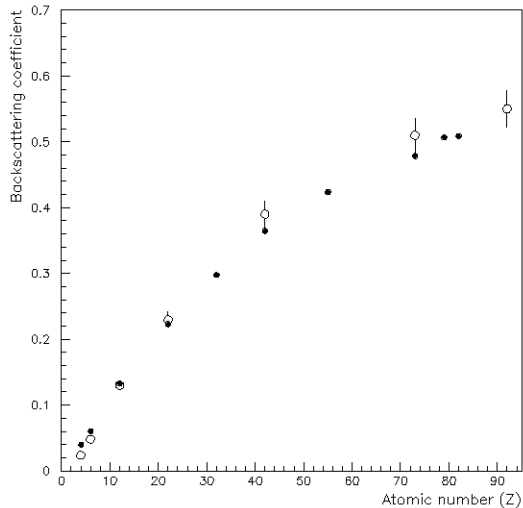


Figure 3. Backscattering coefficient for 100 keV electrons vs. atomic number. The GEANT4 simulations with the lowE electron models (\bullet) is superimposed with the experimental data (\circ) from Lockwood *et al.*, Sandia Lab. Tech. Rep. SAND80-1968 (1981).

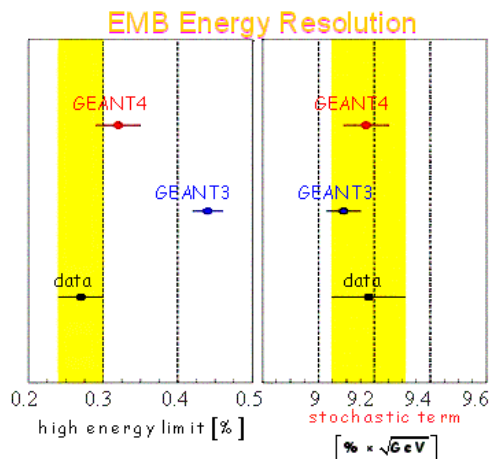


Figure 4. Electron energy resolution in the ATLAS electromagnetic calorimeter. The results obtained with the GEANT4 and GEANT3 Monte Carlo simulations are compared with the experimental data from test-beam.

code) the average electron signal as a function of incident energy in all the ATLAS calorimeters [7]; moreover, the signal fluctuations in the electromagnetic barrel are also corrected reproduced. The agreement of GEANT4 simulations with experimental data in the accelerator physics domain has been extensively verified taking into account a great number of test-beam measurements, provided mainly from the ATLAS, CMS and LHCb groups at CERN and from the BaBar group at SLAC.

A further macroscopic validation test of GEANT4, in a completely different physics domain, has been performed in the context of planetary astrophysics. From an application developed for the characterisation of the rocks composition of Mercury [8] in the Bepi-Colombo mission of European Space Agency, GEANT4 has been able to reproduce with great accuracy the measured fluorescence emission from pure and composite materials irradiated with an electron beam of continuous energy spectrum (see Fig. 5).

An other example of validation, involving a different experimental domain, has been carried out in the framework of the CATANA project [9], which is devoted to the eye cancer therapy with proton beams. The GEANT4 simulation of the Bragg peak of 62 MeV protons in water (see Fig. 6) has been successfully validated against dedicated experimental data collected at the INFN Laboratori Nazionali del Sud proton beam [10].

4. Conclusions

The GEANT4 toolkit encompasses an ample set of physics models, specialised for particle type, energy range and detector applications, and of functionality, ranging from geometry to tracking, visualisation and event biasing. All those components are continuously tested and upgraded in order to improve the robustness and the performances of the toolkit. The physics content is subject to a systematic validation process, both at the microscopic and macroscopic level, in order to monitor the physics performance and to ensure a highly-reliable simulation toolkit. This is a major effort, involving many people, sites and collabo-

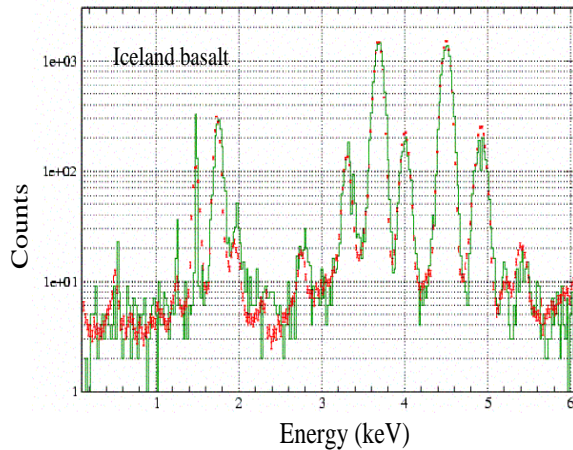


Figure 5. Fluorescence emission from Iceland basalt rocks irradiated with an electron beam.

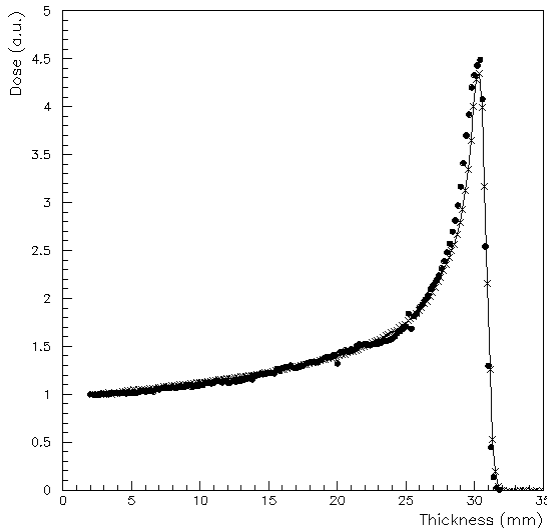


Figure 6. Bragg peak depth position for 62 MeV protons on water. Experimental data (\times and solid line) from the Laboratori Nazionali del Sud, Italy, simulation (\bullet) with GEANT4 lowE.

rating groups, that triggered the development of a new general toolkit for statistical analysis and a system for test automation.

An extensive set of results (plots and quantitative goodness-of-fit values) for the electromagnetic processes is presently available from the microscopic tests of basic physics distributions. Moreover, many significant contributions to the validation of GEANT4 physics at the macroscopic level come from test-beams and user applications in the experiments, from different domains of physics research.

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