New Geant4 Developments for Doppler Broadening Simulation in Compton Scattering - Development of Charge Transfer Simulation Models in Geant4

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***Abstract*—Two topics concerning recent developments in the Geant4 toolkit are described: the simulation of Doppler broadening in Compton scattering and of charge transfer of protons interacting with a variety of materials.**

***Index Terms*—Monte Carlo, simulation, Geant4.**

I. INTRODUCTION

TWO extensions of the simulation capabilities in the electromagnetic physics domain have been recently introduced in the Geant4 [1], [2] toolkit. They concern the simulation of Doppler broadening in Compton scattering and models to describe the charge transfer process involving protons. Both these processes are relevant at low energies.

These developments have been first available in Geant4 9.2-beta version released in July 2008.

II. DOPPLER BROADENING IN COMPTON SCATTERING

Doppler broadening is a fundamental limit to the angular resolution of Compton scattering-based telescopes. This effect is also relevant to other experimental domains: for instance, it adds to the effect of finite energy resolution of the detector in Compton cameras used in medical imaging.

Two alternative sets of physics processes for photon interactions are currently included in Geant4 Low Energy Electromagnetic [3], [4] package, respectively based [5] on the EPDL97 [6] evaluated data library and on analytical models originally developed for the Penelope [7] Monte Carlo system.

Geant4 accounted for Doppler broadening in the Compton Scattering process based on Penelope models (*G4PenelopeCompton*); this functionality has been incorporated also into the library-based process *G4LowEnergyCompton*.

An external package [8] had been developed for the simulation of Doppler broadening in Compton scattering for Geant4-based applications, based on the same modeeling approach as [9]; however, this package does not appear consistent with established good object oriented programming practices: for instance, some classes have public data members and the implementation adopts deprecated procedural programming features like the use of "GOTO" statements.

Due to the interest to provide a variety of modelling approaches in Geant4, the implementation in the library-based process has followed a different path than the one in the Penelope-like process: the latter applies a fully analytical method [10], while the new implementation in *G4LowEnergyCompton* exploits the method originally developed in [9] for the EGS4 [12] Monte Carlo code, based on tabulations of so-called "Compton profiles".

A design iteration in the data management sub-domain has been performed to accommodate the new simulation capabilities required for Doppler broadening. Responsibilities for additional functionality associated to the description of atomic properties at the shell level (shell occupancy) have been added to the *G4ShellData* class; the responsibilities of the *G4VEMDataSet* and derived classes have been extended to include the management of random number generations according to the probability density functions associated to predefined physical distributions; capabilities to manage Doppler profile data have been incorporated in a new class used by Compton scattering. Finally, the generation of the final state in the *G4LowEnergyCompton* process has been modified to account for Doppler broadening due to scattering with bound electrons. The same approach has also been included in *G4LowEnergyPolarizedCompton* to account for Doppler broadening in polarized Compton scattering.

An example of the new simulation capabilities is illustrated in Fig. 1; it concerns the energy distribution of photons between 89° and 91° resulting from Compton scattering of 40 keV photons orthogonally impinging onto a silicon target. The broadening of the original distribution resulting from the new implementation of *G4LowEnergyCompton* with respect to the previous version is evident; the figure also report the equivalent distribution produced by the Penelope-like process.

The respective capabilities of the two Doppler broadening algorithms implemented in Geant4 have been evaluated for what concerns the physics and computational performance.

Regards the photon energy distribution, the two methods produce equivalent results: this is illustrated in Fig. 2 to Fig. 4, respectively for 50 keV photons interacting with aluminium and gold, and 500 keV photons interacting with gold. These plots also show the photon energy distribution resulting from the Klein-Nishina [13] formula: the difference of the distributions produced by the two Geant4 Compton scattering processes with respect to the behaviour predicted

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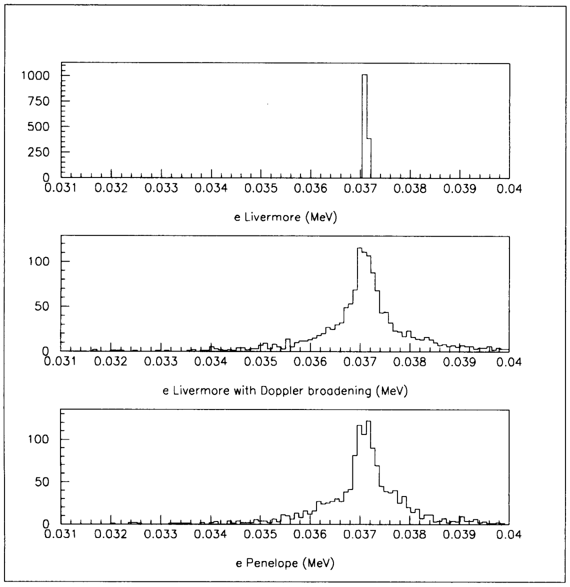

Fig. 1. Energy distribution of photons between 89° and 91° resulting from Compton scattering of 40 keV photons orthogonally impinging onto a silicon target: previous *G4LowEnergyCompton* implementation not accounting for Doppler broadening, new extension of *G4LowEnergyCompton* to model Doppler broadening and Penelope-like *G4PenelopeCompton* process.

TABLE I
COMPUTATIONAL PERFORMANCE OF GEANT4 LIBRARY-BASED AND PENELOPE-LIKE COMPTON SCATTERING PROCESSES

Target	Library-based (s)	Penelope-based (s)	Speed difference (%)
C	5.60	6.08	8.6
Si	6.01	8.37	39.3
Cu	6.17	10.78	74.7
W	7.07	19.18	271.3

by the Klein-Nishina formula is more evident at lower energy.

The computational performance of the final state generation in the two Compton scattering processes was evaluated by measuring the time spent to simulate one million calls to the respective *PostStepDoIt* member function on an Intel Core2 Duo Processor E6420, equipped with a 2.13 GHz processor and 4 GB RAM. The results are summarized in Table I for various materials; the speed difference reported in the table represents the percent difference of execution time of the Penelope-based process with respect to the library-based one. The library-based process is faster than the Penelope-like one; the speed difference increases with the atomic number of the target element. Weak dependence on the photon energy is observed in the energy range relevant to Doppler broadening effects.

III. CHARGE TRANSFER SIMULATION

A new design technique, exploiting policy-based class design [14], was first introduced in Geant4 [15] to model a set of processes specialized for very low energy interactions in water. The new design has been exploited to extend the provision of specialized physics models to other materials than water. This

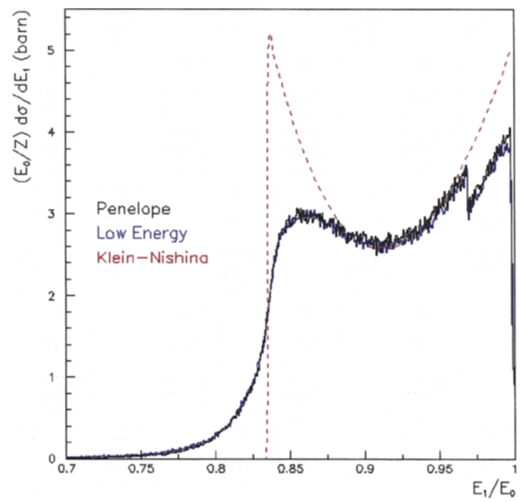

Fig. 2. Differential cross section for Compton scattering vs. energy ratio of scattered photons over incident ones, 50 keV photons impinging onto an aluminum target: *G4LowEnergyCompton* (blue) and Penelope-like *G4PenelopeCompton* (black) process; the red dashed curve represents the result of the Klein-Nishina formula.

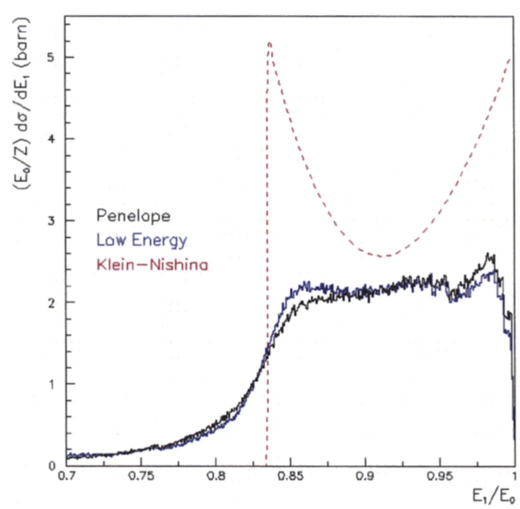

Fig. 3. Differential cross section for Compton scattering vs. energy ratio of scattered photons over incident ones, 50 keV photons impinging onto a gold target: *G4LowEnergyCompton* (blue) and Penelope-like *G4PenelopeCompton* (black) process; the red dashed curve represents the result of the Klein-Nishina formula.

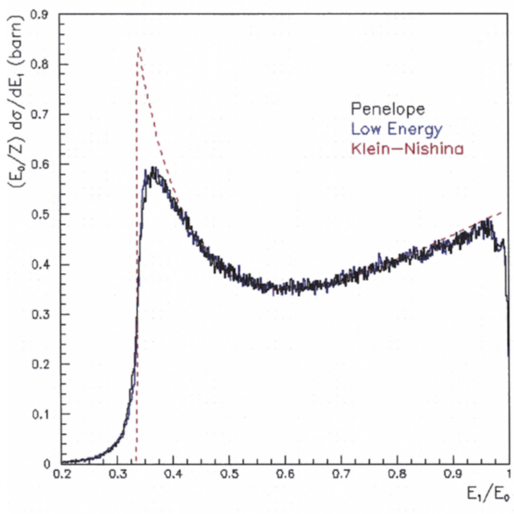

Fig. 4. Differential cross section for Compton scattering vs. energy ratio of scattered photons over incident ones, 500 keV photons impinging onto a gold target: *G4LowEnergyCompton* (blue) and Penelope-like *G4PenelopeCompton* (black) process; the red dashed curve represents the result of the Klein-Nishina formula.

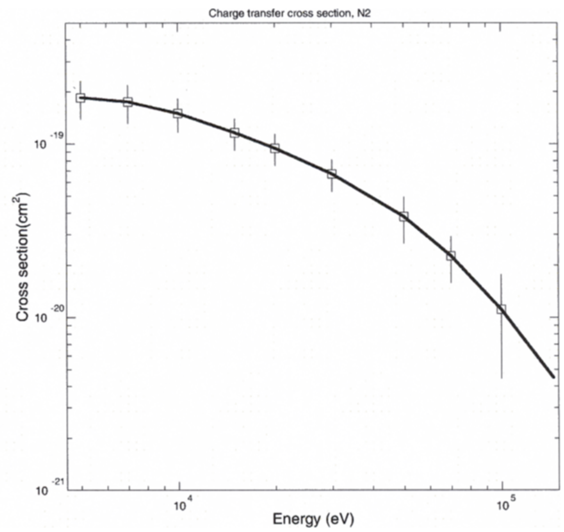

Fig. 5. Cross section for proton charge transfer in interactions with N_2: an example of an analytical cross section model; the black symbols are experimental data from [18].

extension was meant as an investigation of the suitability of the design to address generic materials outside the domain of radiobiology.

To assess the capabilities of the design, a physics domain specific to very low energy has been addressed, concerning the process of charge transfer, Charge transfer, occurring in a very large range of astrophysical environments, can be decisive in establishing ionization structure, energy transfer, and inducing infrared to X-ray radiative relaxation. It is also relevant to plasma interactions in

This process becomes negligible at energies above a few MeV approximately. This kind of interactions has not been handled by Geant4 electromagnetic packages, with the exception of the model developed for proton and α particles (in their charge states) interactions with water.

Little comprehensive data exist for this process. A reference collection is available in the ORNL/UGA Charge Transfer Database for Astrophysics [16], a database for charge transfer reactions of astrophysically important atomic ions with various atoms and selected molecular targets. It gathers experimental and theoretical references from various sources in literature, and encompasses experimental data and analytical parameterisations of cross sections for particle interaction with various materials.

The information available in this database concerning proton interactions has been used to develop new charge exchange simulation models for all the different materials currently included in it, ranging from pure elements to molecules: He, N_2, CO, CO_2, CH, CH_2, CH_3, CH_4, C_2H and C_2H_2.

The new cross section implemented in Geant4 include both data-driven models and analytical ones [17]. A final state model to complement the cross section calculations has been originally developed to complete the simulation of the process.

An example of results of this development is illustrated in Fig. 5 and Fig. 6, respectively for CO and N_2 charge exchange cross sections: the black lines correspond to Geant4 simulation models, while the available experimental data [18]- [22] and theoretical predictions [23] are plotted in white symbols.

IV. Conclusion and Outlook

The capabilities of Geant4 in the electromagnetic physics domain have been extended regards the simulation of Compton scattering and charge transfer processes.

Doppler broadening has been introduced in the library based Compton scattering process and in the corresponding polarized version too. The new implementation has been compared to the previously exiting one of the Penelope-like Compton scattering process: the two modelling approaches produce equivalent physics distributions, but differ significantly in terms of computational performance.

New models for charge transfer concerning protons interacting with a variety of materials have been developed; they appear to describe existing experimental data adequately.

Further developments related to these topics will be pursued in the context of a new project recently launched as part of the INFN research programme, which encompasses design investigations addressing simulation applications in emerging physics domains.

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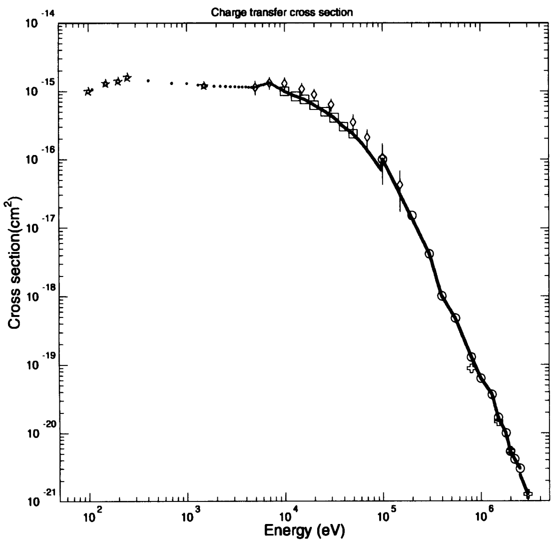

Fig. 6. Cross section for proton charge transfer in interactions with CO: an example of a data-driven cross section model; the black line represents Geant4 simulation model; the white symbols report experimental data in [18]- [22], with the exception of white stars, which correspond to theoretical predictions in [23].

while F. Longo and L. Pandola contributed to the Doppler broadening study only.

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