

Validation of Compton Scattering Monte Carlo Simulation Models

**G. Weidenspointner, M. Batič, S. Hauf, G. Hoff,
M. Kuster, P. Saracco, M.G. Pia**

**2013 NSS-MIC
Seoul, South Korea
Oct. 27 – Nov. 2, 2013**

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

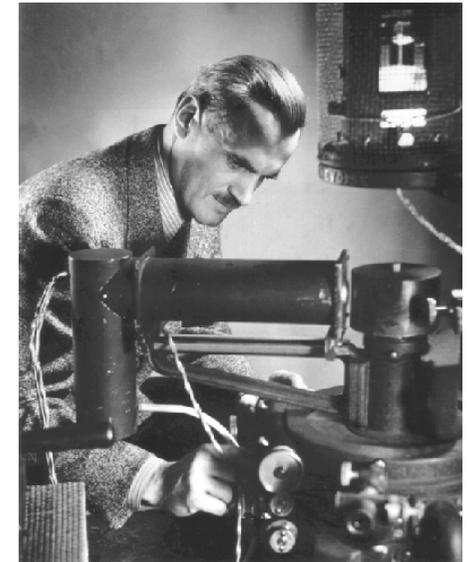
Nano5 conference contributions:

- 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)

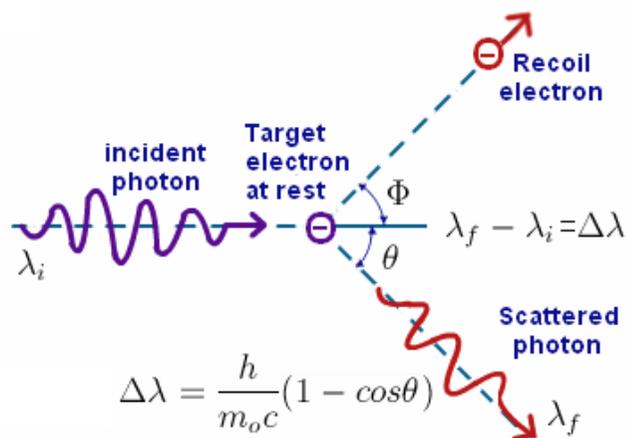
Compton Scattering

Compton scattering

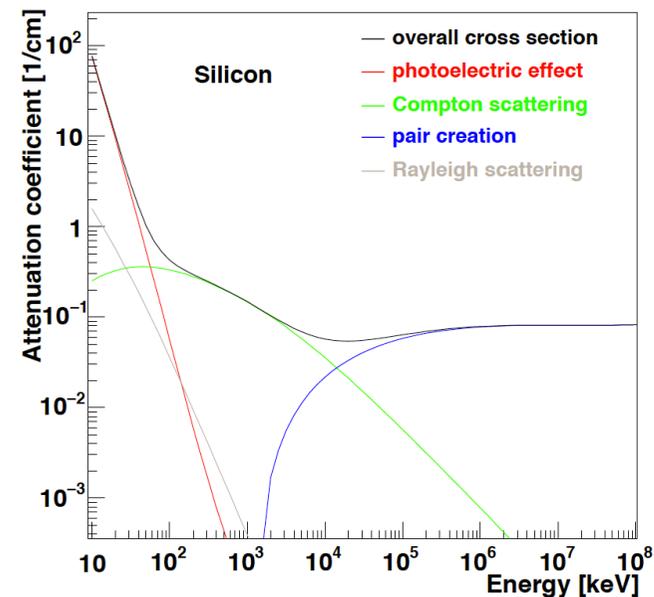
- inelastic scattering of a photon off an electron
- one of the fundamental interaction processes of photons with matter (A.H. Compton, Nobel price 1927)
- dominates at hard X-ray and soft gamma-ray energies
- differential cross section depends on photon polarization



A.H. Compton



theory: Klein-Nishina



Experimental Applications of Compton Scattering

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

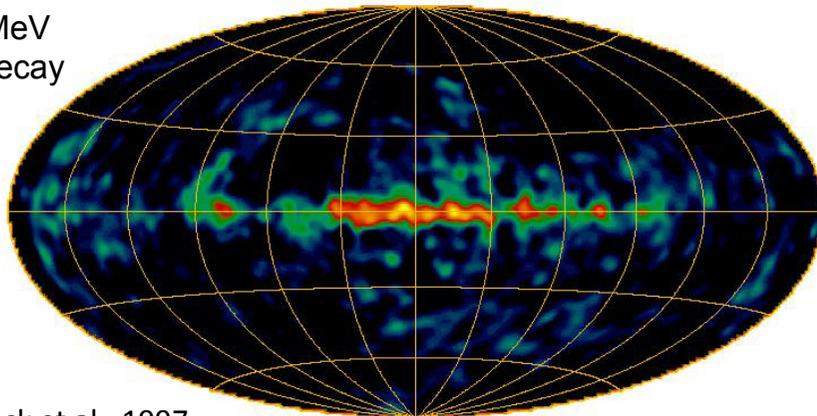
CGRO



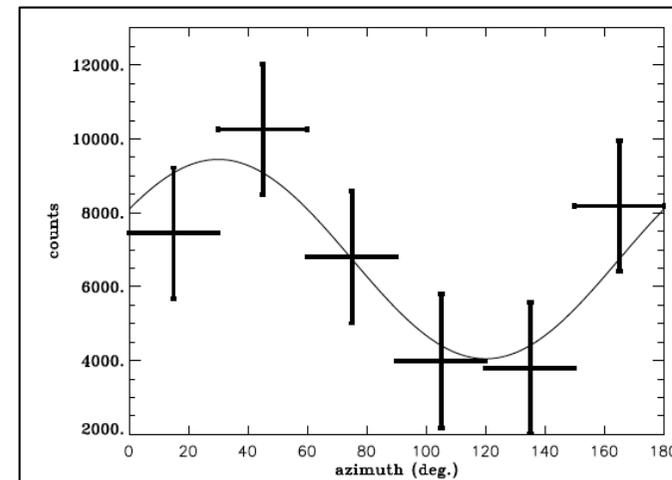
INTEGRAL



1.8 MeV
 ^{26}Al decay



Oberlack et al., 1997



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

Experimental Applications of Compton Scattering

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

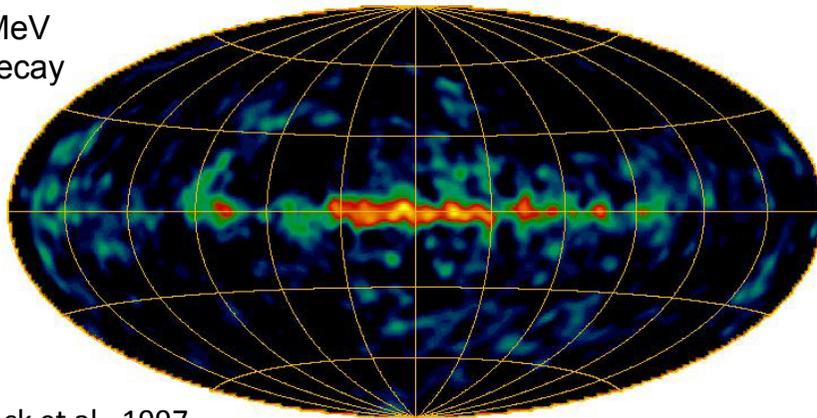
CGRO



INTEGRAL

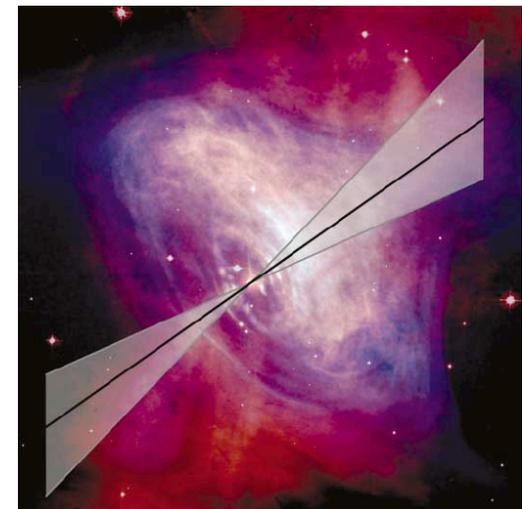


1.8 MeV
 ^{26}Al decay



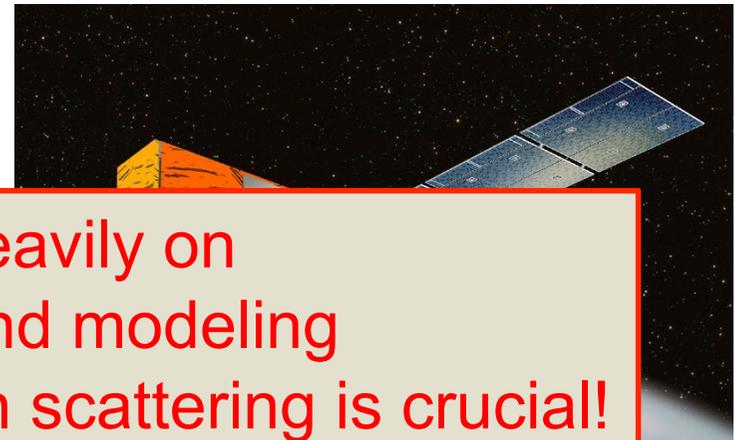
Oberlack et al., 1997

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



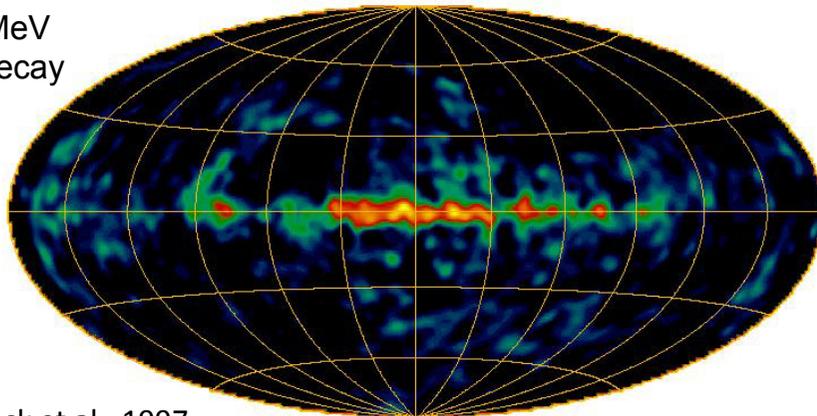
Experimental Applications of Compton Scattering

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



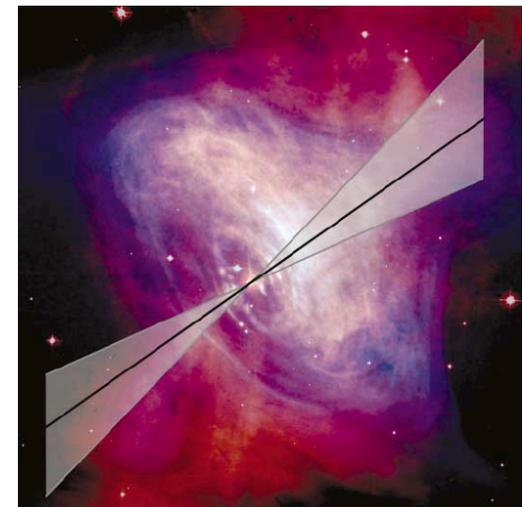
Data analysis relies heavily on Monte Carlo simulation and modeling
⇒ accurate description of Compton scattering is crucial!

1.8 MeV
 ^{26}Al decay



Oberlack et al., 1997

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

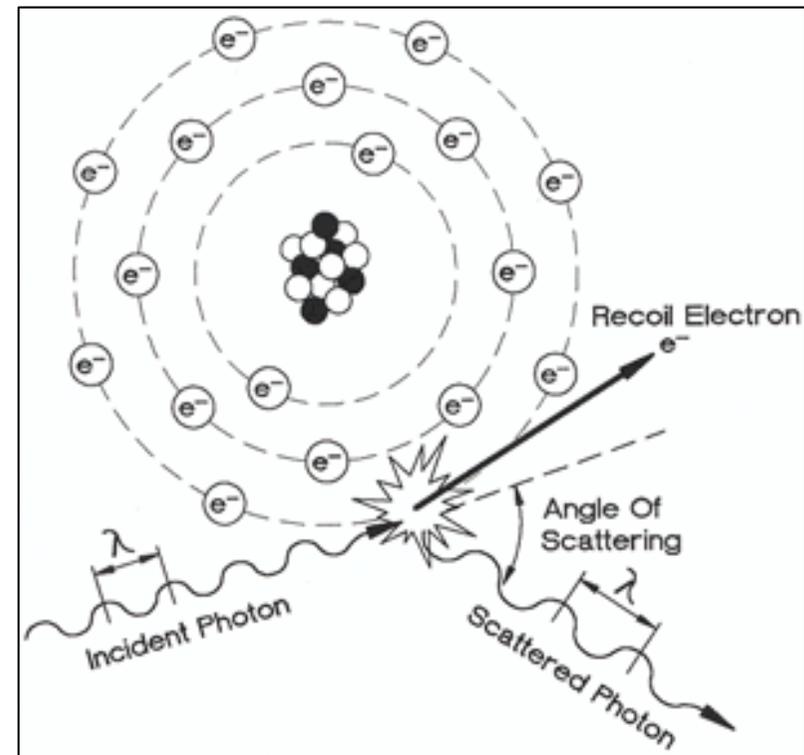


Compton Scattering in Multi-purpose Monte Carlo Codes

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



Validation Strategy

- evaluate large number of cross section models
 - tabulated theoretical calculations
 - (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

- evaluate large number of cross section models
 - tabulated theoretical calculations
 - (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

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
 - most elements from H to U
 - about 230 data points
- differential cross section
 - most elements from H to U
 - about 2600 data points
 - some data for K or L shell only
- required for validation:
 - identification of systematic effects
 - identification of outliers

Validation Analysis: Statistics

- **Compatibility** of model with experimental data:

- goodness-of-fit test using χ^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

$$\epsilon_{model} = \frac{N_{p>0.01}}{N_{tot}}$$

- 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

Total Cross Section Models

Total cross section σ 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
 - used by Geant4 “Livermore” models
- Penelope
 - used by Geant4 Penelope models
- Klein-Nishina
 - used by Geant4 standard physics models
- models based on:
 - Brusa et al., 1996, NIM A, 379, 167-175
 - Biggs et al., 1975,
Atomic Data and Nuclear Data Tables 16, 201
 - Hubbell et al., 1975, J. Phys. Chem. Ref. Data, 4, 417

Differential Cross Section: Preliminary Validation Results

model	efficiency	error
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

Preliminary conclusions:

- all models describe experimental data equally well
- **exception**: Klein-Nishina models in Geant4 standard physics (neglect binding effects...)

Differential Cross Section: Preliminary Validation Results

model	efficiency	error
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

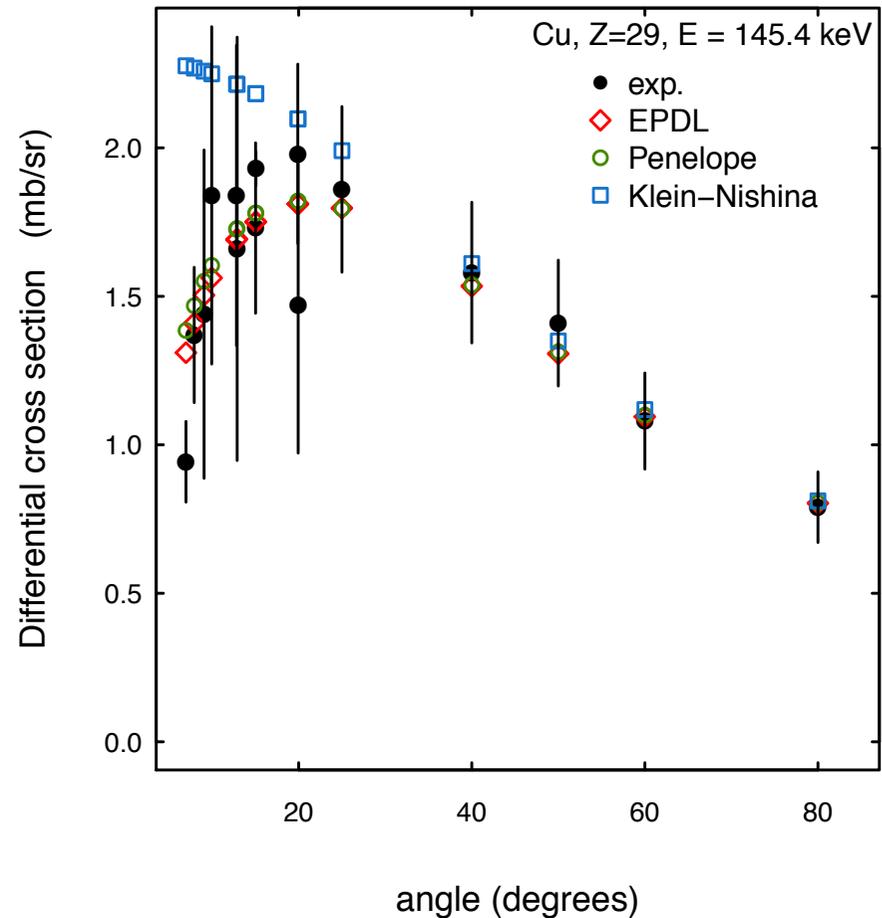
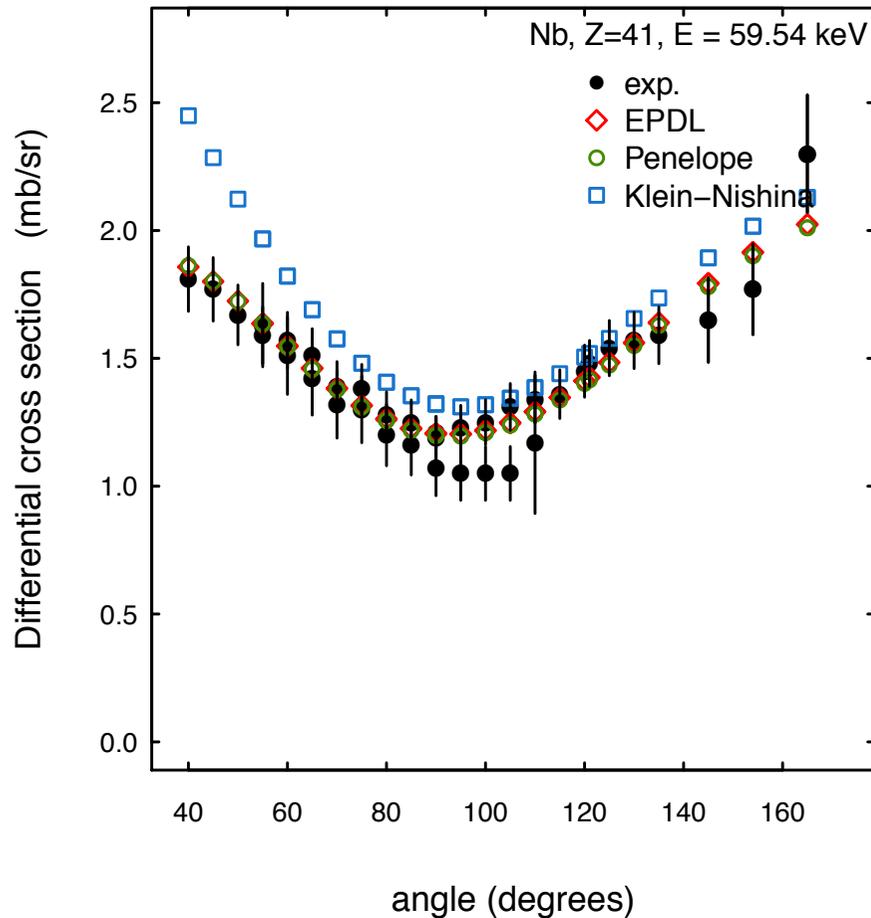
Preliminary conclusions:

- all models describe experimental data equally well
- **exception:** Klein-Nishina models in Geant4 standard physics (neglect binding effects...)

Work in progress:

- elimination of outliers
- identification of systematic effects
- further validations:
 - shell cross sections
 - Compton profiles / Doppler broadening
 - computational performance
 - polarization

Differential Cross Section: Preliminary Examples



- ⇒ 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...