Geant4 Low Energy Electromagnetic Physics

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***Abstract*— The Geant4 Simulation Toolkit includes a specialised package, implementing a precise treatment of electromagnetic interactions of particles with matter below 1 keV. The Geant4 Low Energy Electromagnetic package provides a variety of models describing the electromagnetic processes of electrons and positrons, photons, charged hadrons and ions, taking into account detailed features, such as atomic shell effects and charge dependence. These features are relevant to several experimental domains, such as astrophysics, space science and bio-medical research, and have enabled new simulation studies beyond the conventional applications of Geant4 in high energy physics. The design of the package and the physics models implemented are presented.**

I. Introduction

THE precise simulation of electromagnetic interactions of particles with matter is a critical requirement in various experimental fields. In radiotherapy very precise simulation of the energy loss in tissue of both the incident particles and their secondary particles is required. To maximise patient safety, accurate knowledge is needed of the 3-dimentional distribution of the radiation dose within small volumes, implying low energy production thresholds and small step lengths in particle tracking. In space instrumentation, on the other hand, reduction in component size has led to higher susceptibility to the so-called Single Event Upsets. These phenomena are primarily due to incident protons and ions in space, and are characterised by large energy deposits in small sensitive volumes, particularly near the end of the particle track. Such phenomena usually cause memory bit-flips, and may result either in a temporary operational glitch of an instrument in the spacecraft or, in the worst case, in the deterioration of the capabilities of an entire mission. The detailed simulation of secondary effects, such as the atomic relaxation resulting from a vacancy in an atom left by a primary interaction process, is required in a variety of applications investigating material composition from the spectrum of their characteristic X-rays. More in general, an accurate simulation of electromagnetic processes is useful for precision studies of tracking detectors in high energy and nuclear physics experiments.

All such experimental research problems can profit of a versatile software instrument for the simulation of the experimental configuration and the study of radiation effects, offering precise models of electromagnetic processes down to low energies for any particle type.

The Geant4 [1] Simulation Toolkit includes a series of packages for the simulation of electromagnetic interactions of particles with matter, specialised for different particle types, energy range or approach in physics modelling. Among them, the *Low Energy Electromagnetic* package [2] provides implementations of physics processes for electrons, photons, charged hadrons and ions, extended down to lower energies (< 1 keV) than those included in the so-called *standard* Geant4 package, the one first developed in Geant4.

Like other general-purpose Monte Carlo codes, Geant4 can deal with electromagnetic interactions down to 1 keV. The *standard* package, implementing electromagnetic processes down to 1 keV, has been released as part of the Geant4 Toolkit since its first public version in 1998. Specialised codes for the simulation of electromagnetic interactions at low energies have been available to the scientific community; however, apart from the restriction of particle types they can track, these

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specialized systems lack the detector modelling capabilities and wide functionality offered by general-purpose simulation systems.

Geant4 Low Energy Electromagnetic package represents a significant improvement with respect to other simulations of electromagnetic interactions available to the experimental community: for the first time, it offers the precise physics modelling typical of specialized simulation codes in a general-purpose Monte Carlo system. Moreover, the toolkit architecture of Geant4, allowing the user to select the components he/she actually needs for his/her specific application, out of all those available in the toolkit, does not impose any unnecessary complexity to small applications; therefore, the power of precise electromagnetic models is made accessible to agile simulations for simple experimental configurations, as well as to the complex simulation systems of large scale experiments.

II. Architecture and General Features

A. *Object oriented design*

The architecture of the Low Energy Electromagnetic package exploits the opportunities offered by Geant4 flexible design and by the object oriented technology.

Geant4 design makes particle tracking independent from the physics processes particles are subject to. All processes are handled by tracking transparently through an abstract interface, *G4VProcess*. Therefore, thanks to the object oriented technology, it is possible to extend Geant4 physics capabilities, providing new processes, or new models of a given physics process, as classes inheriting from the *G4VProcess* class, without affecting Geant4 kernel or existing user applications. The Low Energy Electromagnetic package, providing new implementations of electromagnetic processes, has been developed as a further extension to Geant4 first release, originally encompassing the *standard* electromagnetic processes.

Geant4 distinguishes two base classes, *G4VDiscreteProcess* and *G4VContinuousDiscreteProcess*, both derived from *G4VProcess*, relevant to electromagnetic processes. *G4VDiscreteProcess* acts as a base class for describing positron annihilation and photon interactions: the photoelectric effect, the Compton (incoherent) and Rayleigh (coherent) scattering, the pair production.

G4VContinuousDiscreteProcess represents a base class for the processes describing the interactions of charged particles: ionisation and Bremsstrahlung.

The architectural design of the Low Energy Electromagnetic package is illustrated in Fig. 1.

B. *Overview of the physics models*

The Geant4 Low Energy Electromagnetic package handles the physics processes of photons (photoelectric effect, Compton scattering, Rayleigh scattering and pair production), electrons (ionisation and Bremsstrahlung) and positrons (annihilation, as well as the same processes as of electrons).

Two different modelling approaches are provided for electron and photon processes: models based on evaluated data libraries and analytical models. Positrons are handled by analytical models only.

X-ray fluorescence and Auger electron emission from excited atoms are also generated.

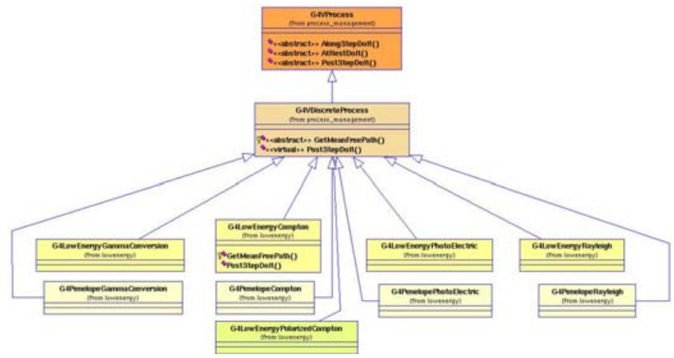

Fig. 1. The architectural design of Geant4 Low Energy Electromagnetic package.

III. Simulation of Interactions of Photons, Electrons and Positrons.

A. *The parameterised models*

The parameterised models for photon and electron processes are based on the exploitation of evaluated data libraries, EEDL (Evaluated Electrons Data Library) [3] and EPDL97 [4] (Evaluated Photons Data Library), that provide data for the determination of cross-sections and the sampling of the final state.

These libraries provide the following data relevant to the simulation, for elements with atomic number between 1 and 99: total cross sections for photoelectric effect, Compton scattering, Rayleigh effect and Bremsstrahlung; sub-shell integrated cross sections for photoelectric effect and ionization; energy spectra of the secondary particles for electron processes; scattering functions for the Compton effect; form factors for the Rayleigh effect.

The energy range covered by the data libraries extends from 100 GeV down to 1 eV for the Rayleigh and Compton effects, down to the lowest binding energy for each element for the photoelectric effect, down to 10 eV for Bremsstrahlung and down to the lowest sub-shell binding energy for each element for ionization. The current implementation of Geant4 Low Energy electron and photon is, in principle, usable over the same energy range covered by the data libraries; however, because of the degradation of the accuracy of the library themselves and of the intrinsic limits of the material properties modelling at lower energies, it is recommended to use it for energies above 250 eV.

All processes involve two distinct phases: the calculation of interaction cross sections and the generation of the final state.

For each process the total cross section at a given energy *E* is obtained by interpolating the data provided by the evaluated library, according to a logarithmic interpolation algorithm. For performance reasons, the processes build and store in memory look-up tables for the calculation of the particle mean free path, of coarser granularity than the data libraries. The precision of the interpolation through these re-formatted tables, with respect to the original data, is better than 1%.

The four-momenta of the final state products of the processes are determined according to distributions derived from the evaluated data. The energy dependence of the parameters characterizing the sampling distributions is taken into account either by interpolation to the data available in the libraries directly, or by interpolation to values obtained from fits to the data.

Particular attention is paid to reproduce precise final state distributions, which are especially relevant at low energies.

In the Compton scattering the scattered photon energy is distributed according to the product of the Klein-Nishina formula times the scattering functions. The scattering functions $F(q)$ at the transferred momentum $q = E \cdot \sin^2(\theta/2)$ corresponding to the energy E are calculated from the values available in the EPDL97 data library. The angular distribution of the scattered photons is obtained from the same procedure.

In the Rayleigh scattering process the angular distribution of the scattered photon is described by $F(E,q)=[1+\cos^2(q)]\cdot F^2(q)$, where $q = E \cdot \sin^2(\theta/2)$ is the transferred momentum corresponding to energy E and F(q) is the form factor. Form factors are obtained from the EPDL97 data library; their dependence on the momentum transfer is taken into account by interpolating the library data.

An example of precise simulation of photon interactions based on Geant4 Low Energy Electromagnetic parameterized models is shown in Figure 2, where shell effects are evident.

B. *The analytical models*

The complete set of physics models originally implemented in the FORTRAN Monte Carlo Code Penelope [6] has been reengineered into Geant4 Low Energy Electromagnetic package, with the only exception of the multiple scattering process, for which Geant4 provides an original, advanced model in its standard electromagnetic package. The easy inclusion of these models into the package demonstrates the versatility of the object oriented technology, which facilitates the provision of alternative physics approaches, all handled transparently through the same abstract interfaces, without affecting the existing code.

The analytical models of the Compton scattering offers two additional features with respect to the corresponding parameterised model: Doppler broadening and the atomic relaxation resulting from the vacancy generated by the primary scattering.

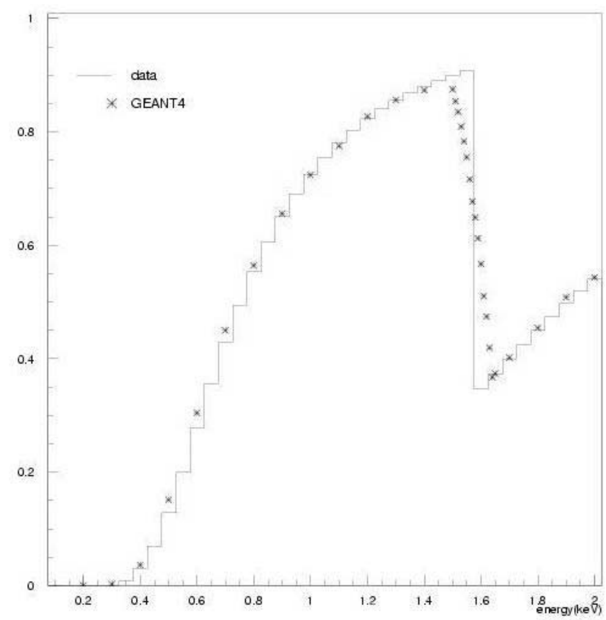

Fig. 2. Simulation of photon transmission in 1 μm Al layer, showing the evidence of shell effects; the solid line represents experimental data from[4], the dots are the simulation results with Geant4 Low Energy Electromagnetic package.

IV. Simulation of the Interactions of Charged Hadrons and Ions

At relatively high energies the mean value of the continuous energy loss is given by the restricted Bethe-Bloch formula [7].

For a velocity of a charged hadron $\beta<0.05$, corresponding to approximately 1 MeV for protons, the Bethe-Bloch formula becomes inaccurate. In that case the velocity of the incident hadron is comparable to the velocity of atomic electrons. At very low energies, when $\beta<0.01$, the model of a free electron gas [8] predicts the stopping power to be proportional to the hadron velocity, but it is not as accurate as the Bethe-Bloch formalism at higher energies. The intermediate region $0.01 < \beta < 0.05$ is not covered by precise theories; this energy interval is relevant for effects in detectors and dosimetry applications, since the Bragg peak of ionisation loss occurs here. Various authoritative reviews [9]-[12] have established procedures to evaluate the existing experimental data and to determine fitting functions depending on few phenomenological parameters, which describe the stopping power for protons from 1 keV to 1 GeV.

The Geant4 Low Energy Electromagnetic package adopts a flexible modelling approach, to take into account the body of knowledge available in this field. The design is shown in Figure 3.

The G4hLowEnergyIonisation process handles the ionisation by hadrons and ions. It adopts different models depending on the energy range and the particle charge. In the high energy domain (E > 2 MeV) the Bethe-Bloch formula and in the low energy one (E < 1 keV for protons) the free electron gas model are applied respectively. In the intermediate energy range parameterized models based on experimental data from the Ziegler [9] [10] [11] and ICRU [12] reviews are implemented; corrections due to the molecular structure of materials and to the effect of the nuclear stopping power are taken into account. The Barkas effect is taken into account; a specialized quantum harmonic oscillator model for negative charged hadrons, valid down to 50 keV, is implemented. Figure 3 shows a comparison with experimental data for ions.

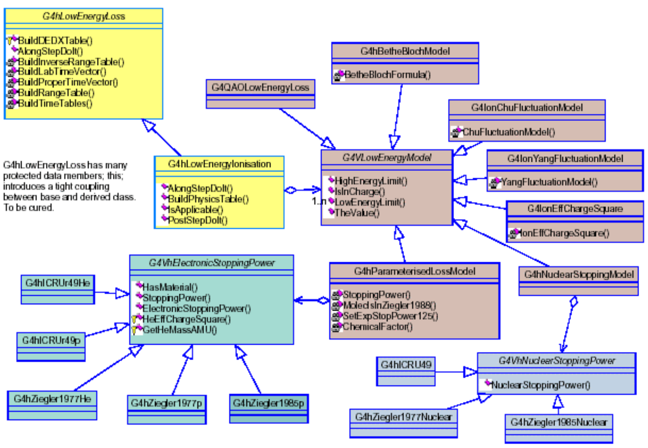

Fig. 3. Object oriented design of hadron physics modeling in Geant4 Low Energy Electromagnetic package.

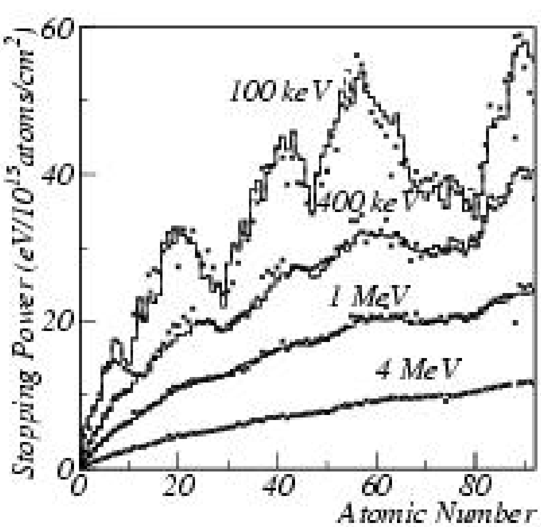

Fig. 4. Stopping power of protons for elements with atomic number up to 93, at proton energy of 100 keV, 400 keV, 1 MeV and 4 MeV, for various parameterisation models implemented in Geant4: the dots represent Ziegler-85 parameterisation [9], the solid line is ICRU-93 **Error! Reference source not found.** parameterisation, the dashed line is Ziegler-77 **Error! Reference source not found.** parameterisation. ICRu-93 and Ziegler-77 parameterisation practically coincide.

V. SIMULATION OF ATOMIC RELAXATION

A component of the Low Energy Electromagnetic package is responsible for the atomic relaxation. It handles the atomic de-excitation following processes leaving an atom in an excited state, with the generation of X-ray fluorescence and Auger electrons. The simulation of atomic relaxation in Geant4 is described in detail in another paper [13] of these Proceedings.

VI. SOFTWARE PROCESS

A rigorous approach to Software Engineering plays a fundamental role in Geant4 Low Energy Electromagnetic package. The general guidelines of Geant4 software process [14] are adopted, and a software process specifically tailored to the project has been optimized.

User Requirements have been formally collected, and are systematically reviewed and updated following the PSS-05 [15] framework standards. Object-Oriented methods - and the respective tools - have been employed for the analysis and design of the software, and to produce the corresponding deliverables. By adopting object oriented methodologies and quality assurance techniques, one ensures that the code quality will not degrade with time; a coherent development is also facilitated, where coupling will not increase with the complexity of the software. The software process adopted in the development of Geant4 Low Energy Electromagnetic Physics, based on the Unified Software Development Process [16] framework, is described in detail in another paper [17] of these proceedings.

The software process is complemented by a goal-directed project management. Extensive interaction with the user communities ranges from the collection of user requirements to collaboration in validation of the simulation models and code by comparison to experimental data.

VII. TESTING AND VALIDATION

Testing procedures are applied extensively, both at granular unit level and integration level. Physics validation is performed by comparison to experimental data, over a wide set of use cases. The validation of the Geant4 Low Energy Electromagnetic package is described extensively in another paper [18] of these proceedings.

VIII. CONCLUSIONS

The Geant4 Low Energy Electromagnetic Physics package provides powerful and versatile tools for the simulation of particle interactions with matter down to low energies. Accurate models, specialized for particle type and energy range, are available for the calculation of the cross sections of the physics processes and for the generation of the final state distributions. The object oriented technology adopted for the design of the package has demonstrated an essential tool to provide alternative and complementary physics models within the same package. A rigorous software process ensures the quality of the software; extensive validation tests demonstrate the behaviour of the simulation models against established references.

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