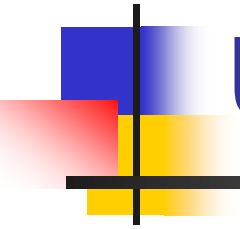

Upgrade of G4Penelope models

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for the Geant4 EM Working Groups

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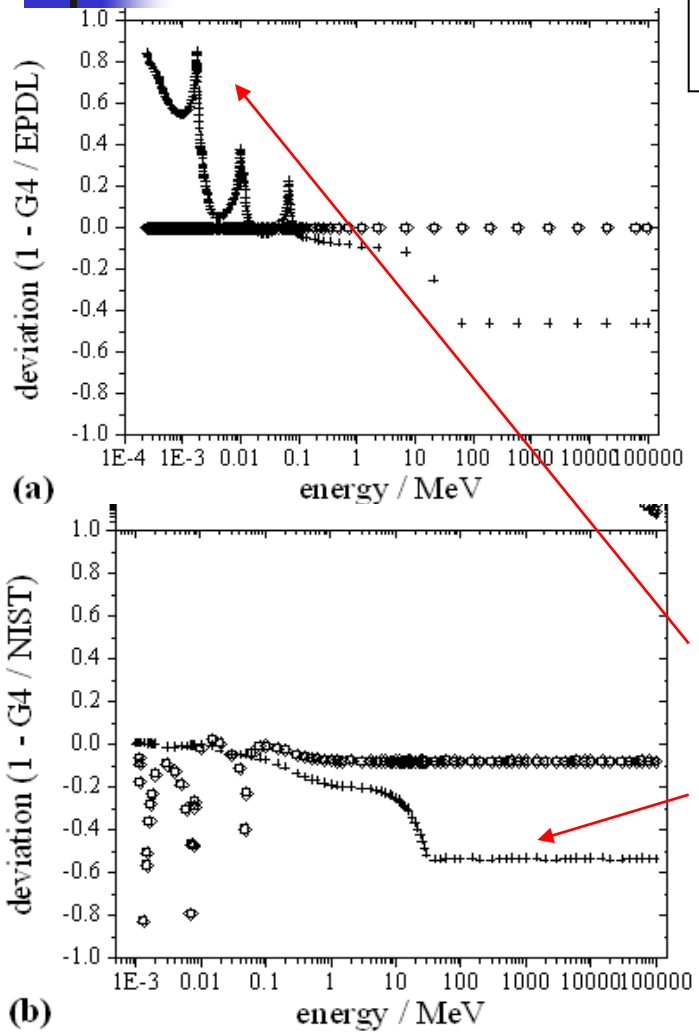
The G4Penelope package

- The Penelope models (from PENELOPE v2001) have been made available in Geant4/LowEnergyEM since versions 5.2 (γ-rays) and 6.0 ($e^{\pm}$)
  - **`G4VDiscreteProcess`** or **`G4VContinuousDiscreteProcess`**
  - Included in the comparison project against **NIST** data (eventually published on IEEE-TNS, 2005)
- Migrated to the new EM design (i.e. inherit from **`G4VEmModel`**) from version 9.3
  - Old processes presently kept for backward-compatibility (warning issued on screen)
  - Naming scheme: **`G4PenelopeXXXXModel`**
  - Used for the new comparison project against **NIST**, **EPDL97** and **SANDIA** databases (NIM A, 2010)

Comparison against databases (NIMA 618,315): a short reminder

- Photon cross sections in different elements/materials from Geant4 models compared against databases (**NIST**, **EPDL**, **SANDIA**) between 100 eV and 100 GeV
  - To be interpreted with some care, because databases are **mutually inconsistent** in some cases (especially at low energy), e.g. Compton and Rayleigh scattering
  - Livermore models are based on EPDL: only a consistency check
- All models (Standard, Livermore, Penelope) do **fairly well**
  - Only visible **problem**: Rayleigh scattering with Penelope model (problems vs. both EPDL and NIST)
  - Notice that EPDL (= Livermore) and NIST databases are inconsistent for Rayleigh scattering at low energy (NIST does not have oscillations due to atomic form factor)

Comparison: Rayleigh scattering

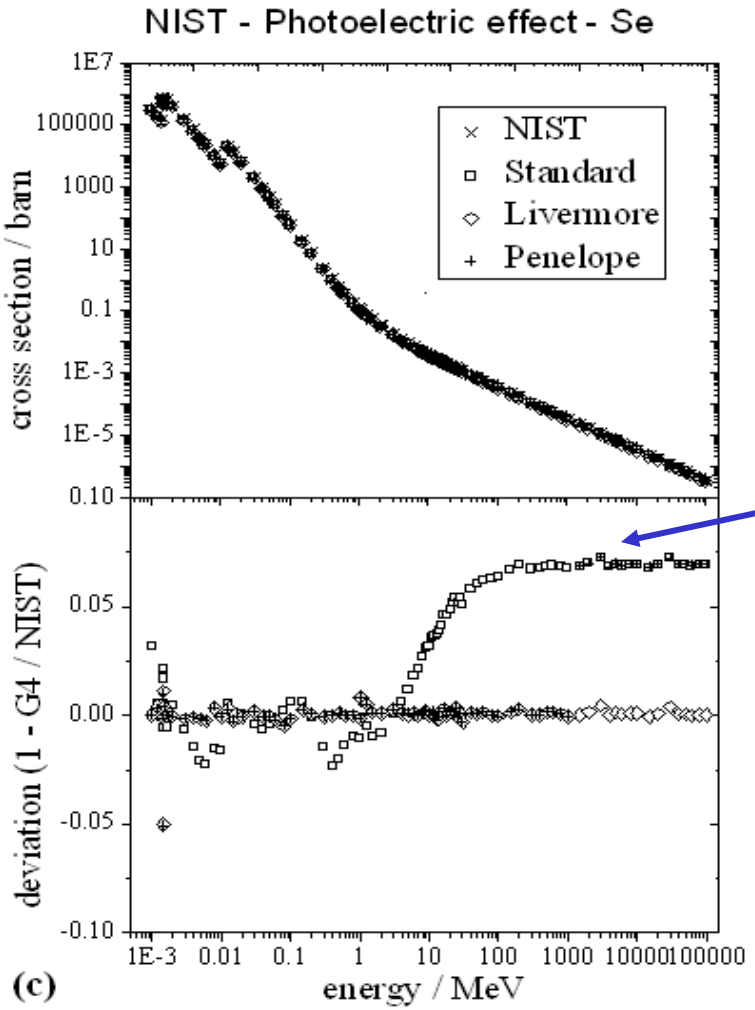


EPDL: Rayleigh on W

- **Standard model** not available for Rayleigh scattering.
- **Livermore model**: ok. Of course = EPDL. Difference to NIST < 10% above 100 keV. At lower energy, databases inconsistent
- **Penelope model**: problems both against EPDL and NIST. Model does not include atomic form factor at low energy (as NIST) and fails to reproduce the high energy behaviour

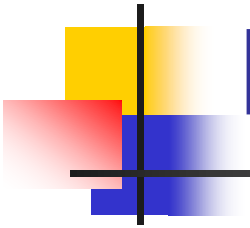
NIST: Rayleigh on Eu

Comparison: photoelectric effect



- Cross sections for photoelectric effect are better than **5%** for all models and all datasets (in the full energy range)
- Small differences in the Standard model (→ SANDIA), but in an energy range (> 10 MeV) where PE effect is irrelevant!
- Same conclusions hold for gamma conversion

Penelope v2008

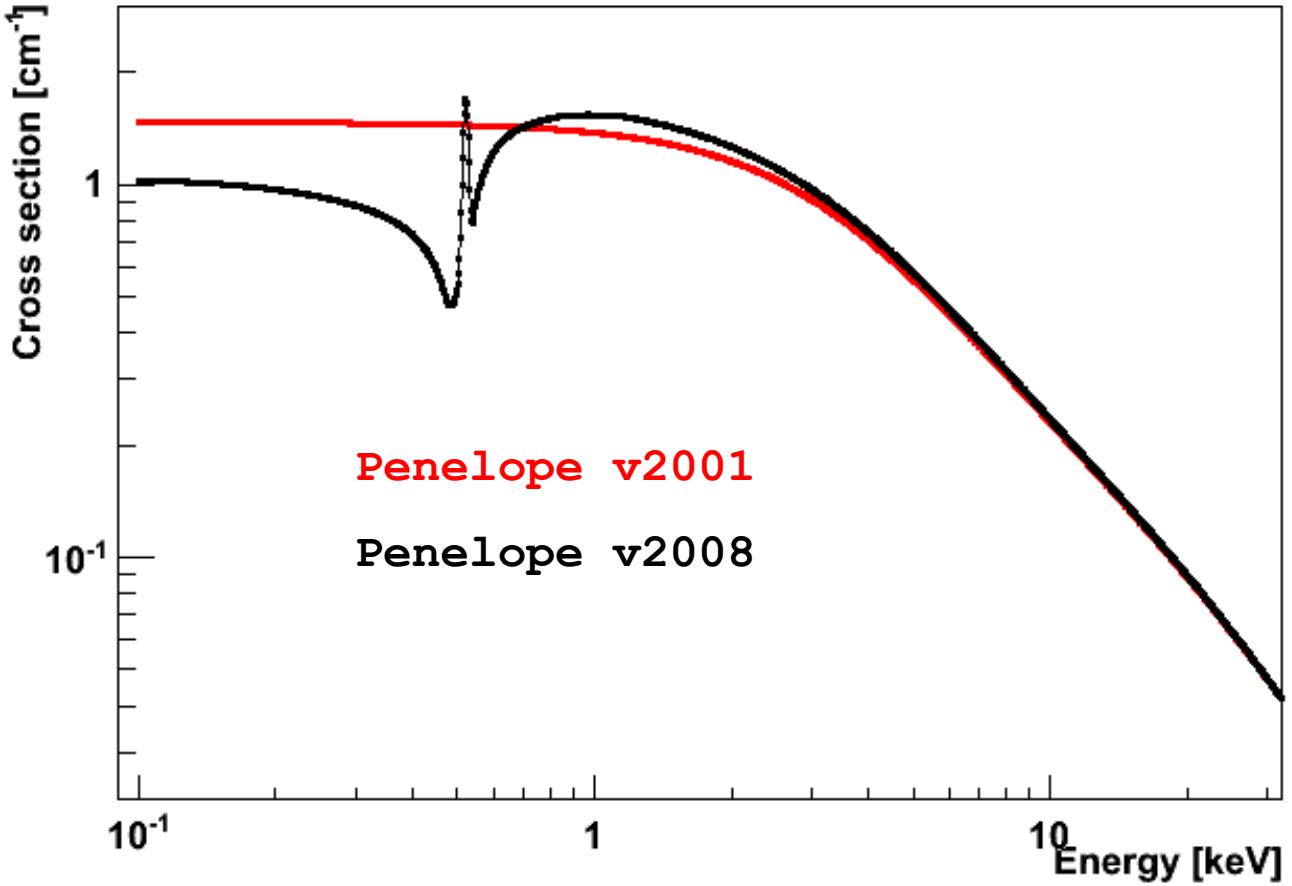


- Since v2001, the FORTRAN Penelope code had **four** releases, v2003, v2005, v2006 and v2008
- Rayleigh model underwent a major restructuring
  - Cross section is not anymore calculated analytically but read from a **database** (based on the EPDL97)
    - Different results below a few keV
  - Changed algorithm of sampling of the final state
- Other small changes in models
  - Sampling algorithm for $e^{\pm}$ ionisation
  - Changed numerical interpolations
  - Polarization effects for Rayleigh and Compton scattering
- Improvements also in the CPU

Rayleigh v2001 vs. v2008

Rayleigh scattering inverse mean free path in water

Analytical approach used in version 2001 does **not account** for **atomic structure** → difference w.r.t. database data for energies below a few keV. Use database data (from EPDL97) in v2008

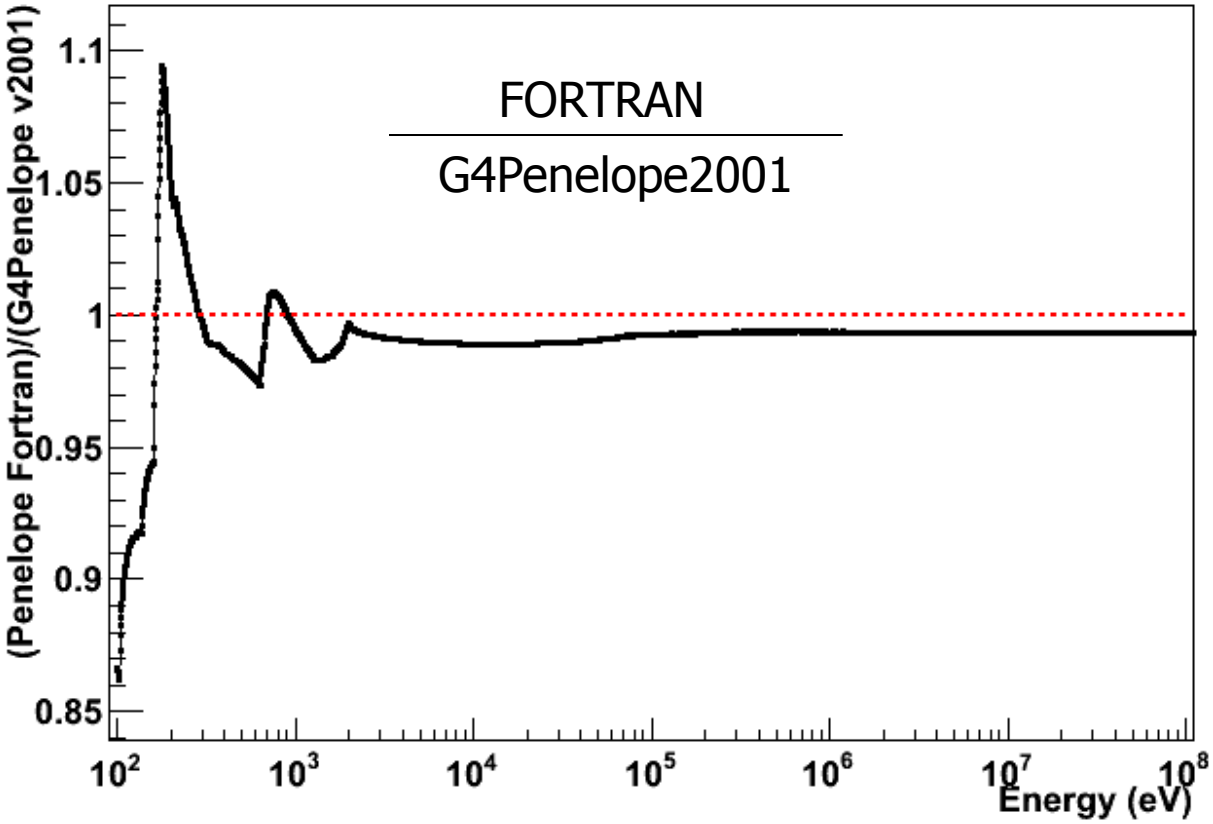


Motivations to upgrade G4Penelope to v2008

- Profit of all improvements (including CPU time) of the original FORTRAN code
  - Rayleigh scattering cross section (→ NIMA paper)
- Verify again G4Penelope models again and make sure they give the same results as FORTRAN
  - **`G4PenelopeIonisationModel`** has small fleas w.r.t. the parent FORTRAN model (but < few % and irrelevant for most sensible applications)
  - Implement the concept of molecular oscillators that is present in the FORTRAN version, but not in G4Penelope
- Take the chance for further improvements and polishing of the C++ implementation (e.g. more efficient use of memory, reduction of CPU time) w.r.t. G4PenelopeModels v2001

Fleas in G4PenelopeIonisationModel (v2001)

e- **stopping power** for ionisation in Au



Due to different approach to materials (molecular oscillators used in Penelope)

Difference **<10%** for all energies, about 1% asymptotic bias w.r.t. FORTRAN calculations

Work done up to now

G4Penelope v08 models **ready** for

- `G4Penelope08ComptonModel` ✓
- `G4Penelope08RayleighModel` ✓
- `G4Penelope08GammaConversionModel` ✓
- `G4Penelope08PhotoElectricModel` ✓
- `G4Penelope08IonisationModel` ✓

} **All** models involving **γ-rays**

To be done for

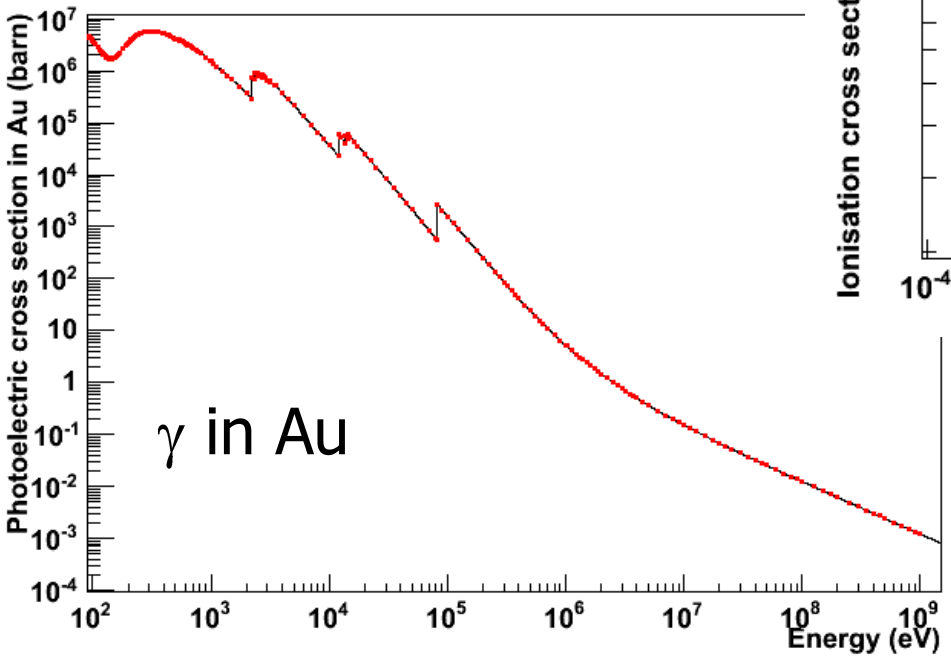
- `G4Penelope08BremsstrahlungModel` ✗ (work in progress)
- `G4Penelope08AnnihilationModel` ✗

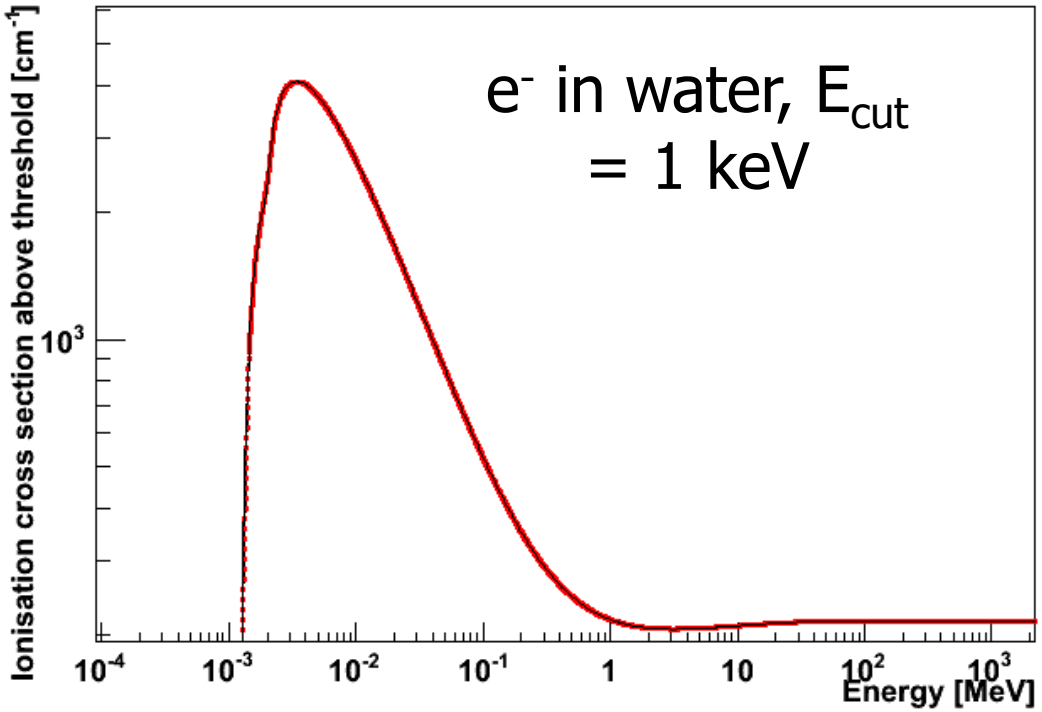
γ-ray models already **released** in **June** (9.4.beta). $e^{\pm}$ models perhaps ready for the **December release** (9.4)

A few examples (XSs)

PENELOPE Fortran

G4Penelope08

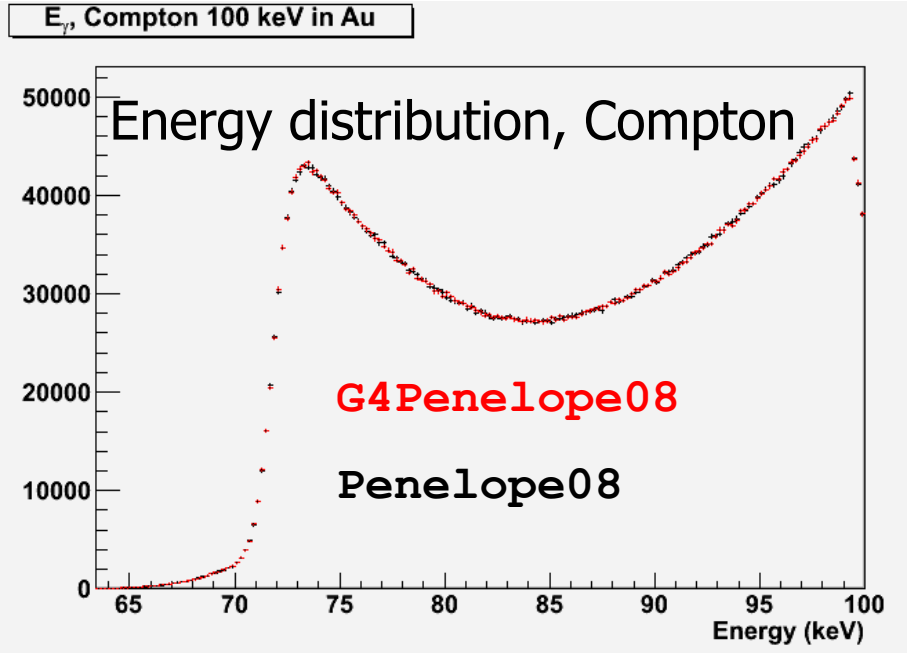


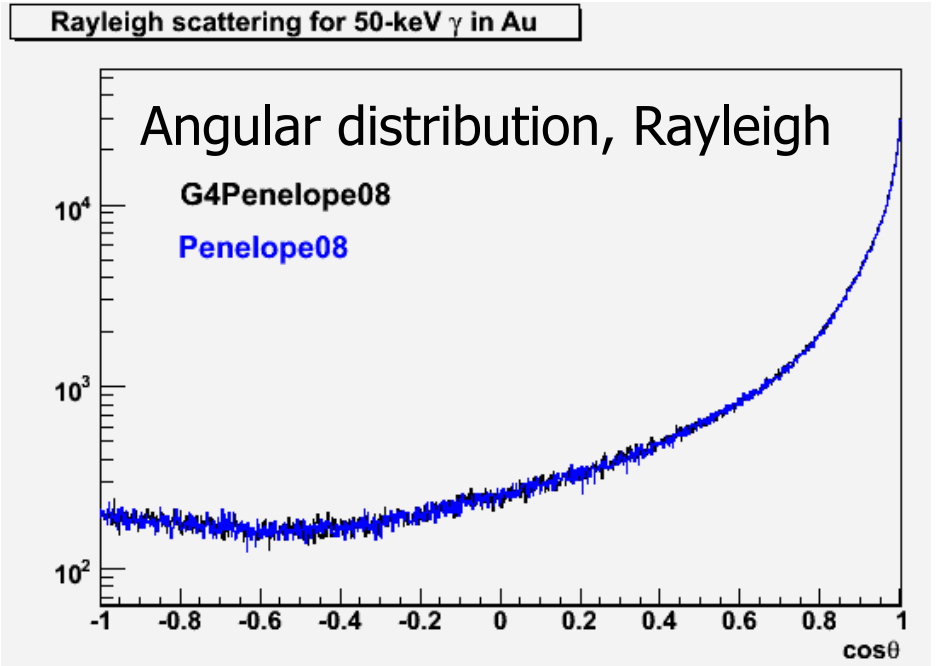


The G4Penelope models reproduce the same cross section and stopping power tables as FORTRAN

A few examples (final states)

- Final states less straightforward to compare than cross sections. Produce 10^7 events per each run using **TestEm14**.
- Test at least two materials (e.g. Water and Au) with two energies (<100 keV and >1 MeV)

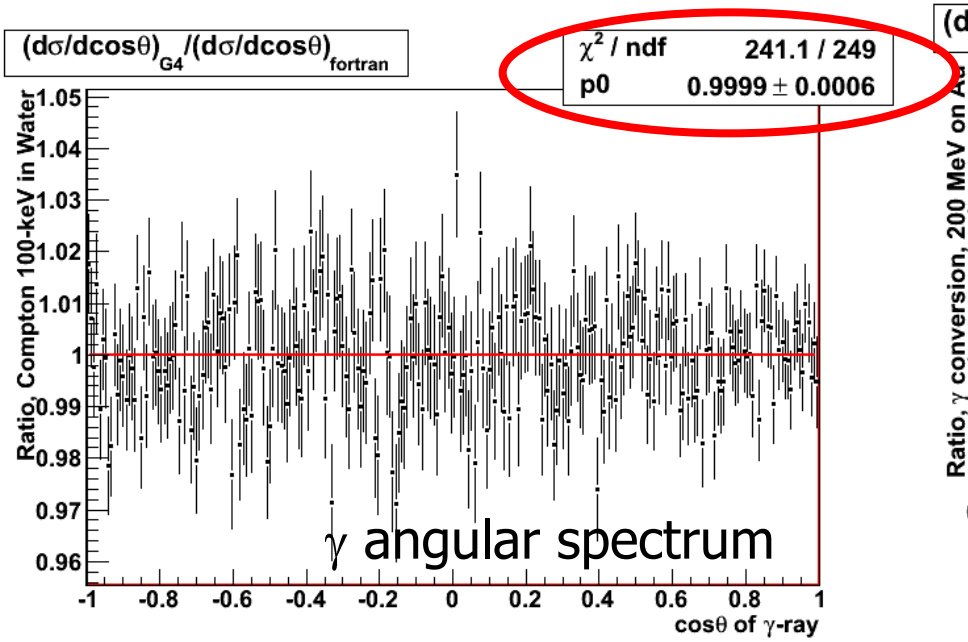




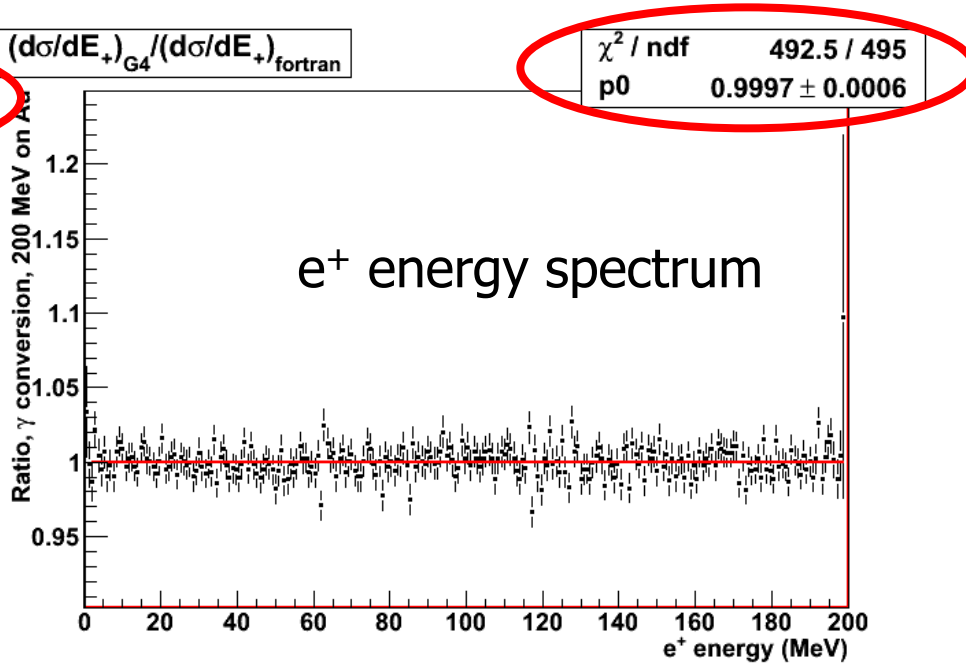
A few examples (final states)

- Quantitative agreement measured by χ^2
  - test that the **bin-per-bin histogram ratio** is flat and consistent with 1

Compton, 100 keV in Water



γ-conversion, 200 MeV in Au



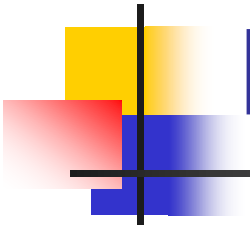
Interplay v2001 and v2008

- In a while, there will be **3 different classes** for each Penelope model
  - **`G4PenelopeXXXX`** (old process, v2001)
  - **`G4PenelopeXXXXModel`** (v2001 model, migrated)
  - **`G4Penelope08XXXXModel`** (v2008 model)

  } Same physics

- Plan: avoid the excessive proliferation of physics models (confusing to user).
  - In 9.4 give both v2001 and v2008 (v2008 as "beta"), with their database files
  - From December 2011, keep only v2008 (**renamed** as **`G4PenelopeXXXXModel`**) → **transparent** upgrade to users. Remove completely v2001 and the corresponding database files
  - Old processes will be erased anyway (obsolete)

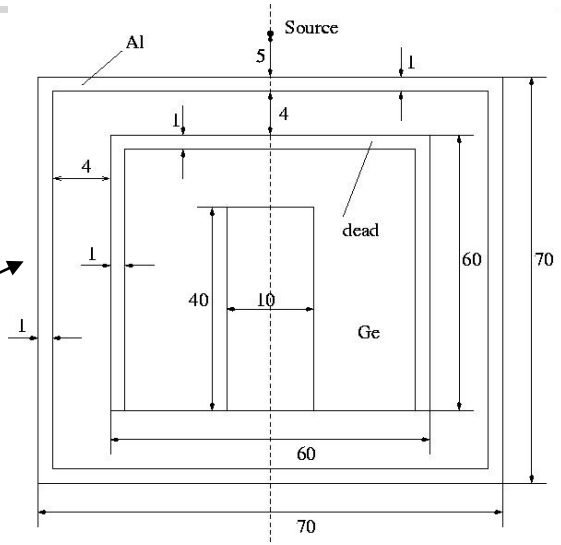
Database organization

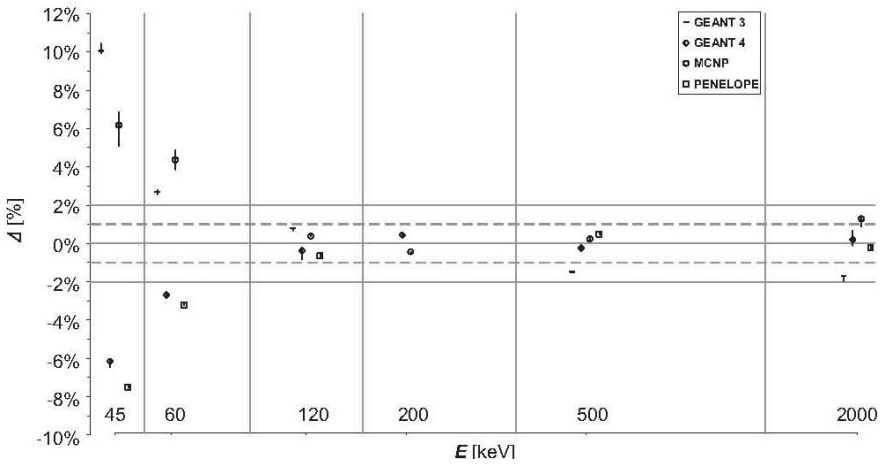


- A few G4Penelope08 models require database files
  - In some cases, the information is the same as in the files used for G4Penelope01
- General policy now:
  - **`$G4LEDATA/penelope/[process]/*.p08`**
    - E.g. **`$G4LEDATA/penelope/rayleigh/pdgra01.p08`**
    - More tidy than for G4Penelope01 (all files in the main directory **`$G4LEDATA/penelope`**)
  - The format of the database files is **exactly the same** as in PENELOPE/FORTRAN
    - Files used for G4Penelope v2001 have a different format (conversion step from the original file)
    - At the moment, a lot of information is duplicated in the database (same info contained in two files, having different format)
- Plan: dismiss the old database files together with the G4Penelope v2001 models (and processes)

Intercomparison exercise

- In 2007 a **"comparison exercise"** has been performed within the **γ-ray spectrometry** community
- Goal: compare detection efficiencies predicted by different MC codes for a given (simplified) geometry of interest
  - each participant submitted the results calculated with his/her favourite MC code
  - participants used Geant4, Geant3, PENELOPE, MCNP, EGS et al.
- Appl. Rad. Isotopes 66 (2008) 764
  - found differences **up to 10%** at very low energy. Typically < few %
- Use this setup as a benchmark for the existing and new EM models in Geant4

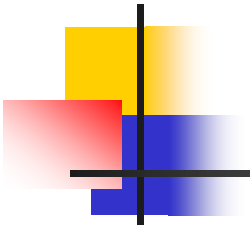




Intercomparison exercise

- For instance, geant4-09-03-ref-07 at E=120 keV
  - ε = (2.49 ± 0.05)% with Penelope08*
    *bremsstrahlung from Penelope01
  - ε = (2.51 ± 0.05)% with Livermore
  - ε = (2.57 ± 0.05)% with StdOption3
- Reference from the intercomparison:
  - ε = (2.556 ± 0.003)% median from Geant3 (3 res.)
  - ε = (2.527 ± 0.002)% median from Geant4 (5 res)
  - ε = (2.546 ± 0.004)% median from MCNP (3 res)
  - ε = (2.520 ± 0.003)% median from Penelope (7 res)

Work in progress



Summary

- All EM physics processes available in the LowEnergy package **migrated** to the new design as **`G4VEmModel`** since version 9.3
- Cross sections for γ-ray models compared to various databases
  - found a **fair agreement**
- The upgrade of Penelope models in Geant4 from v2001 to v2008 is ongoing
  - fixes the issue of Rayleigh cross section
  - other improvements in physics modeling
  - try to improve also CPU performances and memory management
  - full set possibly ready for release in December
- Plan to **dismiss** the **old models** and processes (and **database**) with Penelope2001 physics