Validation of Compton Scattering Monte Carlo Simulation Models

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Compton Validation in the Context of Nano5

**NANO5**: New Architecture for Novel simulation domains

http://www.ge.infn.it/geant4/nano5/index.html

**NANO5** is international, inter-disciplinary (particle physics, astronomy, photon science, medical science, …) collaboration.

**Research program:**
- address fundamental issues in radiation transport simulation
- investigate conceptual and technological software solutions to extend current capabilities of Geant4 toolkit to cope with new experimental requirements
- one main activity: Geant4 (low energy) electromagnetic physics design

**Nano5 conference contributions:**
- Uncertainty quantification (N18-5)
- Physics methods for the simulation of photo-ionization (N29-4)
- Negative improvements, relative validity and elusive goodness (N29-6)
- Validation of Geant4 electron pair production by photons (NPO2-141)
Compton Scattering

Compton scattering
• inelastic scattering of a photon off an electron
• one of the fundamental interaction processes of photons with matter (A.H. Compton, Nobel price 1927)
• dominates at hard X-ray and soft gamma-ray energies
• differential cross section depends on photon polarization

\[ \Delta \lambda = \frac{h}{m_e c} (1 - \cos \theta) \]

theory: Klein-Nishina
Experimental Applications of Compton Scattering

Nuclear science, medical science, radiation safety, astronomy, ...:
- imaging
- and
- polarization

CGRO

INTEGRAL

1.8 MeV
$^{26}$Al decay

Crab supernova remnant: polarized emission 0.2-0.8 MeV (Laurent et al., 2012)

Oberlack et al., 1997
Experimental Applications of Compton Scattering

Nuclear science, medical science, radiation safety, astronomy, …:
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1.8 MeV $^{26}$Al decay

Oberlack et al., 1997

INTEGRAL

Crab supernova remnant: polarized emission 0.1-1.0 MeV (Dean et al., 2008)
Experimental Applications of Compton Scattering

Nuclear science, medical science, radiation safety, astronomy, …:

imaging and polarization

Data analysis relies heavily on Monte Carlo simulation and modeling
⇒ accurate description of Compton scattering is crucial!

1.8 MeV $^{26}$Al decay

Crab supernova remnant: polarized emission 0.1-1.0 MeV (Dean et al., 2008)

CGRO

INTEGRAL

Oberlack et al., 1997
Compton Scattering in Multi-purpose Monte Carlo Codes

Multi-purpose Monte Carlo codes such as Geant4: scattering of a photon off a bound electron in an atomic shell

⇒ electron binding energy
⇒ final state:
  • scattered photon
  • Compton (recoil) electron
  • shell vacancy

theory e.g. Klein-Nishina × incoherent scattering function

whs.wsd.wednet.edu
Validation Strategy

• evaluate large number of cross section models
  o tabulated theoretical calculations
  o (simple) analytical formulae

• same computational environment for all evaluations

• objective, quantitative evaluation of physical accuracy based on rigorous statistical analysis

• measure computational performance

⇒ objective identification of best available model(s)

First evaluation cycle:
  total and differential cross sections
Validation Strategy

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First evaluation cycle:
  total and differential cross sections

Note: extraction of cross sections from out-of-the-box Geant4 is very tedious, requires full simulation…!
⇒ used re-factored code in Nano5 design
  (separated: cross section calculation and final state generation)
Experimental Data

Literature search:

• total cross section
  o most elements from H to U
  o about 230 data points

• differential cross section
  o most elements from H to U
  o about 2600 data points
  o some data for K or L shell only

• required for validation:
  o identification of systematic effects
  o identification of outliers
Validation Analysis: Statistics

**Compatibility** of model with experimental data:
- goodness-of-fit test using $\chi^2$
- significance: $\alpha = 0.01$
  - $p(\chi^2) \geq \alpha$: pass
  - $p(\chi^2) < \alpha$: fail

**Efficiency** of a cross section model:
- fraction of test cases in which model is compatible with experimental data
- definition of test cases:
  - total cross section: all available data
  - differential cross section: all data for given energy and scattering angle

**Significance** of difference in accuracy between models:
- categorical analysis

\[ \varepsilon_{\text{model}} = \frac{N_{p>0.01}}{N_{\text{tot}}} \]
Total Cross Section Models

Total cross section $\sigma$ is integral over differential cross section $d\sigma/d\Omega$

- EPDL
  - used by Geant4 “Livermore” models
- Penelope
  - used by Geant4 Penelope models
- Klein-Nishina
  - used by Geant4 standard physics models
Total Cross Section:

*Preliminary* Validation Results

All models are consistent with experimental data!
Differential Cross Section Models

• EPDL
  o used by Geant4 “Livermore” models
• Penelope
  o used by Geant4 Penelope models
• Klein-Nishina
  o used by Geant4 standard physics models

• models based on:
  o Brusa et al., 1996, NIM A, 379, 167-175
  o Biggs et al., 1975,
    Atomic Data and Nuclear Data Tables 16, 201
Differential Cross Section: Preliminary Validation Results

<table>
<thead>
<tr>
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Preliminary conclusions:
- all models describe experimental data equally well
- exception: Klein-Nishina models in Geant4 standard physics (neglect binding effects...)
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Work in progress:
- elimination of outliers
- identification of systematic effects
- further validations:
  - shell cross sections
  - Compton profiles / Doppler broadening
  - computational performance
  - polarization
more vetting of experimental data is needed…

EPDL and Penelope differential cross sections are very similar, but computational expense is different…

Klein-Nishina tends to overestimate forward scattering
Thank you…