Upgrade of G4Penelope models

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The G4Penelope package

- The Penelope models (from PENEOLOPE v2001) have been made available in Geant4/LowEnergyEM since versions 5.2 ($\gamma$-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± 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.

Penelope v2001
Penelope 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 $\gamma$-rays

To be done for
- G4Penelope08BremsstrahlungModel × (work in progress)
- G4Penelope08AnnihilationModel ×

$\gamma$-ray models already released in June (9.4.beta). $e^\pm$ models perhaps ready for the December release (9.4)
A few examples (XSSs)

PENELOPE Fortran
G4Penelope08

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

\[ e^{-} \text{ in water, } E_{\text{cut}} = 1 \text{ keV} \]

\[ \gamma \text{ in Au} \]

[Graphs showing cross sections and ionisation cross sections above threshold]
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)

**Energy distribution, Compton**
- G4Penelope08
- Penelope08

**Angular distribution, Rayleigh**
- G4Penelope08
- Penelope08
A few examples (final states)

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

**Compton, 100 keV in Water**

![Compton, 100 keV in Water](image)

$\gamma$ angular spectrum

$\frac{\langle d\sigma/d\cos\theta \rangle_{G4}}{\langle d\sigma/d\cos\theta \rangle_{\text{fortran}}} \chi^2 / \text{ndf} = 241.1 / 249$

$p0 = 0.9999 \pm 0.0006$

**$\gamma$-conversion, 200 MeV in Au**

![$\gamma$-conversion, 200 MeV in Au](image)

$\frac{\langle d\sigma/dE_+ \rangle_{G4}}{\langle d\sigma/dE_+ \rangle_{\text{fortran}}} \chi^2 / \text{ndf} = 492.5 / 495$

$p0 = 0.9997 \pm 0.0006$

$e^+$ energy spectrum
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)

- **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 \(\gamma\)-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.
  - 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
  - $\varepsilon = (2.49 \pm 0.05)\%$ with Penelope08*
    *bremsstrahlung from Penelope01
  - $\varepsilon = (2.51 \pm 0.05)\%$ with Livermore
  - $\varepsilon = (2.57 \pm 0.05)\%$ with StdOption3

- Reference from the intercomparison:
  - $\varepsilon = (2.556 \pm 0.003)\%$ median from Geant3 (3 res.)
  - $\varepsilon = (2.527 \pm 0.002)\%$ median from Geant4 (5 res)
  - $\varepsilon = (2.546 \pm 0.004)\%$ median from MCNP (3 res)
  - $\varepsilon = (2.520 \pm 0.003)\%$ median from Penelope (7 res)
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