

Validation of Geant4 electromagnetic physics versus protocol data

K. Amako, S. Guatelli, V. Ivanchenko, M. Maire, B. Mascialino, K. Murakami, L. Pandola, S. Parlati, M.G. Pia, M. Piergentili, T. Sasaki, L. Urban.

Abstract—The Geant4 Simulation Toolkit provides an ample set of complementary and alternative physics models for both electromagnetic and hadronic processes, describing the interaction of particles with matter. We present a short overview of the actual state of the physics models provided by Geant4 and the results of a series of detailed tests for the quantitative validation of the electromagnetic processes. The Geant4-based test results are compared to protocol references commonly adopted in the medical physics domain (NIST and ICRU).

Index Terms—Geant4, Electromagnetic Physics, Validation, Protocol Data.

I. INTRODUCTION

GEANT4 is an Object-Oriented Toolkit [1] for the simulation of the passage of particles through matter.

Geant4 offers an ample set of complementary and alternative physics models based either on theory, on experimental data or on parameterisations. In particular, Geant4 provides Packages specialized for modeling both electromagnetic and hadronic physics interactions.

The validation of Geant4 physics models with respect to experimental data and protocol references is obviously a critical issue, fundamental to the reliability of the Geant4 physics models.

This paper presents the results of the validation of Geant4 electromagnetic models with respect to recognised reference data: protocols of the *International Commission on Radiation Units and Measurements* (ICRU) [2] and reference data provided by the *National Institute of Standards and Technologies* (NIST) [3]. The aim is to demonstrate the accuracy and reliability of the Geant4 electromagnetic physics models by means of a set of tests concerning the electromagnetic processes of photons,

electrons, protons and alpha particles. These tests include the calculation of:

- the total attenuation coefficients,
- the cross sections of the singular processes of photons,
- electron stopping power and continuously slowing down approximation (CSDA) range,
- proton stopping power and continuously slowing down approximation (CSDA) range,
- α particles stopping power and continuously slowing down approximation (CSDA) range,

in a set of selected materials. The validation has involved both Standard and Low Energy electromagnetic Geant4 Packages.

The testing activity has involved simple experimental setups, with the scope of observing the behavior of the various models with respect to the reference data, independently from the specific geometrical configuration adopted and from the detector features. Under these conditions, it has been possible to observe the different behavior of the specific Geant4 electromagnetic Packages in the same experimental set-up.

II. GEANT4 ELECTROMAGNETIC PHYSICS PACKAGES

The Geant4 electromagnetic Packages handle the electromagnetic interactions of leptons, photons, hadrons and ions. In particular they include multiple scattering, ionization, bremsstrahlung, positron annihilation, photoelectric effect, Compton and Rayleigh scattering, gamma conversion, synchrotron and transition radiation, Čerenkov effect, refraction, reflection, absorption, scintillation, fluorescence, Auger effect, Particle Induced X-ray Emission (PIXE) [1].

In this study we present the results concerning the following Geant4 electromagnetic Packages:

- Standard Package;
- Low Energy Package, based on the Livermore data libraries [4], [5], [6];
- Low Energy Package, based on Penelope analytical approach [7].

A. Standard Package

The Standard Package [1] provides a variety of models based on an analytical approach to describe the interactions of electrons, positrons, photons, and charged hadrons in the energy range between 1. keV and 100. TeV. The models assume that the atomic electrons are quasi-free (*i.e.*, their binding energy is neglected except for photoelectric effect)

Manuscript received November 1, 2004.

K. Amako, K. Murakami and T. Sasaki are with KEK, 1-1 Oho, Tsukuba, Ibaraki, Japan (e-mail: Katsuya.Amako@kek.jp, Koichi.Murakami@kek.jp, Takashi.Sasaki@kek.jp).

S. Guatelli, B. Mascialino, M. G. Pia, M. Piergentili are with the Italian Institute for Nuclear Research, via Dodecaneso 33, 16146 Genova - Italy (e-mail: Susanna.Guatelli@ge.infn.it, Barbara.Mascialino@ge.infn.it, Maria-Grazia.Pia@ge.infn.it, Michela.Piergentili@ge.infn.it).

V. Ivanchenko is with CERN, CH 1122, Geneve 23 - Switzerland (e-mail: Vladimir.Ivanchenko@cern.ch).

M. Maire is with the LAPP, Annecy, France (e-mail: Michel.Maire@cern.ch).

L. Pandola and S. Parlati are with the Italian Institute for Nuclear Research, Strada Statale 17bis del Gran Sasso, 67010 Assergi - L'Aquila - Italy (e-mail: Luciano.Pandola@lngs.infn.it, Sandra.Parlati@lngs.infn.it).

L. Urban is with Kfki Research Institute for Particle and Nuclear Physics, Konkoly Thege Miklos ut 29-33, H-1121 Budapest, Hungary (e-mail: Laszlo.Urban@cern.ch).

while the atomic nucleus is fixed (*i.e.*, the recoil momentum is neglected). The Standard Package is mainly addressed to the high energy physics domain.

B. Low Energy Package: evaluated data driven approach

The Low Energy Package [1], [9] extends the range of accuracy of electromagnetic interactions down to lower energy than the Standard Package. This Low Energy Package approach exploits evaluated data libraries (EPDL97 [4], EEDL [5] and EADL [6]) that provide data for the calculation of the cross-sections and the sampling of the final state for the modeling of photon and electron interactions with matter. The current implementation of low energy electron and photon processes can be used down to 250. eV. The Low Energy Package handles the ionization by hadrons and ions [10], [11]. It adopts different models depending on the energy range and the particle charge. In the high energy domain ($> 2.$ MeV) the Bethe-Bloch formula, while in the low energy one ($< 1.$ keV for protons) the free electron model are applied respectively. In the intermediate energy range parameterized models based on experimental data from the Ziegler [12] and ICRU [2] reviews are implemented; corrections due to the molecular structure of materials and the effect of the nuclear stopping power are taken into account.

C. Low Energy Package: analytic approach

The physics models developed for the Penelope Simulation Toolkit (PENetration and Energy Loss of Positrons and Electrons) [7] have been implemented in Geant4 as an alternative and independent set of processes in the Low Energy Package. The models, that have been specifically developed for Monte Carlo simulation, are based on an approach which combines numerical databases with analytical cross section models for the different interaction mechanisms. In particular, they include low-energy and atomic effects (*e.g.* Doppler broadening, shell effects) and can be applied to energies from a few hundred eV to about 1. GeV [8].

III. EXPERIMENTAL SET-UP OF THE TESTS

The experimental set-up was specific to the the physics quantity object of the test, and it reproduced the same experimental conditions of the reference data.

In each test, we evaluated the behavior of the electromagnetic models in a selected group of materials: beryllium, aluminum, silicon, iron, germanium, silver, gold, lead, uranium and water with the aim of studying the particles interaction with materials covering the entire periodic table of the elements in terms of the atomic number Z . The behavior of particles in water was studied as well because of the importance of this material in medical physics applications.

The conditions of the tests were fixed to reach a good compromise between the calculation accuracy and the use of CPU resources.

The next subsections describe in detail the specific experimental set-up adopted in each test.

A. Photon attenuation coefficients

Monochromatic photon beams impinge on a slab of a chosen material. The result of the test is the attenuation coefficient $\frac{\mu}{\rho}$, calculated as follows:

$$\frac{\mu}{\rho} = -\frac{1}{d\rho} \ln\left(\frac{N}{N_0}\right),$$

where ρ is the density of the target material, d is the thickness of the slab along the photon incident direction, N_0 is the number of incident monochromatic photons, N is the number of photons emerging from the target without interacting.

The photon total attenuation coefficients have been calculated activating the photoelectric effect, the Compton effect, the pair production. In the case of testing the Low Energy Package, the Rayleigh effect is also modeled¹.

The singular photon processes are activated one by one to validate the individual cross sections.

B. Stopping power and CSDA range

The stopping power and the CSDA range have been calculated for electrons, protons and α particles. The experimental conditions are the same for the three types of particles.

Each type of particle is generated with a chosen energy from the center of a box, filled with one of the materials listed above.

The multiple scattering and the energy loss fluctuations are not active, in agreement with the stopping power and CSDA range definitions.

IV. REFERENCE DATA

The reference data adopted are ICRU and NIST. The XCOM database reports the photon cross sections and attenuation coefficients. The sum of the interaction coefficients for the individual processes is equal to the total attenuation coefficient. This database comprehends all the elements of the periodic table over a wide range of energies. The XCOM database derives from references: [13], [14], [15], [16].

ESTAR generates stopping powers and CSDA ranges for electrons which are the same as those tabulated in ICRU Report 37 [17], while PSTAR and ASTAR generate the stopping powers and CSDA ranges for protons and α particles on the basis of ICRU Report 49 [18].

V. STATISTICAL ANALYSIS

Comparisons between reference data and Geant4 simulations obtained by means of the specific electromagnetic Packages have been performed by means of a Goodness-of-Fit Statistical Toolkit [21], specialised in the comparison of data distributions. This Toolkit was selected because it is an updated, versatile, flexible tool providing a variety of powerful and sophisticated Goodness-of-Fit algorithms for physics data analysis.

For any physical quantity of interest and for any element considered, the aim of the comparison was to test whether the

¹The Rayleigh effect is not available in the Geant4 Standard electromagnetic physics Package.

TABLE I
GEANT4 ELECTROMAGNETIC MODELS UNDER TEST.

Particle	Geant4 Packages
Photon	Geant4 Low Energy
Photon	Geant4 Penelope
Photon	Geant4 Standard
Electron	Geant4 Low Energy
Electron	Geant4 Penelope
Electron	Geant4 Standard
Proton	Geant4 Low Energy - ICRU 49
Proton	Geant4 Low Energy - ZIEGLER 1985
Proton	Geant4 Low Energy - ZIEGLER 2000
Proton	Geant4 Standard
α particle	Geant4 Low Energy - ICRU 49
α particle	Geant4 Low Energy - ZIEGLER 1977
α particle	Geant4 Standard

physical quantity obtained with Geant4 specific electromagnetic Packages agreed with reference data all over the range of energies E . Table I summarises the specific Geant4 models activated for the specific particles considered.

Among the ones available in the Goodness-of-Fit Statistical Toolkit, we selected the Chi-squared test, as this is the only Goodness-of-Fit algorithm including data uncertainties in the computation of the test statistics. The Goodness-of-Fit Statistical Toolkit returned the computed Chi-squared value together with the number of degrees of freedom and the p-value of the comparison. The p-value represents the probability that the test statistics has a value at least as extreme as that observed, assuming that the null hypothesis is true. Obviously p-values higher than the confidence level $\alpha = 0.05$ set a priori led to the acceptance of the null hypothesis, stating the equivalence between reference data and Geant4 simulations.

VI. RESULTS

For all the physical quantities considered, Geant4 is able to reproduce with high accuracy the reference data with any physical electromagnetic model. As an example, a few of the results of the test are shown in the following figures:

- *photons*: Fig. 1 shows the x-ray total attenuation coefficient in uranium,
- *electrons*: Fig. 2 represents the CSDA range of electrons in lead,
- *protons*: Fig. 3 represents the stopping power of protons in aluminum,
- *α particles*: Fig. 4 represents the stopping power of α particles in silver.

The Goodness-of-Fit tests performed for all the selected elements demonstrate that all the Geant4 electromagnetic Packages can simulate with great accuracy all the specific physical quantities considered in the whole energy range selected. All the statistical comparisons, in fact, led to the acceptance of the null hypothesis, stating that there is not a statistical difference between reference data and the specific Geant4 simulations. Fig. 5, 6 and 7 represent three examples of the Goodness-of-Fit test results: the p-values (respectively

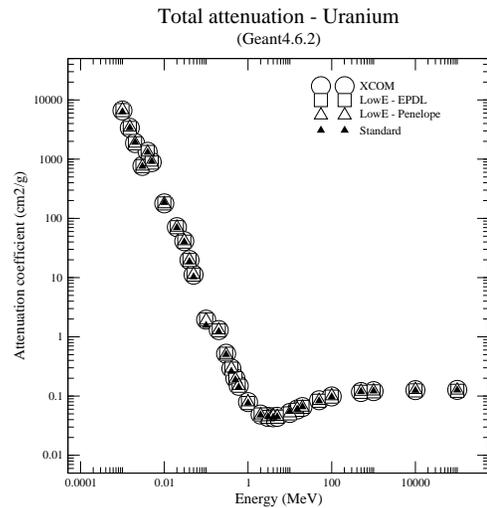


Fig. 1. Total attenuation coefficient in uranium as a function of the photon incident energy.

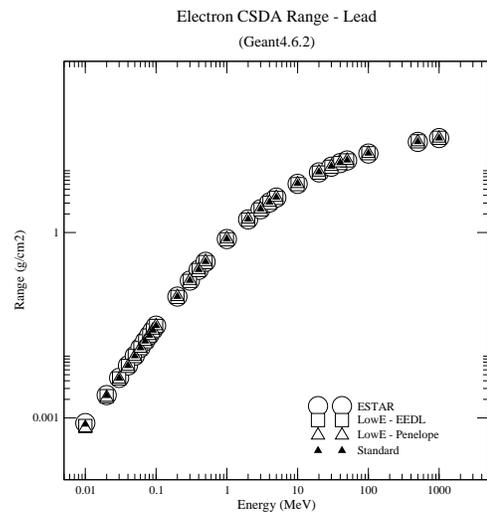


Fig. 2. Electron CSDA range in lead as a function of the electron incident energy.

of the total attenuation coefficient, electron stopping power and proton stopping power tests) are plotted as a function of the atomic number Z of the selected elements. In any case, as visible in the three figures, we obtained a p-value higher than the confidence level set. This led to the acceptance of the null hypothesis, stating that there is no difference between reference data and Geant4 simulations. The oscillations of the p-values as a functions of the atomic number Z are ascribable to the differences of the physics models contained in Geant4.

VII. CRITICAL DISCUSSION AND CONCLUSIONS

A. Photons

- The three Geant4 models reproduce total attenuation coefficients with high accuracy, the two Low Energy approaches exhibiting the best agreement with reference data.
- Concerning photoelectric cross section, the three Geant4 models reproduce reference data with high accuracy;

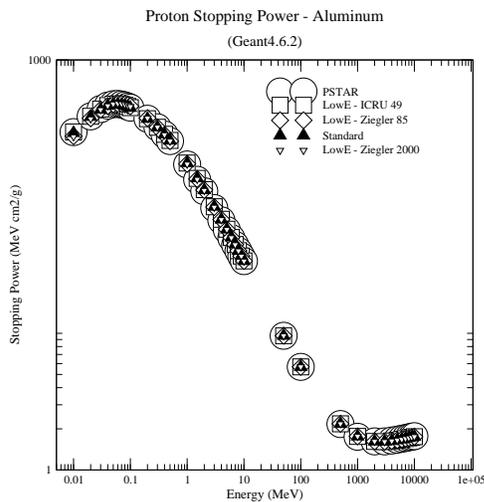


Fig. 3. Proton stopping power in aluminum as a function of the proton incident energy.

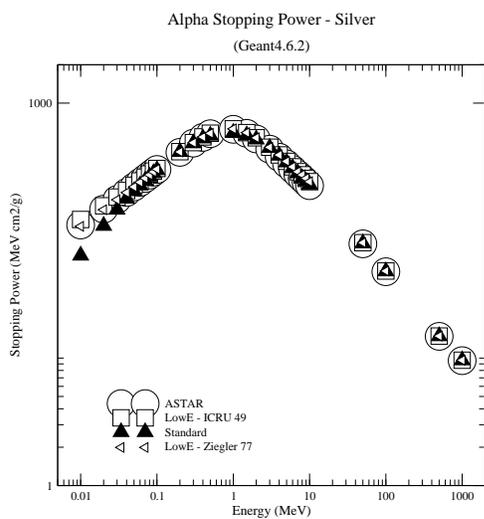


Fig. 4. α stopping power in silver as a function of the α incident energy.

the two Geant4 Low Energy models exhibit the best agreement.

- Both Compton scattering and pair production cross sections are reproduced with high accuracy by the three Geant4 models; the Geant4 Low Energy EPDL model exhibits the best agreement with reference data.
- In the case of Rayleigh scattering cross sections, the Geant4 models seemed to be in disagreement with the reference data for some materials. The disagreement between NIST reference data and data coming from the recent library EPDL97 within the range of energies between 1. keV and 1. MeV has been already underlined and discussed in a recent paper [22]. In his paper the author concluded that EPDL97 [4] is the most up-dated, complete and consistent data library available at the moment. As shown in Fig. 8 in the case of a gold slab, Rayleigh cross section from XCOM and EPDL present major deviations. The results obtained with the Geant4 Low Energy EPDL approach reproduce the EPDL

Attenuation Test

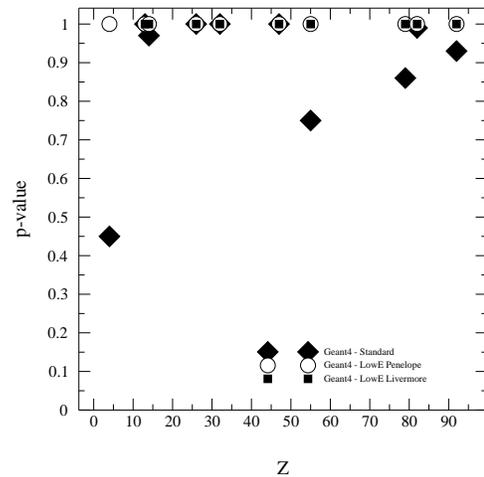


Fig. 5. Goodness-of-Fit test results concerning the total attenuation coefficient plotted as a function of the atomic number Z of the selected elements (Standard: black diamonds, Low Energy EPDL: black squares, Low Energy Penelope approach: empty circles). All the p-values obtained are higher than the confidence level set ($\alpha = 0.05$).

Electron Stopping Power Test

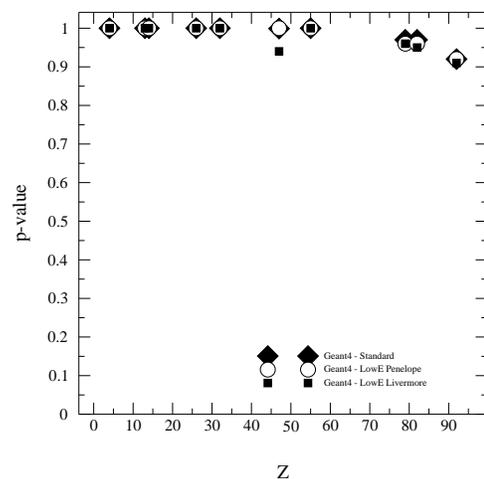


Fig. 6. Goodness-of-Fit test results concerning the electron stopping power plotted as a function of the atomic number Z of the selected elements (Standard: black diamonds, Low Energy EPDL: black squares, Low Energy Penelope approach: empty circles). All the p-values obtained are higher than the confidence level set ($\alpha = 0.05$).

original data; this is meant to be a verification of the Geant4 simulation dedicated to this specific test.

B. Electrons

The validation test exhibited that all the three Geant4 physics models are in excellent agreement with the NIST reference data; the test has not pointed out any particular difference among the three approaches.

C. Protons and α particles

The Geant4 Low Energy Package contains ICRU 49 parameterisation as one of its models. In this case the comparison between Geant4 simulations and reference data is to be

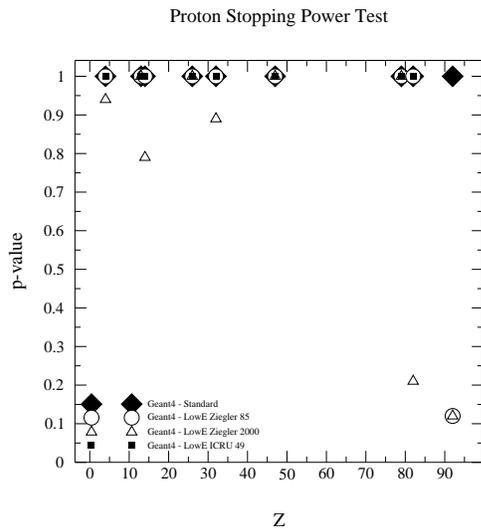


Fig. 7. Goodness-of-Fit test results concerning the proton stopping power plotted as a function of the atomic number Z of the selected elements (Standard: black diamonds, Low Energy ICRU 49: black squares, Low Energy Ziegler 1985: empty circles, Low Energy Ziegler 2000: empty triangles). All the p -values obtained are higher than the confidence level set ($\alpha = 0.05$).

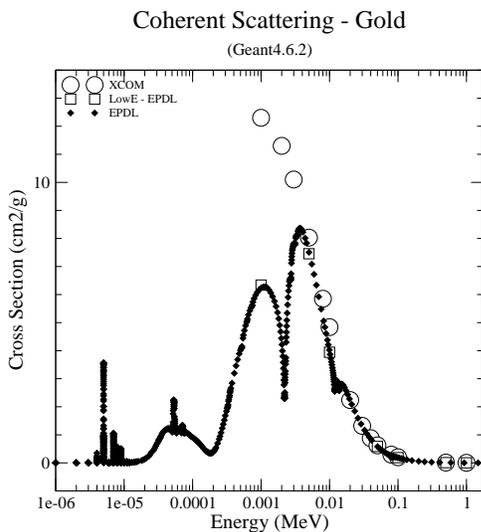


Fig. 8. Comparison between Rayleigh cross section from XCOM (black circles) and EPDL (white circles) in the specific case of a gold slab. Note the major deviations between the two data sets. The results obtained with the Geant4 Low Energy Package (black triangles) are in perfect agreement with the EPDL data; this is meant to be a verification of the Geant4 simulation dedicated to this specific test. For more details see text.

considered as a verification, rather than as a validation. The test showed some apparent discrepancies between the Low Energy Package based on Ziegler parametrizations; however the Ziegler models represent an authoritative reference in this physics domain, of comparable relevance as the ICRU 49 reference; in this case the comparison between the models should be retained for its intrinsic interest, but it should not be considered as the validation of one with respect to the other. As expected, the Low Energy Package shows a more precise agreement with respect to the Standard Package in the lower energy range ($E < 2$.MeV).

A systematic test has been performed comparing all the

Geant4 simulation models for electrons, photon, protons and α particles with respect to the ICRU and NIST references. All the models for electrons, photons and protons are found in good agreement with the reference data; for α particles the Geant4 Low Energy Package exhibits a good agreement over the whole energy range, while the Standard Package is in agreement with the reference for energies above 0.05 MeV. A quantitative statistical analysis has allowed to point out the respective strengths of the various Geant4 models in detail, for each of the physics distributions reported in the ICRU and NIST references.

REFERENCES

- [1] Geant4 Collaboration, "Geant4 - a simulation toolkit", NIM A 506 pp. 250-303, 2003.
- [2] A. Allisy, et al., *ICRU Report 49*, 1993.
- [3] <http://www.nist.gov>
- [4] D. Cullen, J.H. Hubbell, L. Kissel, *The Evaluated Photon Data Library, '97 version*, UCRL-50400, Vol.6, Rev.5.
- [5] S.T. Perkins, D.E. Cullen, S.M. Seltzer *Tables and Graphs of Electron-Interaction Cross-Sections from 10 eV to 100 GeV Derived from the LLNL Evaluated Electron Data Library (EEDL), Z=1-100* UCRL-50400 Vol.31.
- [6] S.T. Perkins, D.E. Cullen, M.H. Chen, J.H. Hubbell, J. Rathkopf, J. Scofield, *Tables and Graphs of Atomic Subshell and Relaxation Data Derived from the LLNL Evaluated Atomic Data Library (EADL), Z=1-100* UCRL-50400 Vol.30.
- [7] J. Sempau, J.M. Fernández-Varea, E. Acosta, F. Salvat, "Experimental benchmarks of the Monte Carlo code PENELOPE" NIM B vol. 207 pp. 107-123, 2003.
- [8] "Penelope - A code system for Monte Carlo simulation of electron and photon transport" Workshop Proceedings, Issy-les-Moulineaux, France, AEN-NEA, 2001.
- [9] S. Chauvie, G. Depaola, V. Ivanchenko, F. Longo, P. Nieminen, M.G. Pia, "Geant4 Low Energy Electromagnetic Physics" Proceedings of CHEP 2001, Beijing (China), pp. 337-340, 2001.
- [10] S. Giani, et al., CERN-OPEN-99-121 and INFN/AE-99/20, 1999.
- [11] S. Giani, et al., CERN-OPEN-99-300 and INFN/AE-99/21, 1999.
- [12] H.H. Andersen, J.F. Ziegler, "The Stopping and Ranges of Ions in Matter" Vol.3, Pergamon Press, Oxford, 1997.
- [13] J.H. Hubbell "Photon Mass Attenuation and Energy Absorption Coefficients from 1 keV to 20 MeV" *Int. J. Appl. Radiat/Isotopes*, vol. 33 pp. 1269-1290, 1982.
- [14] J.H. Hubbell, W.J. Veigele, E.A. Briggs, R.T. Brown, D.T. Cromer, R.J. Howerton "Atomic Form Factors, Incoherent Scattering Functions, and Photon Scattering Cross Sections" *J. Phys. Chem. Ref. Data*, vol. 4 pp. 471-538, 1975.
- [15] J.H. Hubbell, Overbo "Relativistic Atomic Form Factors and Photon Coherent Scattering Cross Sections" *J. Phys. Chem. Ref. Data*, vol. 8 pp. 69-105, 1979.
- [16] J. Leroux, T.P. Tinh "Revised Tables of X-ray Mass Attenuation Coefficients" *Corporation Scientifique Classique, Quebec*, 1977.
- [17] ICRU International Commission on Radiation Units and Measurements. "ICRU Report 37, Stopping Powers for Electrons and Positrons", 1984.
- [18] ICRU International Commission on Radiation Units and Measurements. "ICRU Report 49, Stopping Powers and Ranges for Protons and Alpha Particles", 1993.
- [19] H.H. Andersen, J.F. Ziegler "Hydrogen: Stopping Powers and Ranges in All Elements. Vol. 3 of The Stopping and Ranges of Ions in Matter", Pergamon Press, Elmsford, New York, 1977.
- [20] J.F. Ziegler "Helium: Stopping Powers and Ranges in all Elemental Matter. Vol. 4 of The Stopping and Ranges of Ions in Matter", Pergamon Press, New York, 1977.
- [21] G.A.P. Cirrone, S. Donadio, S. Guatelli, A. Mantero, B. Mascialino, S. Parlati M.G. Pia, A. Pfeiffer, A. Ribon, P. Viarengo "A Goodness-of-Fit Statistical Toolkit" *IEEE-Transactions on Nuclear Science*, vol. 51 (5) pp. 2056-2063, 2004.
- [22] H. Zaidi, "Comparative evaluation of photon cross section libraries for materials of interest in PET Monte Carlo simulation" *IEEE Transaction on Nuclear Science*, vol. 47, pp. 2722-2735, 2000.