Validation of Compton Scattering Monte Carlo Simulation Models

Georg Weidenspointner, Matej Batič, Steffen Hauf, Gabriela Hoff, Markus Kuster, Maria Grazia Pia, and Paolo Saracco

Abstract—Several models for the Monte Carlo simulation of Compton scattering on electrons are quantitatively evaluated with respect to a large collection of experimental data retrieved from the literature. Some of these models are currently implemented in general purpose Monte Carlo systems; some have been implemented and evaluated for possible use in Monte Carlo particle transport for the first time in this study. Here we present first and preliminary results concerning total and differential Compton scattering cross sections.

I. INTRODUCTION

Compton scattering is of fundamental importance for hard X-ray and soft γ-ray imaging and polarimetry systems in a wide range of applications in nuclear science, astronomy, medical science, radiation safety, or homeland security. It is the dominant interaction process of photons with matter at hard X-ray and soft γ-ray energies. The inelastic scattering of photons on electrons was discovered in 1923 by A.H. Compton [1]; for stationary and free electrons, the relativistic theory of this process was presented in 1929 by O. Klein and Y. Nishina [2]. When considering the scattering of photons in matter, electrons are neither stationary nor free, rather they are bound to atomic nuclei and possess non-zero orbital momentum. For photon energies below a few 100 keV, the effect of electron binding is not negligible for inelastic scattering and can be described by a so-called incoherent scattering function (see e.g. [3]).

Compton scattering is simulated by all general purpose Monte Carlo systems that model the transport of photons and other particles in matter (e.g. EGS [4], FLUKA [5], Geant4 [6, 7], ITS [8], MCNP [9], and Penelope [10]). Nevertheless, an objective, quantitative evaluation of the physical accuracy of Compton scattering simulation models is not yet documented in the literature. The validation of Compton scattering models implies their comparison with experimental data [11].

The accuracy of simulation models can then be objectively quantified based on rigorous statistical analysis.

The validation of Compton scattering models presented here is part of a larger effort to validate photon interaction simulation models for general purpose Monte Carlo systems. An overview can be found in [12], validation results for photon elastic scattering have been reported in [13], preliminary results for photo-ionization and electron-positron pair production were presented at this conference (see [14], [15]).

In this article, we present first and preliminary validation results concerning a variety of models for total and differential Compton scattering cross sections, with emphasis on those implemented in Geant4, with respect to a large collection of experimental data retrieved from the literature.

II. COMPTON SCATTERING IN GEANT4 9.6

Geant4, as of version 9.6, currently implements 10 Compton scattering models, and physics processes that use these models. An overview of the models and their dependencies is given in the UML (Unified Modeling Language) class diagram shown in Fig. 1. As is indicated in the class diagram, these models can be subdivided into four general physics scenario categories: standard, low-energy, polarized and adjoint. The following discussion, which summarizes observations on the code with respect to good design practices as given e.g. by Fowler [17], considers only the first two models, as they constitute the most common application scenarios.

The Geant4 “standard” electromagnetic package encompasses two classes implementing Compton scattering models based on the Klein-Nishina [2] approach: G4KleinNishinaCompton and G4KleinNishinaModel. These models are selectable for usage by the G4ComptonScattering process, which is derived from G4VEmProcess, which in turn is a concrete implementation of the G4VDiscreteProcess base class encompassed in the Geant4 kernel. Additionally, a G4HeatedKleinNishinaCompton model is present, which can be used to simulate comptonization in a hot plasma. It does not appear to be documented in the Geant4 physics reference manual [16] and will not be further discussed here.

The initially mentioned two models are in fact very similar, in that they duplicate code for an empirically parameterized cross section calculation [16] derived from theoretical tabulations by [18], [19]. They differ in the final state generation. G4KleinNishinaModel handles the atomic relaxation following the emission of an electron from the target atom by delegating it to G4AtomicDeexcitation, while G4KleinNishinaCompton does not take into account atomic relaxation. The code dupli-
For applications which require the simulation of Compton scattering at lower energies than the 10 keV limit documented for the “standard” models [16], the Livermore- and Penelope-based Compton scattering models can be used.

In Geant4 9.6 these models consist of G4LivermoreComptonModel, G4LivermoreComptonModifiedModel, G4LowEPComptonModel and G4PenelopeComptonModel. Here the first three models implement a cross section calculation based on the EPDL data library [22], while the latter uses an approach reengineered from the Penelope code [25].

In their final state generation the Livermore-based models describe the scattered photon distribution using a scattering function as given by Cullen [24]. G4LivermoreComptonModel and G4LivermoreComptonModifiedModel differ in the modeling of the scattered electron, whereas G4LowEPComptonModel adds a fully relativistic treatment to the final state generation using the Relativistic Impulse Approximation (RIA) [16, 26]. Across all Livermore-based models, code duplication is again a major issue. The code has been fully duplicated for the cross section calculation, and partially duplicated for the final state generation.

### III. Refactored Software

The software design has been refactored based on a sharp domain decomposition, which identified total cross section calculation and final state generation as two distinct entities of the problem domain. A policy-based class design [20] has been adopted: it ensures flexibility at endowing the Compton scattering process with multiple behaviours based on a variety of alternative modeling approaches, while the intrinsic simplicity, restricted responsibilities, and minimized dependencies of policy classes facilitate the testing of the software both in the processes of verification and of validation. The same software design approach has been successfully adopted in the simulation of photon elastic scattering [21]. The physics functionality of policy classes can be tested by means of simple unit tests, whereas the design of the Compton models in Geant4 9.6 hinders testing the physics functionality of the models outside a full simulation environment. The main features of the refactored software design, which does not alter physics functionality, are illustrated in the UML class diagram of Fig. 2.
Fig. 2: A UML class diagram of the refactored policy-based design for Geant4 Compton scattering. Policy classes for final state and cross section generators are bound to the G4TCompton host template class.

In the first development cycle documented in this paper three total cross section policies were implemented, which correspond to the three uniquely distinct modeling approaches documented in Section II: standard (empirical fit to [18], [19]) , EPDL-based and Penelope-based (Penelope).

Similarly, three differential cross section policies were implemented, which correspond to three distinct methods used to sample the scattered photon angular distribution implemented in Geant4: according to the Klein-Nishina formula, according to the Klein-Nishina formula multiplied by a scattering function, and according to the method reengineered from Penelope. In addition to the tabulated scattering function data of EPDL, which are used by Geant4, scattering function tabulations based on work by Brusa et al. [27], Biggs et al. [28], and Hubbell et al. [29] were reformatted to be used by the above mentioned policy class, and included in the validation of differential cross sections. The tabulations identified as “Hubbell” and as EPDL are based on the same calculations [29], but they differ in the $\sin(\theta/2)$ values at which scattering functions were calculated.

IV. Data Extraction

A. Experimental Data

The experimental data were extracted from the literature, yielding 230 data points for total cross sections and 2612 data points for differential cross sections for elements ranging from hydrogen ($Z = 1$) to uranium ($Z = 92$).

For this preliminary analysis the data have been extracted into tabular format and converted to units of barn or barn/sr whenever necessary and appropriate. Cross sections derived from subtracting theoretically calculated photoelectric and elastic scattering contributions from total photon attenuation coefficient measurements were excluded from the validation analysis. The tabular format is such that data are accessible by incident photon energy as well as scattering angle. A full screening for and removal of outliers, as well as a consistency check of experimental uncertainties, has not yet been performed for this conference contribution, but will be included in our final analysis.

B. Simulation models

Total and differential cross sections for the incident photon energies, scattering angles and target elements covered by the experimental data were obtained by means of unit tests.

For the validation of total scattering cross sections unit tests were done for the three distinct policy classes described in Section II: standard (empirical fit to [18], [19]), EPDL-based and Penelope-based (Penelope). Similarly, the validation of differential cross sections involved unit tests associated with the three options mentioned in Section III. In addition to using scattering functions tabulated in EPDL, unit tests were performed using the aforementioned alternative scattering functions.

V. Validation Strategy

For the validation the different models have been compared to the individual experimental data points using a $\chi^2$ goodness-of-fit test. If the $p$-value of a given test exceeded a significance value of $\alpha = 0.01$, i.e. $p(\chi^2) \geq \alpha$, the test was classified as passed, i.e. the model was considered compatible with the data. In cases where $p(\chi^2) < \alpha$ the test was considered as failed, i.e. model and data were considered incompatible. The efficiency of a given cross section model is then determined by the fraction of test cases which were found to be compatible with the data with respect to the total number of test cases for this model:

$$\epsilon = \frac{N_{\chi^2 \geq 0.01}}{N_{\text{total}}}. \quad (1)$$

In the case of total cross sections one test case consists of all available data points. For differential cross sections all data available for a given energy and scattering angle constitute one test case. The total efficiency of a model was then calculated as the mean of the efficiencies obtained from all test cases of this model.
Fig. 3: Validation results for differential cross sections of elements Sc (Z = 21), V (Z = 23), Cu (Z = 29) and Pb (Z = 82). The Penelope- (green circles) and EPDL-based (red diamonds) models are often indistinguishable and generally describe the experimental data well. The Klein-Nishina-based model (blue squares) tends to overestimate the differential cross section in these examples, in particular at low scattering angles. In some cases, there are noticeable differences between experimental data sets.

TABLE I: Comparison of efficiencies of validated differential cross section models. Note that Klein-Nishina represents the implementation in Geant4 standard physics.

| model        | efficiency |
|--------------|------------|
| EPDL         | 0.82 ± 0.02 |
| Penelope     | 0.82 ± 0.02 |
| Klein-Nishina| 0.54 ± 0.03 |
| Brusa        | 0.84 ± 0.02 |
| BrusaF       | 0.84 ± 0.02 |
| PenBrusa     | 0.84 ± 0.02 |
| PenBrusaF    | 0.84 ± 0.02 |
| Biggs        | 0.84 ± 0.02 |
| BiggsF       | 0.85 ± 0.02 |
| Hubbell      | 0.82 ± 0.02 |

VI. RESULTS

Concerning total Compton scattering cross sections our preliminary analysis shows that all tested models reach an efficiency of 1 for all test cases, i.e. all models are capable of modeling the experimental data with a significance of α = 0.01.

Table I shows the mean efficiencies achieved by the different models when compared to experimental differential Compton scattering cross sections. It is apparent that all models except the Klein-Nishina model behave almost equally well. This observation is also qualitatively supported by the exemplary plots of differential cross sections for different elements and energies shown in Fig. 3. A more detailed follow-up to the preliminary analysis presented here, which categorizes e.g. different energy ranges and angles, and corrects for outliers in the experimental data, will likely distinguish more between
these models.

VII. SUMMARY AND PROSPECTS

Our first and preliminary results concerning the validation of total Compton preliminary cross sections suggest that all evaluated models agree equally well with available experimental data. Concerning differential Compton scattering cross sections, we arrive at a similar conclusion, with the notable exception of models based on the original Klein-Nishina theory, as is e.g. the case for the Compton scattering models implemented in Geant4 standard physics. This was to be expected, since the original Klein-Nishina theory describes Compton scattering on free electrons, and therefore by design does not take into account binding effects for electrons bound to an atom.

Before final conclusions can be reached, we will subject our data base of experimental results to a more detailed critical appraisal to identify possible systematic biases or outliers. At the same time, we will evaluate additional Compton scattering models.

Further aspects of Compton scattering that still await validation are shell cross sections, Doppler broadening, polarization, and finally computational efficiency.

The complete set of results of the validation of Compton scattering simulation, including additional physics features and modeling options that are not considered in this paper, will be reported in detail in a forthcoming publication in a refereed journal.

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