Systematic test of gamma-ray models with NIST data

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Geant4 Collaboration Workshop 2015

Project

- K. Amako et al, IEEE TNS, 52(4), 910-918, 2005.
  - Comparison of
    - Attenuation coefficients
    - Stopping Power and Range of e^-, p and α

    With respect to NIST

- The project is to have systematic regression tests on gamma ray processes
  - *trunk/verification/electromagnetic/attenuation*

Comparison of Geant4 Electromagnetic Physics Models Against the NIST Reference Data

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***Abstract*—The Geant4 Simulation Toolkit provides an ample set of physics models describing electromagnetic interactions of particles with matter. This paper presents the results of a series of comparisons for the evaluation of Geant4 electromagnetic processes with respect to United States National Institute of Standards and Technologies (NIST) reference data. A statistical analysis was performed to estimate quantitatively the compatibility of Geant4 electromagnetic models with NIST data; the statistical analysis also highlighted the respective strengths of the different Geant4 models.**

***Index Terms*—Geant4, Monte Carlo, NIST, validation.**

I. Introduction

GEANT4 is an object oriented toolkit [1] for the simulation of the passage of particles through matter. It offers an ample set of complementary and alternative physics models for electromagnetic and hadronic interactions, based on theory, experimental data or parameterizations.

The validation of Geant4 physics models with respect to authoritative reference data is a critical issue, fundamental to establish the reliability of Geant4-based simulations. This paper is focused on the validation of Geant4 electromagnetic models, with the purpose to evaluate their accuracy and to document their respective strengths. It presents the results of comparisons of Geant4 electromagnetic processes of photons, electrons, protons and α particles with respect to reference data of the United States National Institute of Standards and Technologies (NIST) [2], [3] and of the International Commission on Radiation Units and Measurements (ICRU) [4], [5].

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TABLE I
Geant4 Electromagnetic Models in This Comparison Study

Particle	Geant4 Models in Electromagnetic Packages
Photon	Geant4 Low Energy - EPDL
	Geant4 Low Energy - Penelope
	Geant4 Standard
Electron	Geant4 Low Energy - EEDL
	Geant4 Low Energy - Penelope
	Geant4 Standard
Proton	Geant4 Low Energy - ICRU 49
	Geant4 Low Energy - Ziegler 1985
	Geant4 Low Energy - Ziegler 2000
	Geant4 Standard
α	Geant4 Low Energy - ICRU 49
	Geant4 Low Energy - Ziegler 1977
	Geant4 Standard

The simulation results were produced with Geant4 version 6.2. The Geant4 test process verifies that the accuracy of the physics models will not deteriorate in future versions of the toolkit with respect to the results presented in this paper.

II. Overview of Geant4 Electromagnetic Physics Packages

The Geant4 Simulation Toolkit includes a number of packages to handle the electromagnetic interactions of electrons, muons, positrons, photons, hadrons and ions. Geant4 electromagnetic packages are specialised according to the particle type they manage, or the energy range of the processes they cover.

The physics processes modeled in Geant4 electromagnetic packages include: multiple scattering, ionization, Bremsstrahlung, positron annihilation, photoelectric effect, Compton and Rayleigh scattering, pair production, synchrotron and transition radiation, Cherenkov effect, refraction, reflection, absorption, scintillation, fluorescence, and Auger electrons emission [1].

Alternative and complementary models are provided in the various packages for the same process. The Geant4 electromagnetic models studied in this paper are listed in Table I.

A. Standard Electromagnetic Package

The Geant4 Standard electromagnetic package [8] provides a variety of models based on an analytical approach, to describe the interactions of electrons, positrons, photons, charged hadrons and ions in the energy range 1 keV–10 PeV.

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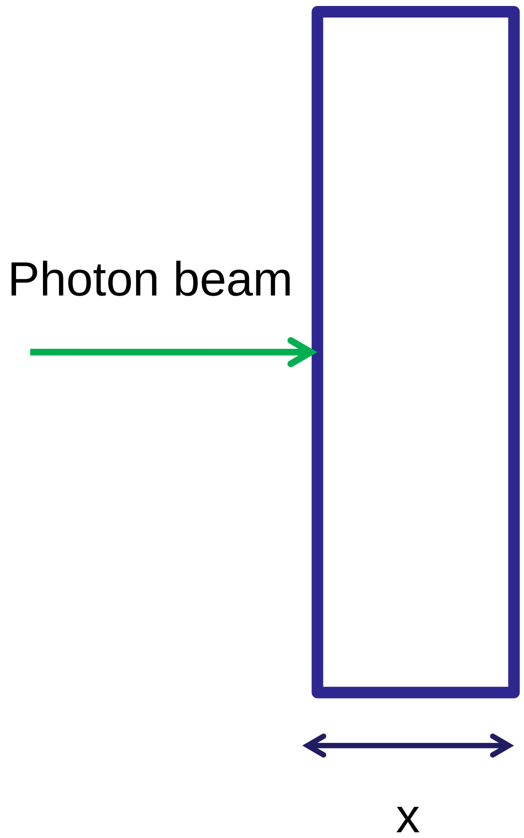
Attenuation coeff tests: on going

- Elements to test: Be (Z=4), C(Z=6), O(Z=8) ,Al (Z=13), Ar (Z=18), Ca (Z=20), Fe(Z=26), Cu(Z=29), Ge (Z=32), Ag (Z=47), Xe (Z=54), Ce(Z=58), Gd (Z=64), W(Z=74), Au(Z=79), Pb (Z=82), Bi (Z=83), U(Z=92)

- Compounds to test: Water, BGO, PMMA, other plastic phantoms used in radiotherapy Quality Assurance

- Attenuation coeff. to test
  - Total
  - Rayleigh scattering
  - Photoelectric effect
  - Compton scattering
  - Gamma conversion

Simulation set-up



$$N = N_0 e^{-\mu x}$$

- User application
  - Calculate **attenuation coefficients**
  - The cut is fixed 1/10 of the target thickness
  - **Physics lists**:
    - EMStandard_opt0
    - EMStandard_opt3
    - EMStandard_opt4
    - Livermore
    - Penelope
  - Same simulation parameters for the alternative physics lists
  - Comparison: **% difference**: abs((NIST-Geant4/NIST)*100)
  - **Regression testing**: G4 10.0 and 10.1

Summary -1

Reference NIST data have 1-5% error

Z	Rayl	Photoel	Compton	Conversion	Total
4	Livermore and Penelope: 1 and 1.5 keV, then ok	Livermore: x Penelope: x Std_opt0 and opt3: diff 3 keV <E < 1MeV Std_opt4: x	Livermore: x Std_opt4 : x Penelope: E< ~5 keV Std_opt0 and opt3: E< 6 keV	Livermore:x Penelope: x Std_opt3: x Std_opt4:x	Livermore:x Penelope: x Std_opt0: 4 keV-40 keV Std_opt3: 4 keV-10 keV Std_opt4:x
13	Livermore: 1-8 keV Penelope: 1-8 keV	Livermore: x Penelope: x Std_opt0: x Std_opt3: x Std_opt4: x	Livermore: x Penelope: 1 keV- 10 keV Std_opt3 and opt0: 1keV- 15 keV Std_opt4: x	Livermore:x Penelope: x Std_opt0:x Std_opt3: x Std_opt4: x	Livermore:x Penelope: x Std_opt0: 15 keV<E< 150 keV Std_opt3: x Std_opt4:x
20	Livermore and Penelope: below 15 keV	Livermore: x Penelope: x Std_opt0 and opt3: 1-3 MeV Std_opt4: x	**Running opt3**	Livermore:x Penelope: x Std_opt3: x Std_opt0:x Std_opt4: x Just first point for penelope, opt0, opt3 and opt4	Livermore: x Penelope: x Std_opt0: 30 keV-200 keV Std_opt3: x Std_opt4: x
26	Livermore and Penelope: below 20 keV	Livermore: x Penelope: x Std_opt0:x Std_opt3: x Std_opt4: x	Livermore: x Penelope: E< 8 keV Std_opt3 and opt0: E< 10 keV Std_opt4: x	Livermore:x Penelope: x Std_opt0:x Std_opt3: x Std_opt4: x	Livermore: x Penelope: x Std_opt0: 40 keV-200keV Std_opt3: x Std_opt4: x
32	Livermore and Penelope: below 40 keV	Livermore: x Penelope: x Std_opt3 and opt0: 20 MeV-1GeV Std_opt4: x	Livermore: x Penelope : 1keV< E< 10 keV Std_opt3 and opt0: 1 keV < E< 10 keV Std_opt4: x	Livermore:x Penelope: x Std_opt3: x Std_opt4: x Just first point for penelope, opt0, opt3	Livermore: x Penelope: x Std_opt0: 50 keV - 300 keV Std_opt3: x Std_opt4: x

X: agreement within 5% red: differences > 5 %

green: differences < 5%
red: differences > 5%

Summary – 2

Reference NIST data have 1-5% error

Z	Rayl	Photoelectric	Compton	Conversion	Total
47	Livermore: x Penelope: x	Livermore: x Penelope: x Std_opt4: x Std_opt0 and std_ opt3 differences between 5% and 20% for E> ~ 50 MeV	Livermore: x Penelope: E < 8 keV Std_opt0: diff up to 10% E< 5 keV Std_opt3: diff up to 10% E< 5 keV Std_opt4: x	Livermore:x Penelope: x Std_opt0:x Std_opt3: x Std_opt4: x	Livermore: x Penelope: x Std_opt0: 15 keV-300keV up to 10% Std_opt3: x Std_opt4: x
74	Livermore: different Penelope: different	**The statistic needs to be improved : running**	Livermore: x Penelope: E < 20 keV Std_opt0: E< 10 keV Std_opt3: E< 10 keV Std_opt4: x	running	Livermore: x Penelope: x Std_opt0: 15 keV-600keV up to 10% Std_opt3:1 keV-10 keV Std_opt4: x
79	**running**	**running**	Livermore: x Penelope: E < 20 keV Std_opt0: E< 1.5 keV Std_opt3: E< 1.5 keV Std_opt4: x	Livermore:x Penelope: x Std_opt0:x Std_opt3: x Std_opt4: x	Livermore, Penelope and opt4 liv: 2.248 keV and 2.507 keV (values just after the M edges) opt0: 1 keV – 600 keV: differences > 5% opt3: 1 keV – 5 keV differences > 5%

Summary – 3

Reference NIST data have 1-5% error

Materials	Rayl	Photoelectric	Compton	Conversion	Total
Water	Livermore: < 5 keV Penelope: < 5 keV	Livermore: x Penelope: x Std_opt0: x Std_opt3: x Std_opt4: x	Livermore: x Penelope: E < 10 keV Std_opt0: E< 10 keV Std_opt3: E< 10 keV Std_opt4: x	Livermore: x Penelope: x Std_opt3: x Std_opt4: x	Livermore: x Penelope: x Std_opt0: x Std_opt3: x Std_opt4: x
BGO	**Running livermore**	Livermore: x Penelope: x Std_opt0: 1keV – 5keV Std_opt3: 1keV – 5keV Std_opt4: x	**running**	Livermore: x Penelope: x Std_opt3: x Std_opt4: x	Livermore: x Penelope: x Std_opt0: 1 keV – 4 keV and 40 keV – 500 keV Std_opt3: 1keV – 5 keV Std_opt4: x

green: differences < 5%
red: differences > 5%

Results: discussion

- In the last year, added:
  - New materials
  - Rayleigh scattering
  - Regression test
  - Standard_option0

- Regression test: Geant4 10.1 agrees with Geant4 10.0 within statistical error bars.

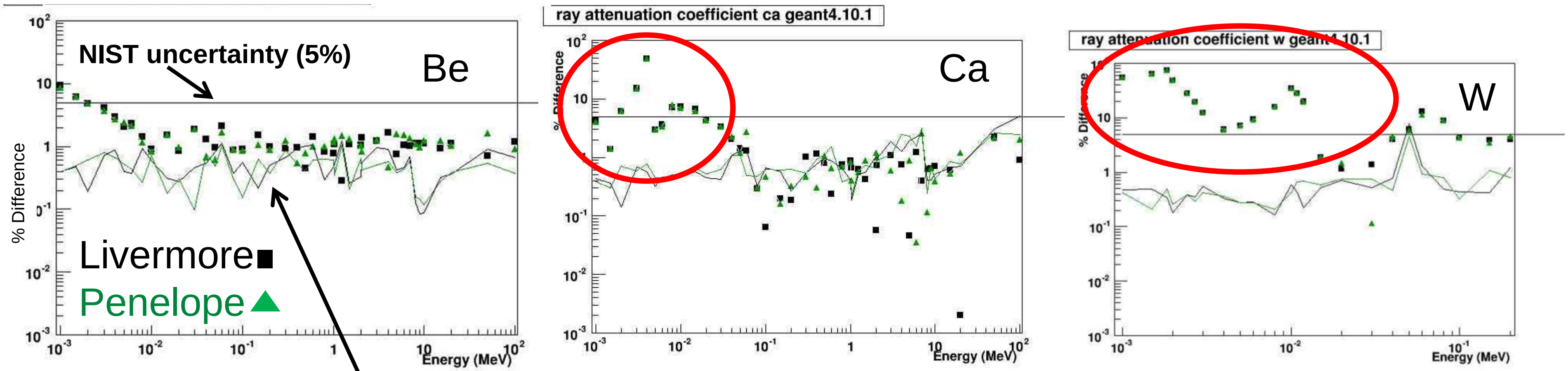
- In general good agreement with NIST (within 5%, which is the NIST uncertainty).

- Penelope approach, Standard Option 0 and 3 Compton scattering report differences below ~20 keV, where this process is negligible

Rayleigh scattering (1)

- Significant differences observed.

% Difference Geant4-NIST



The continued lines are the statistical uncertainties of Geant4 simulations (green: Penelope, black: Livermore)

Rayleigh scattering (2)

- Livermore Rayleigh scattering model is different from NIST.
  - This is known for Livermore approach

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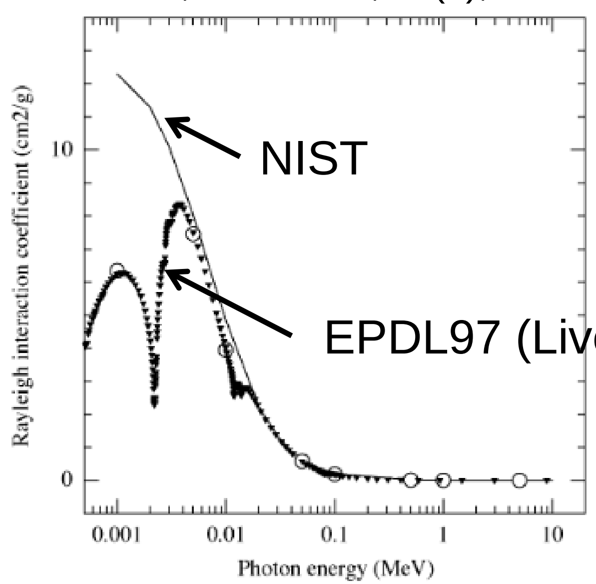

Fig. 11. Comparison between Rayleigh interaction coefficient data from NIST-XCOM (continuous line) and EPDL97 (triangles) in the specific case of a gold slab. Note the major deviations between the two data sets. The results obtained with the Geant4 Low Energy package (circles) are in agreement with the EPDL97 data; this is meant to be a verification of the Geant4 simulation dedicated to this specific test. For more details see text.

To be investigated for Penelope, however Penelope and Livermore seem to agree

Further investigation required

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Next steps

- Finish the materials
- Repeat with next Geant4 public release.
  - The tests have been automatised from execution to analysis.
  - The tests are ran on UOW High Performance Computing Facility (~ 100 CPUs available per day)
- Statistical analysis to do (Chi-squared, Kolmogorov-Smirnov)