PENELOPE. A code system for Monte Carlo simulation of electron and photon transport

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Introduction

- **PENELOPE** is an acronym for "**P**enetration and **ENE**rgy **LO**ss of **P**ositrons and **E**lectrons"
- **A general-purpose Monte Carlo simulation code system** with
  - Realistic, well defined interaction models
  - Fast and accurate random sampling algorithms
  - Efficient tools for tracking particles through complex geometries (constructive quadric geometry)
  - Complementary tools: variance reduction, transport in electro-magnetic fields, tabulation of macroscopic interaction parameters, ...
- **Distributed by the OECD/Nuclear Energy Agency Data Bank (Paris) and the RSICC (Oak Ridge).**
  More than 1,000 copies distributed
  List server: **http://www.oecd-nea.org/lists/penelope.html**
- **Main applications:**
  - Radiotherapy and Nuclear Medicine
  - Dosimetry and radiation metrology
  - Electron microscopy (SEM, electron-probe microanalysis)
  - Detector response, x-ray generators, ...

Introduction

- **Main reference:** very detailed manual, free hard copies available

  F. Salvat, J.M. Fernández-Varea and J. Sempau
  PENELOPE-2011: A Code System for Monte Carlo Simulation of Electron and Photon Transport
  OECD NEA Data Bank/NSC DOC(2011)/5
  (OECD Nuclear Energy Agency, Issy-les-Moulineaux, 2011)
  http://www.oecd-nea.org/dbprog/courses/penelope-2011.pdf

- **Other references:**

  J. Baró, J. Sempau, J.M. Fernández-Varea and F. Salvat
  "PENELOPE: an algorithm for Monte Carlo simulation of the penetration and energy loss of electrons and positrons in matter"
  Nucl. Instrum. Meth. B **100** (1995) 31–46

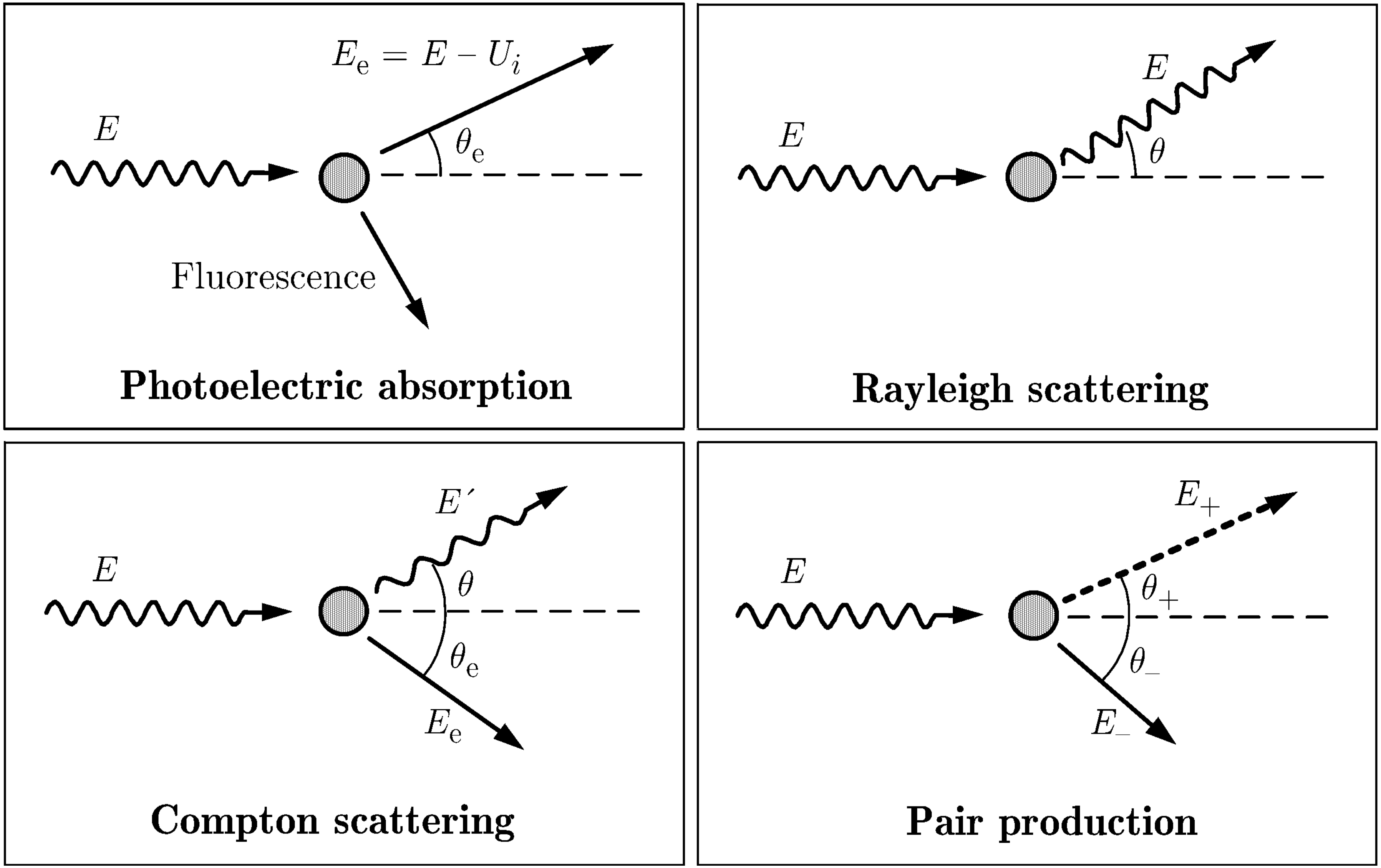
  J. Sempau, J.M. Fernández-Varea, E. Acosta and F. Salvat
  "Experimental benchmarks of the Monte Carlo code PENELOPE"
  Nucl. Instrum. Meth. B **207** (2003) 107-123

  F. Salvat and J. M. Fernández-Varea
  "Overview of physical interaction models for photon and electron transport used in Monte Carlo codes"
  Metrologia **46** (2009) S112–S138

Main features

- All kinds of interactions (except nuclear reactions) in the energy range from 50 eV to 10^9 eV
- Implements the most accurate physical models available, limited only by the required generality
- Uses an elaborate mixed scheme to simulate the transport of high-energy electrons and positrons
- Simulates fluorescent radiation from K, L, M and N shells
- Subroutine package **pengeom** for tracking particles in quadric geometries (*i.e.*, material systems consisting of homogeneous bodies limited by quadric surfaces)
- Electron and positron transport in electric and magnetic fields (in matter)
- Scattering of polarized photon beams (synchrotron)

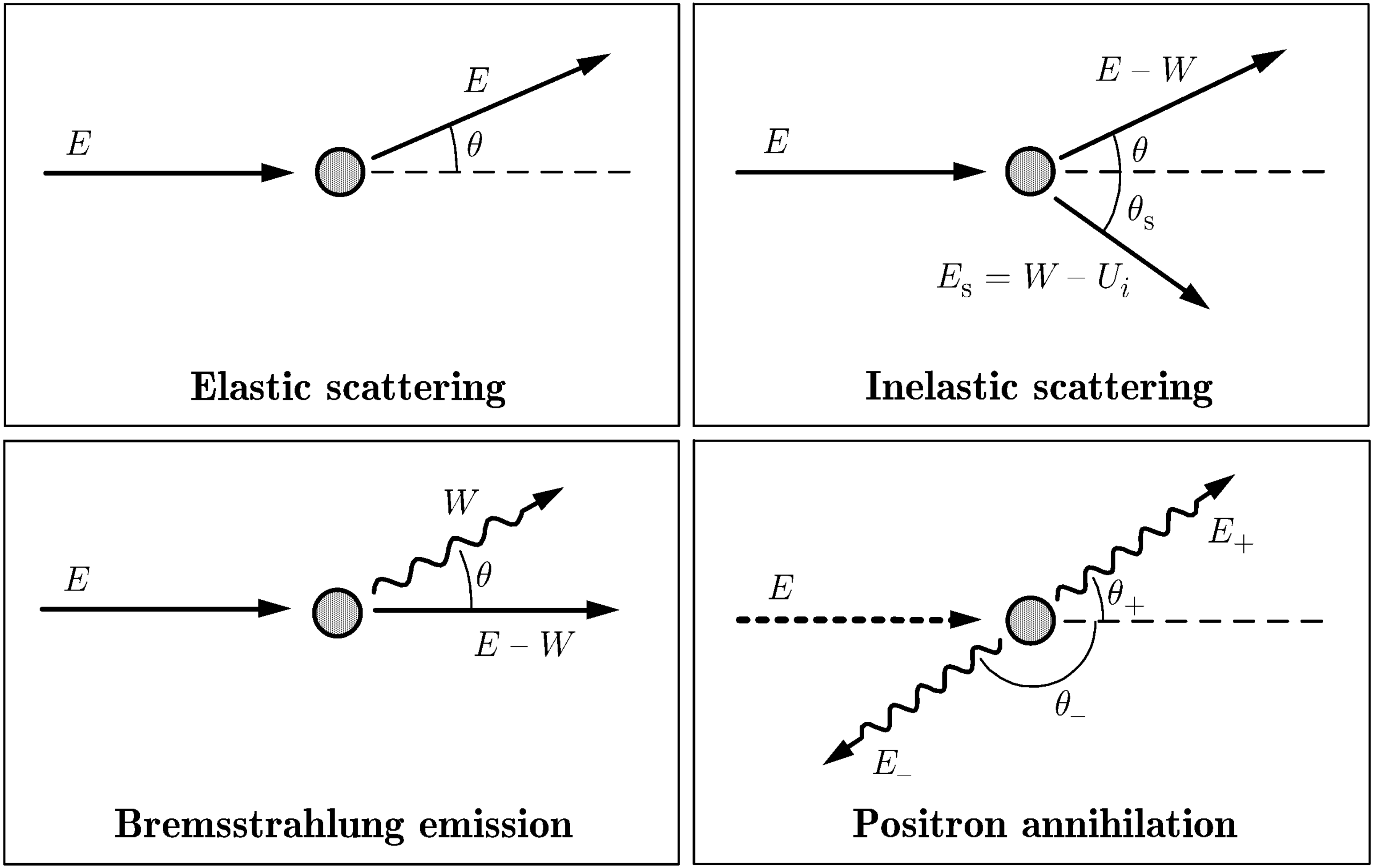
Interactions of photons



$m_e c^2 \simeq 511$ keV, electron rest energy

- **Photoelectric effect:**
  - Total cross sections calculated from the DHFS atomic potential (equivalent to Scofield's LLNL database; Cullen *et al.*, 1997)
  - Angular distribution of photoelectrons from Sauter's (1931) formula (plane-wave Born approximation for K-shell hydrogenic ions)
  - Atomic relaxation from the EADL (Perkins *et al.*, 1991)
- **Coherent (Rayleigh) scattering:**
  - Total cross sections from the EPDL (Cullen *et al.*, 1997), includes anomalous atomic scattering factors
  - Angular distribution from atomic form factors
- **Incoherent (Compton) scattering:**
  - Double-differential cross sections (DDCS) calculated from the relativistic impulse approximation (Ribberfors, 1983) using analytical Compton profiles (Brusa *et al.*, 1996)
  - Total cross sections obtained as integrals of the DDCS
  - Subsequent atomic relaxation from the EADL (Perkins *etal.*, 1991)
- **Electron-positron pair production:**
  - Total cross sections from the EPDL (Cullen *et al.*, 1997), includes triplet production
  - Energies and directions of the pair particles from the Bethe-Heitler theory

Interactions of electrons and positrons



$m_e c^2 \simeq 511$ keV, electron rest energy

- **Elastic collisions:**
  - Atomic differential cross sections (DCS) calculated using the Dirac partial-wave expansion method (ICRU 77, 2007)
  - High-energy modified Wentzel model with correct first and second moments (ICRU 77, 2007) for energies above 100 MeV

- **Inelastic collisions:**
  - DDCS from the Born approximation, using the Sternheimer-Liljequist GOS model, with resonance energies fitted to reproduce the mean excitation energies from ICRU 37 (1984)
  - Secondary electrons emitted in the direction of momentum transfer

- **Bremsstrahlung emission:**
  - Photon-energy scaled DCSs of Seltzer and Berger (1985, 1986)
  - Photon angular distribution fitted to partial-wave data of Kissel *et al.* (1983)

- **Impact ionization of inner shells**
  - Total cross sections for K, L and M shells calculated from the distorted-wave Born approximation (Bote *et al.*, 2009)
  - Subsequent atomic relaxation from the EADL (Perkins *et al.*, 1991)

Electron/positron transport mechanics

- **Mixed simulation algorithm:**

PENELOPE uses a pure class II (mixed) algorithm for electrons/positrons. Allows verifying the stability under variations of simulation parameters

Hard interactions (with angular deflection larger than a cutoff angle θ_c or energy loss larger than selected cutoffs) **are simulated individually**

- **Hard elastic interactions:**

The cutoff angle is determined by two user parameters, C_1 and C_2 , according to the formula (Eq. 4.85 of the manual)

$$\lambda_{\rm el}^{\rm (h)}(E) = \max\left\{\lambda_{\rm el}(E), \min\left[C_1\lambda_{\rm el,1}(E), C_2\frac{E}{S(E)}\right]\right\}$$

- **Hard energy loss events:**

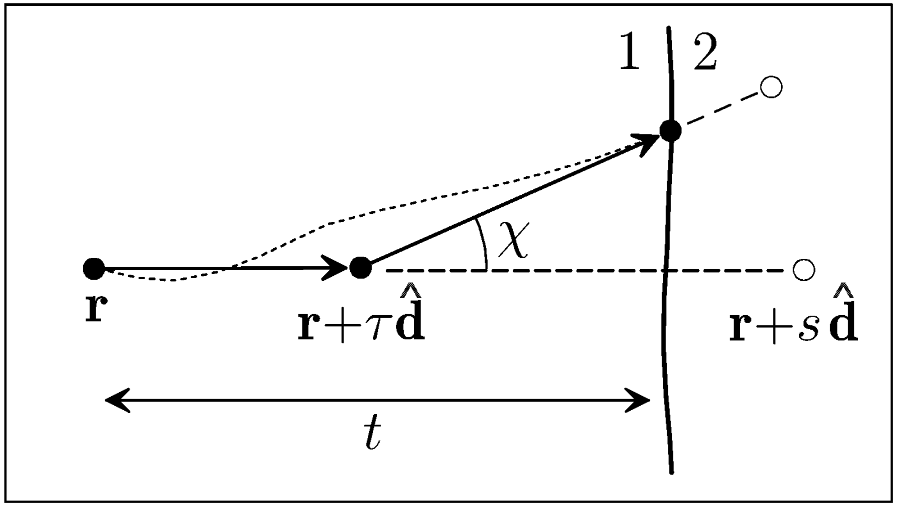
The user defines the cutoff energies $W_{\rm cc}$ (col) and $W_{\rm cr}$ (brems), in accordance with the required energy resolution

- **Maximum allowed step length between hard interactions:**

An additional parameter, $s_{\rm max}$, sets a limit to the step length (needed to account for the variation of energy along the step, and for consistency of the simulation of soft events)

Electron/positron transport mechanics

- **Simulation of soft interactions:** Random hinge method
  - The global effect all the soft interactions in a step s between a pair of hard interactions is simulated as a single event, a **hinge**
  - The angular deflection and the energy loss at the hinge are sampled from approximate distributions having the correct first and second moments
  - The position of the hinge, τ, is sampled uniformly in $(0,s)$
    $\Rightarrow$ simple and accurate scheme for interface crossing



- Includes elaborate corrections to account for the variation of energy along the step

Role/effect of the simulation parameters

- **Step-length control (for each material):**

C_1 limits the average angular deflection per step, $1 - \langle \cos\theta \rangle \lesssim C_1$
Influences the simulation speed only at intermediate energies

C_2 limits the average fractional energy loss per step, $\langle E_0 - E \rangle \lesssim C_2 E_0$
Affects simulation speed only at high energies

- **Energy-straggling control (for each material):**

W_{cc} energy-loss threshold (in eV) for hard inelastic collisions

W_{cr} energy-loss threshold (in eV) for hard bremsstrahlung events

These cutoffs govern energy resolution. Mild effect on speed

- **Geometrical constraints (local):**

s_{max} maximum step length for "critical" geometries (needed for thin bodies, backscattering, ...)

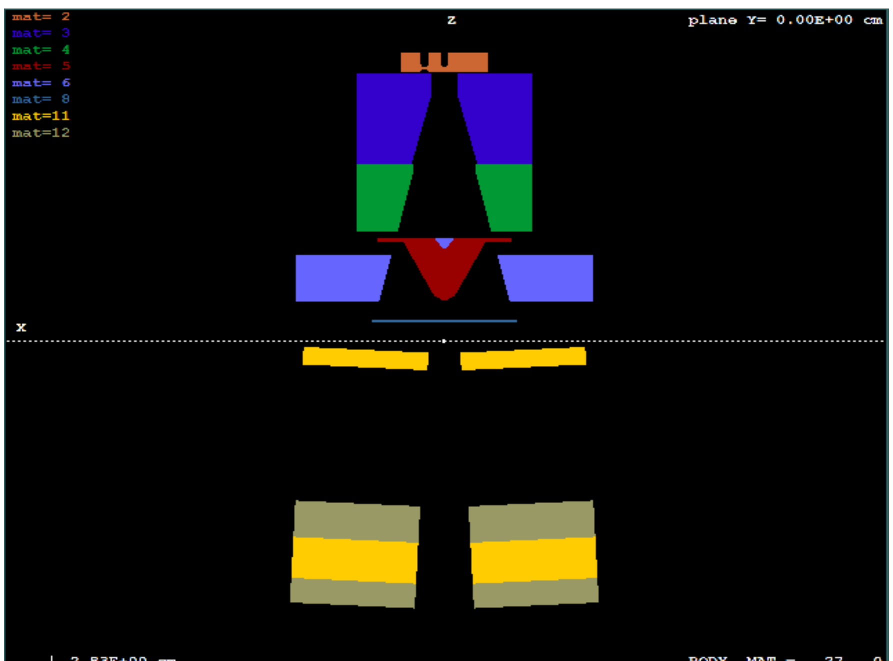
- **Reasonable "blind" choices:**

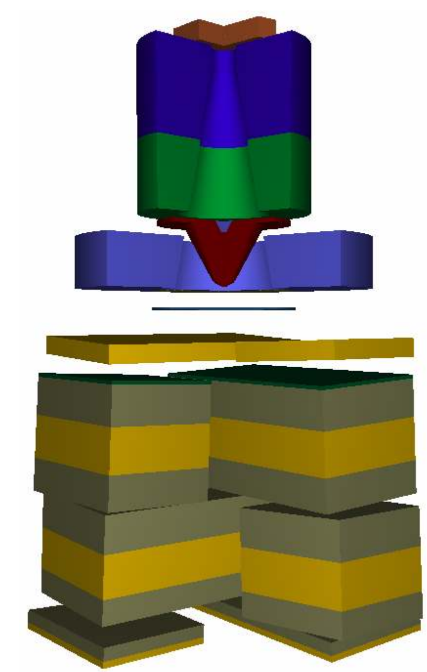
C_1 and C_2 : 0.05 to 0.1; W_{cc} and W_{cr} : ~ 1,000 eV
s_{max} : one tenth of the minimal thickness

Transport in complex geometries

- **The subroutine package PENGEOM**
  - Tracks particles within material systems consisting of homogeneous bodies limited by (fuzzy) quadric surfaces
  - Highly accurate (effective nm resolution near the origin)
  - Tailored to minimize numerical work
  - Generally applicable to detailed and mixed simulations
- **Geometry viewers:** 2- and 3-dimensional viewers are provided
  - Images of the geometry are rendered by using the tracking routines

  $\Rightarrow$ what you see is what is passed to the simulation program





Structure of the code system

- The **PENELOPE** code system consists of
  - The subroutine package **penelope.f**, which defines the interaction properties of materials and performs the simulation of interactions
  - The geometry package **pengeom.f**, and the 2D and 3D viewers (**gview2d.exe** and **gview3d.exe**)
  - The variance-reduction routines **penvared.f** (include particle splitting, Russian roulette, interaction forcing, and delta scattering of photons)
  - The **database**: 995 ascii files with interaction cross sections and other properties of the elements Z=1−99 (hydrogen to einstenium)
  - Steering main programs for cylindrical and quadric geometries, **pencyl.f** and **penmain.f**. They can simulate a variety of radiation sources, allowing scoring of different transport properties
  - Routines **penfield.f** for tracking charged particles in static electro-magnetic fields

- ...

  - Program **tables.f** for displaying plots of energy-dependent interaction properties. Macroscopic quantities are made available numerically and graphically

  - A program for displaying electron-photon showers in material slabs, **shower.exe**

  - Documentation: **Manual and tutorial**

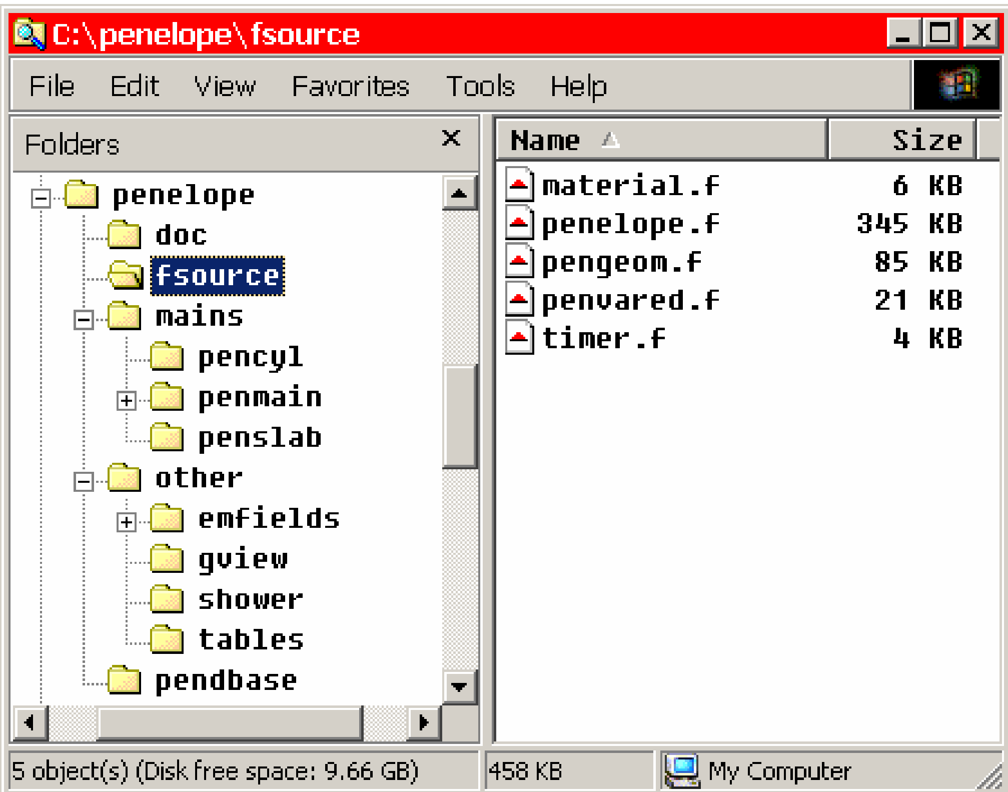
- All source programs are written in Fortran, *i.e.*, they can be run on any operating system with a Fortran compiler

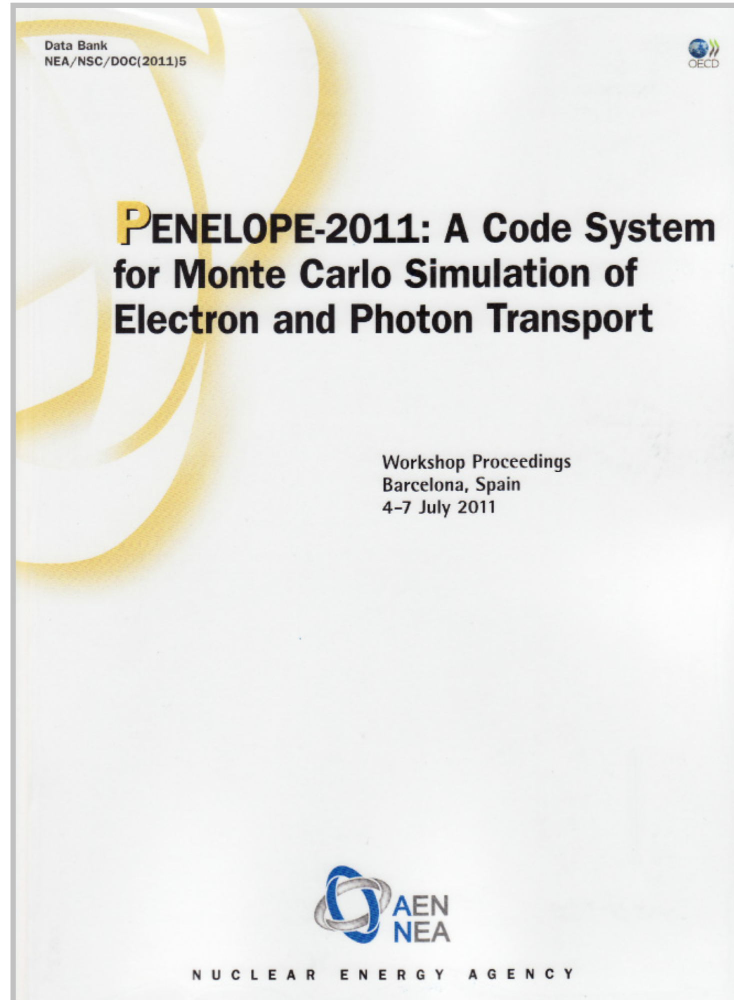
- The geometry viewers **gview2d** and **gview3d**, and the program **shower** work only on MS Windows (for the time being)

- The output of the simulation programs and of **tables.f** is formatted for visualization with the plotting program **gnuplot,** available for Windows and Linux (**http://www.gnuplot.info**)

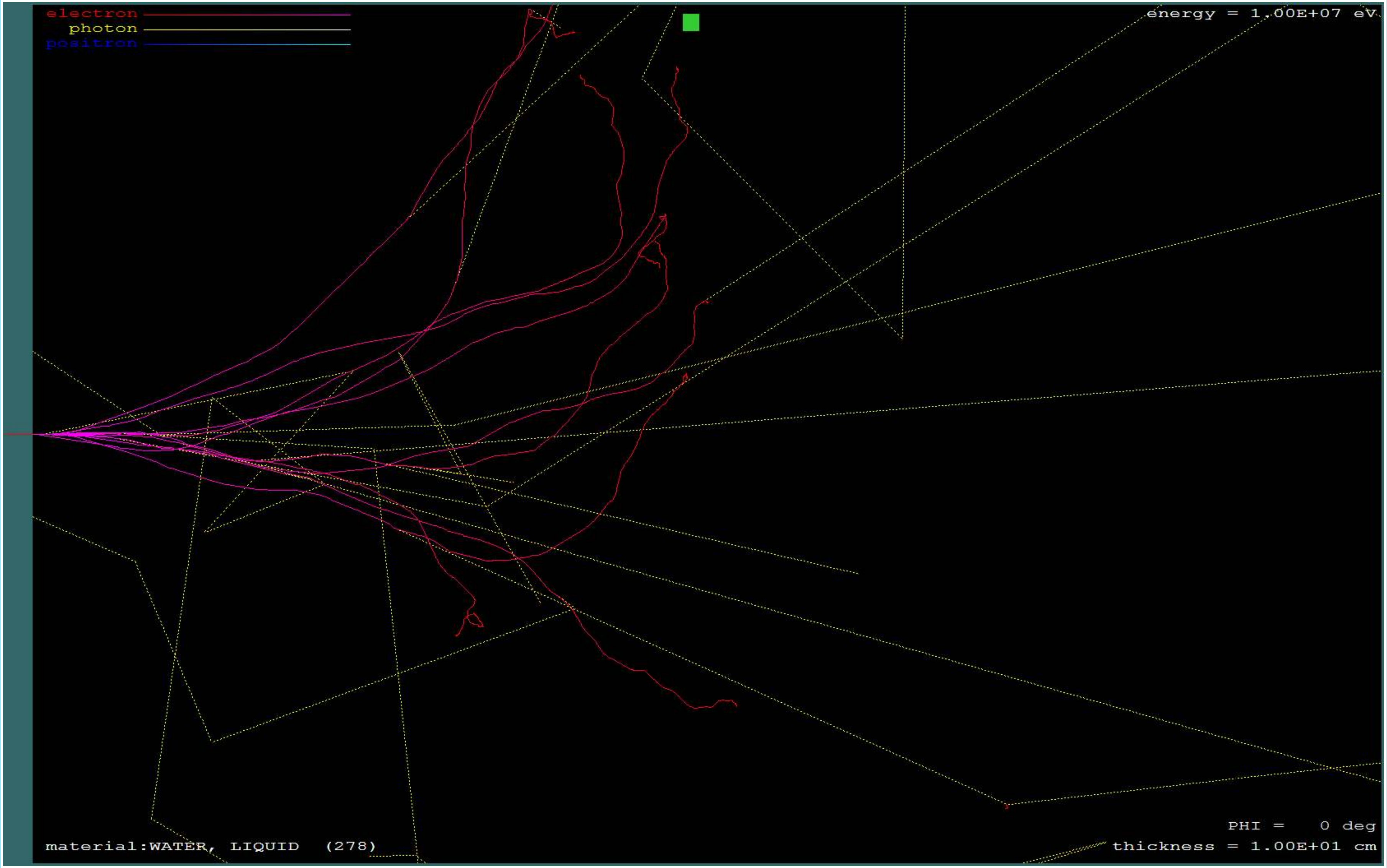
Distribution package

- A single zip compressed file, penelope.zip (~74 Mb)

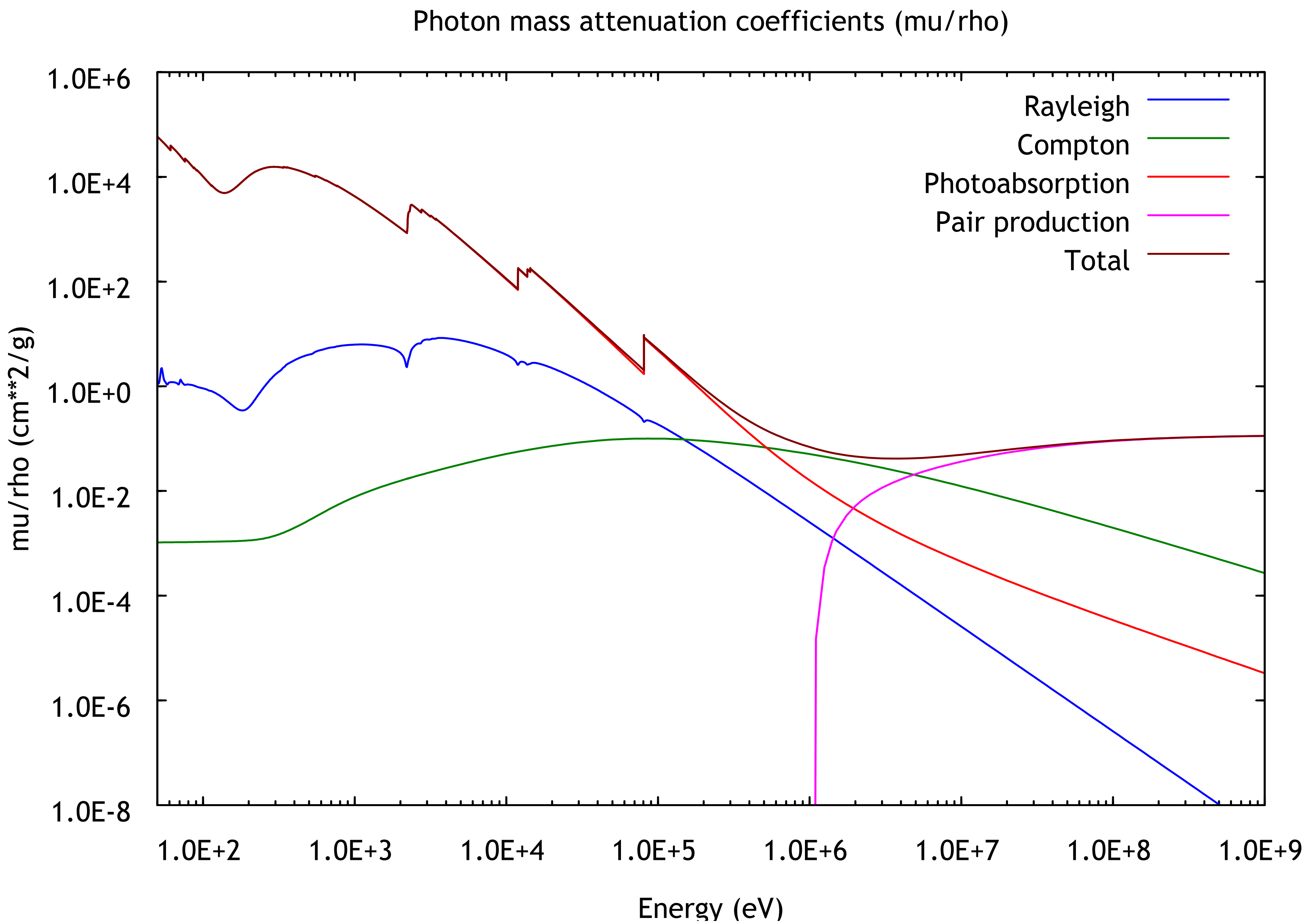




Screenshot of "shower": 10 MeV electrons in water

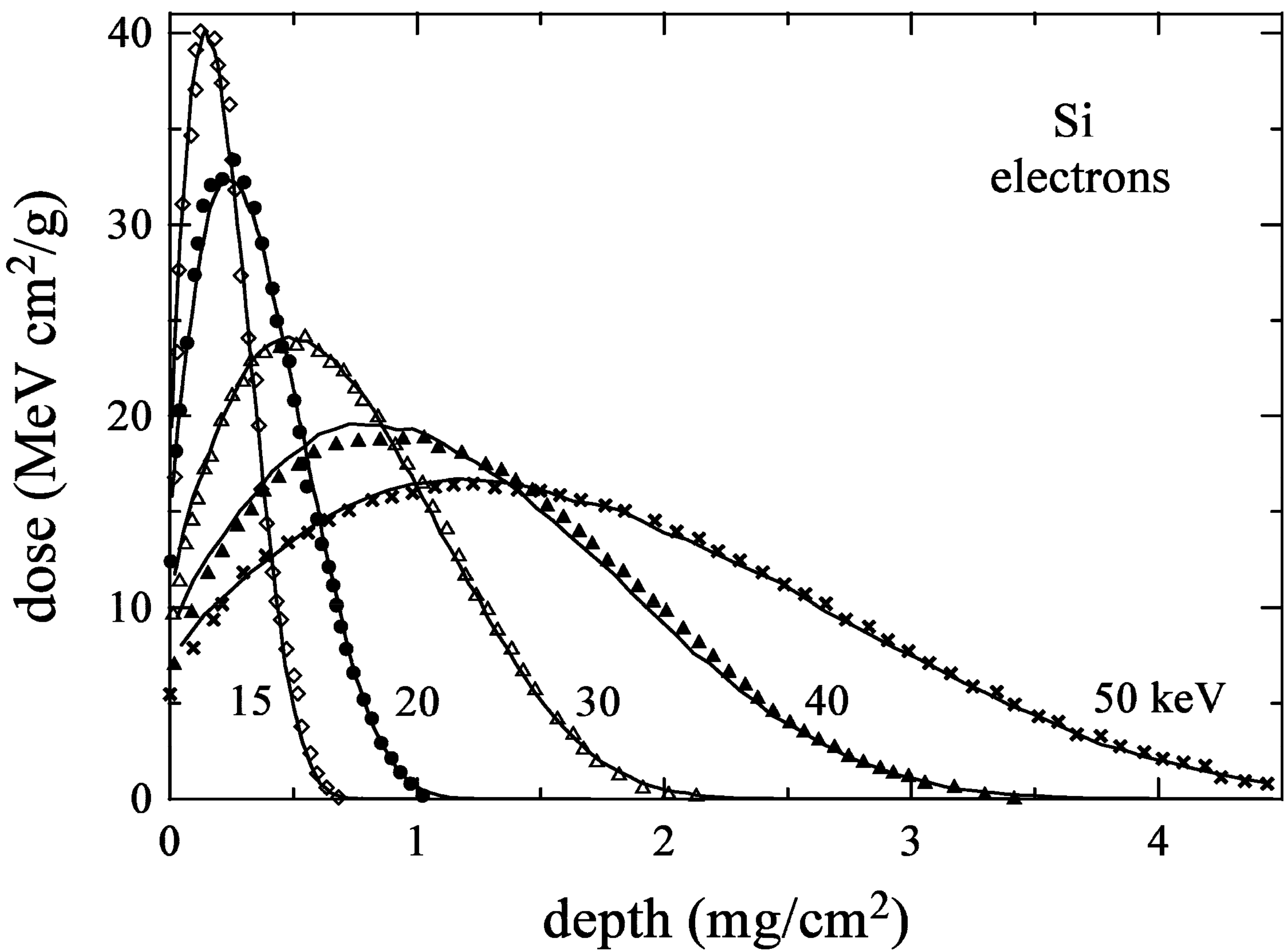


Screenshot of "tables": photons in gold



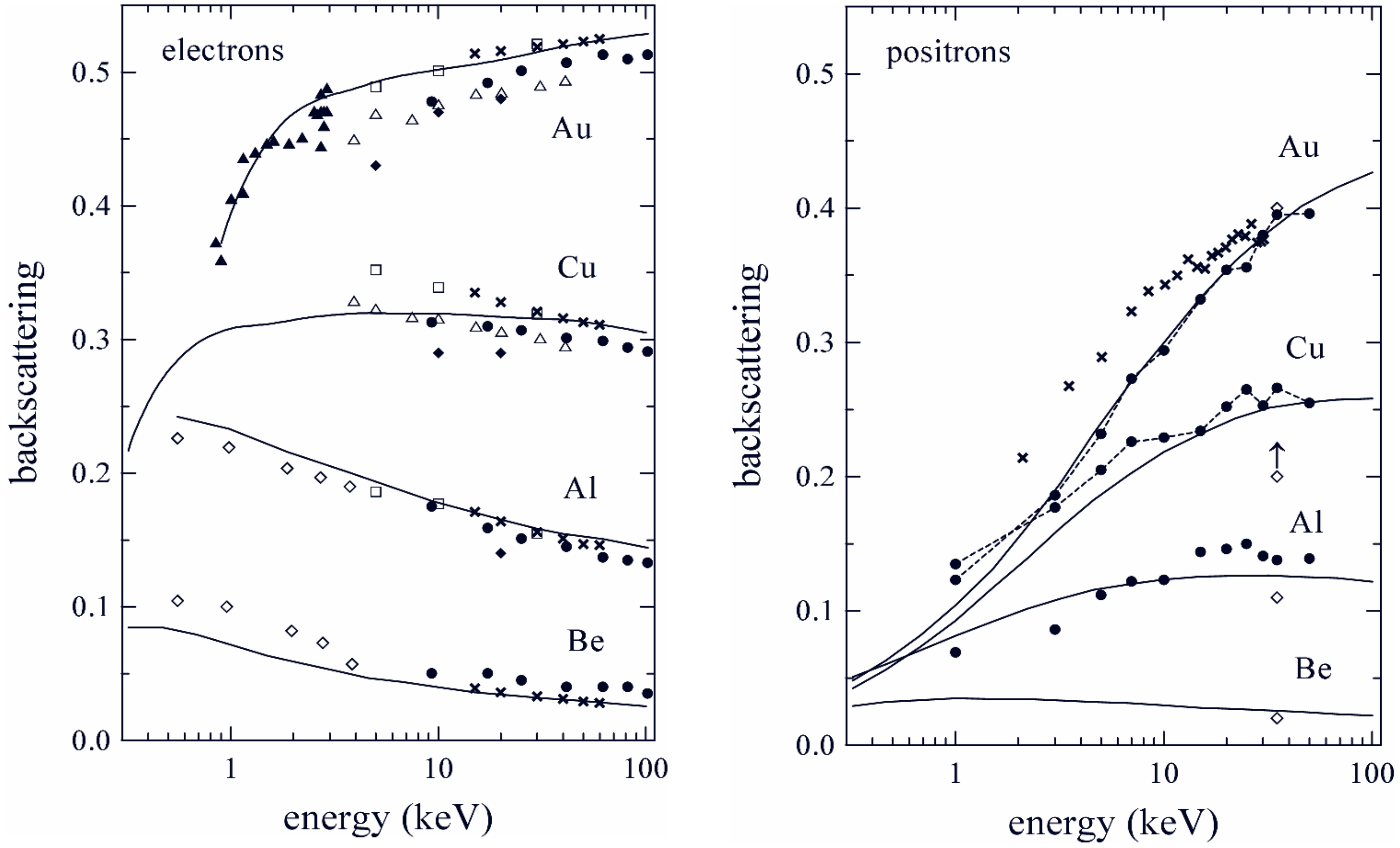
Example: depth-dose distribution, electrons in Al

- Experiment of Werner *et al.*, *JPD* (1988)



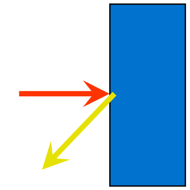
Example: backscattered fractions of electrons and positrons

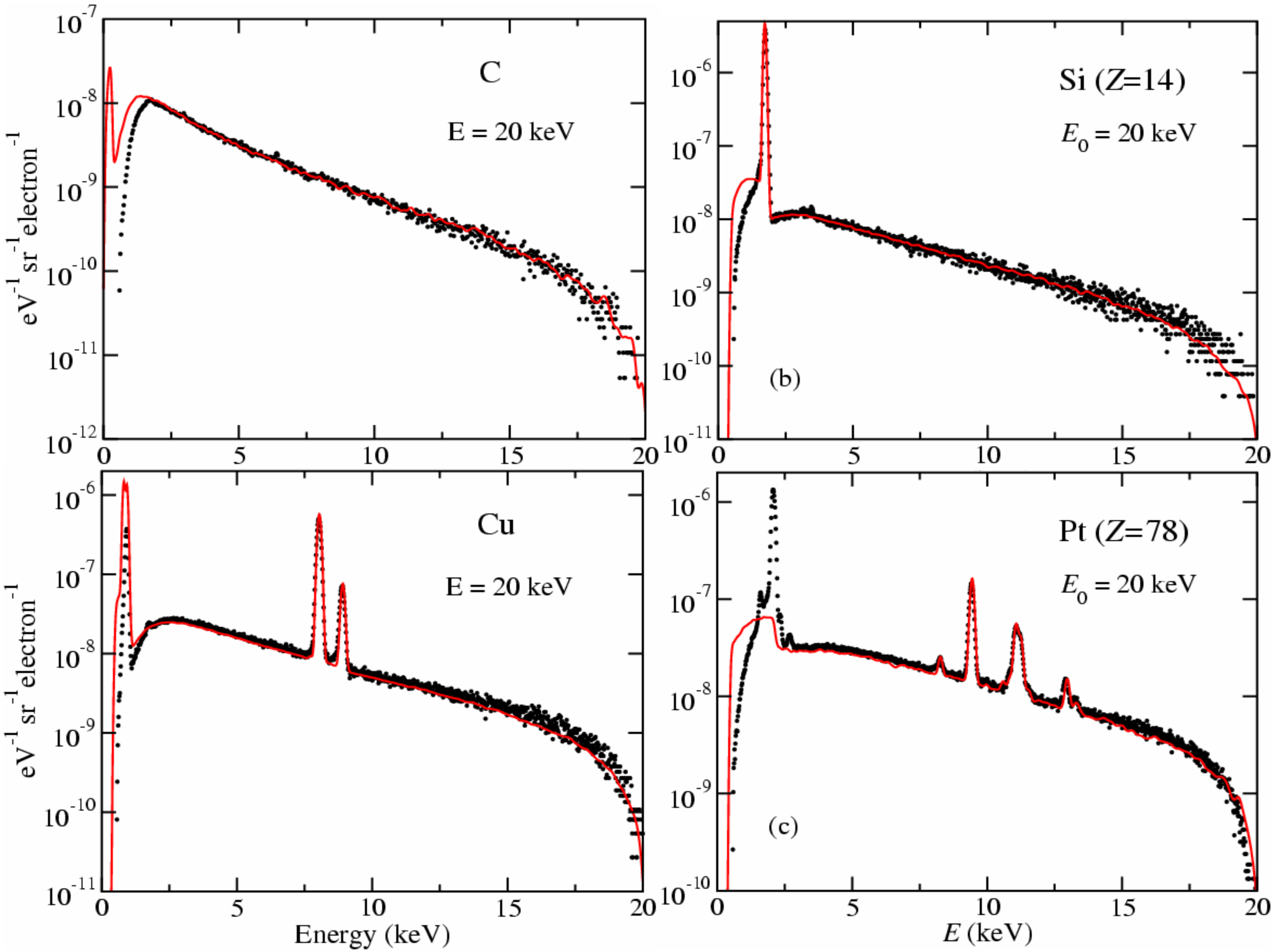
- Experimental data from different authors (Sempau *et al.*, 2003)



Example: x-ray spectra from electron beams

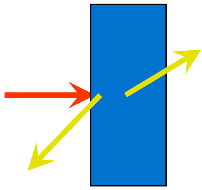
- Measurements by Llovet and Merlet on an electron microprobe

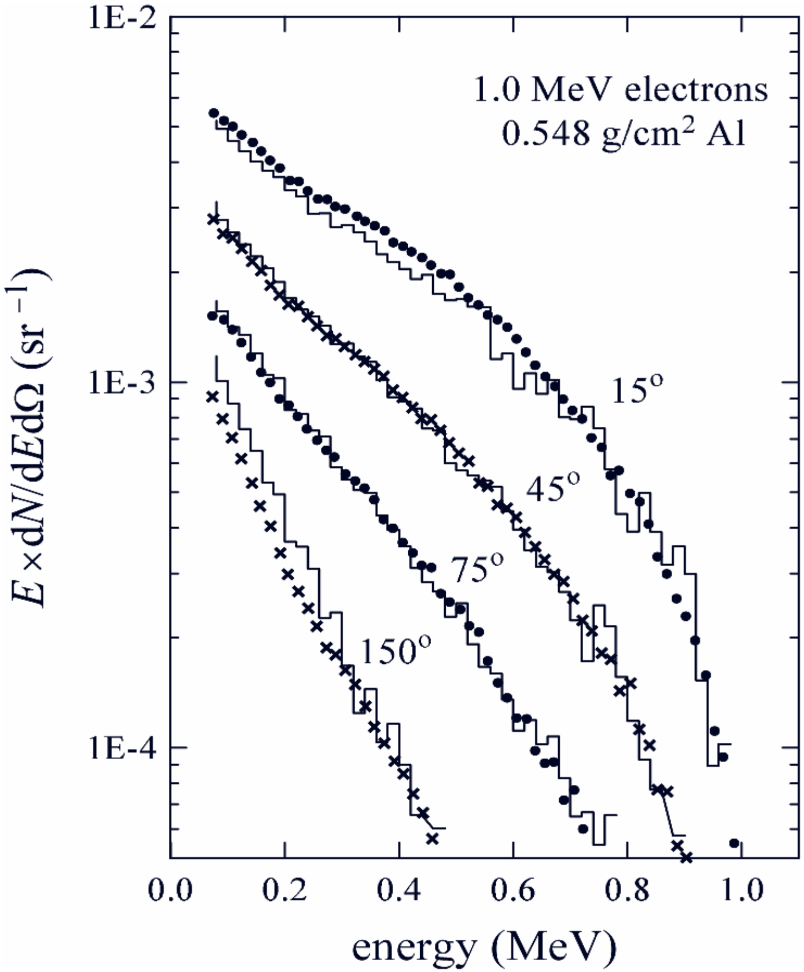


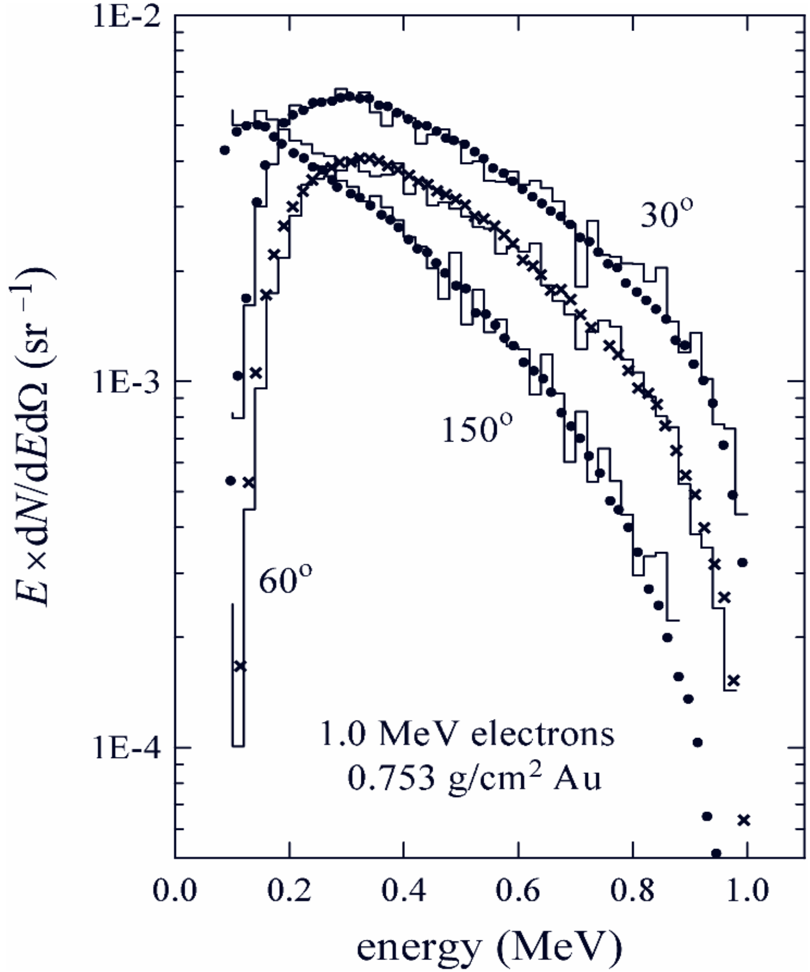


Example: bremsstrahlung energy spectra

- Experiment of Rester *et al.*, *J. Appl. Phys.* (1970)

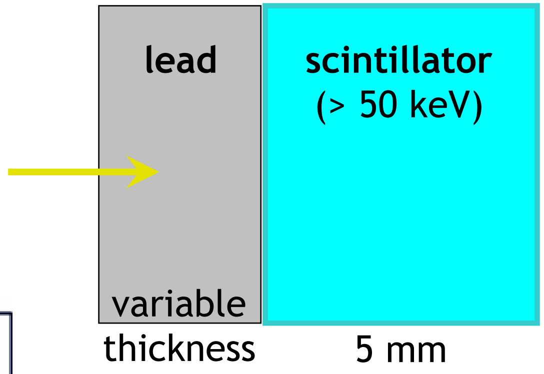


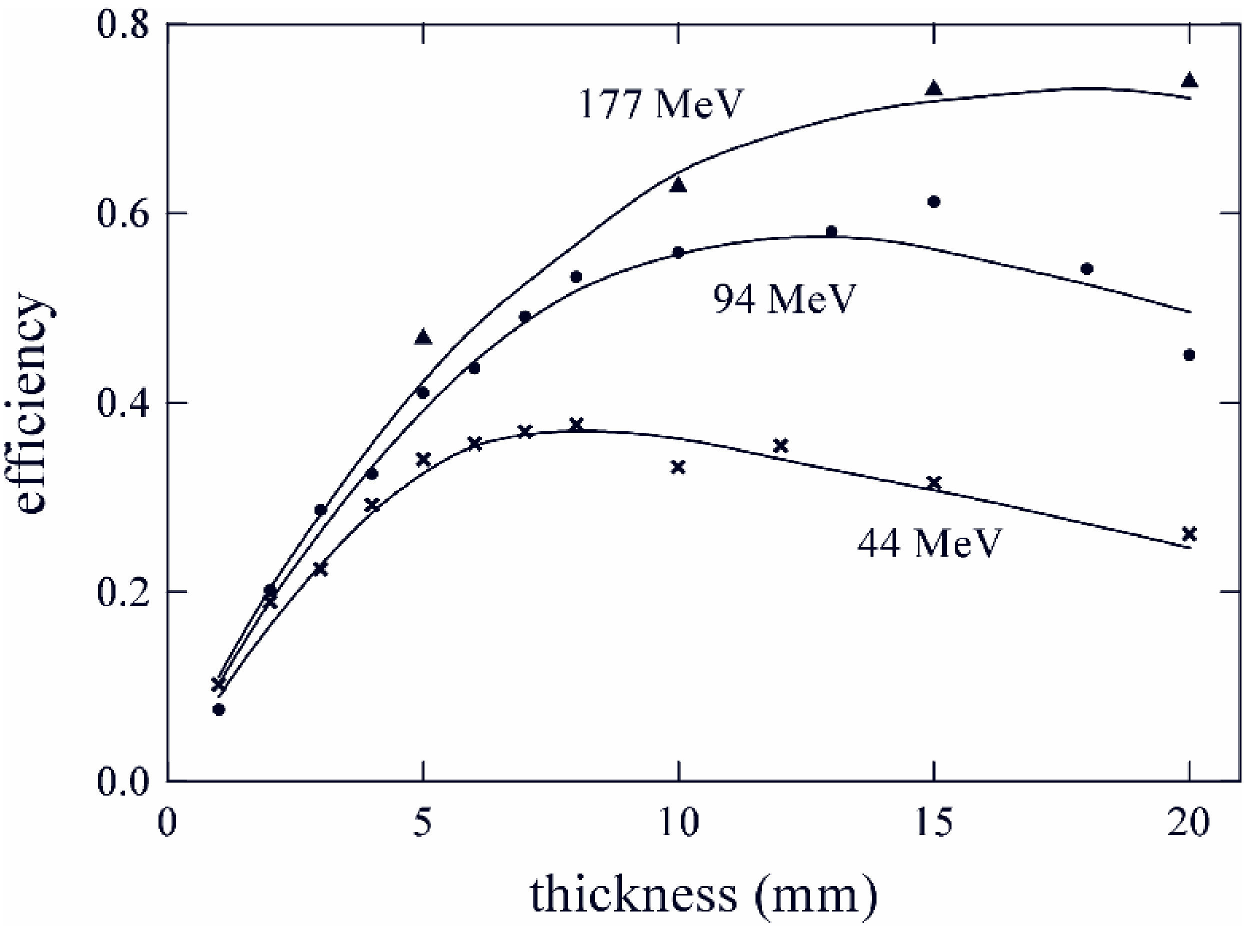




Example: efficiency of a radiation converter

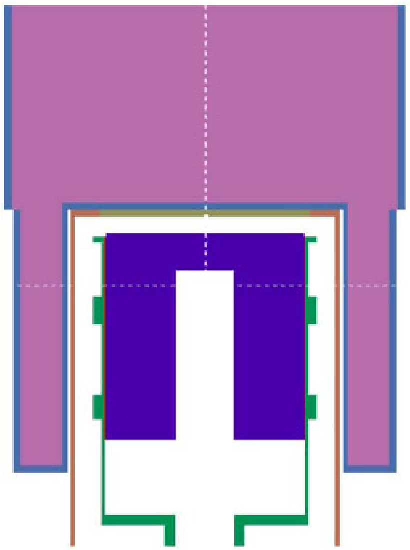
- Experiment of Darriulat *et al.*, *NIM* (1975)

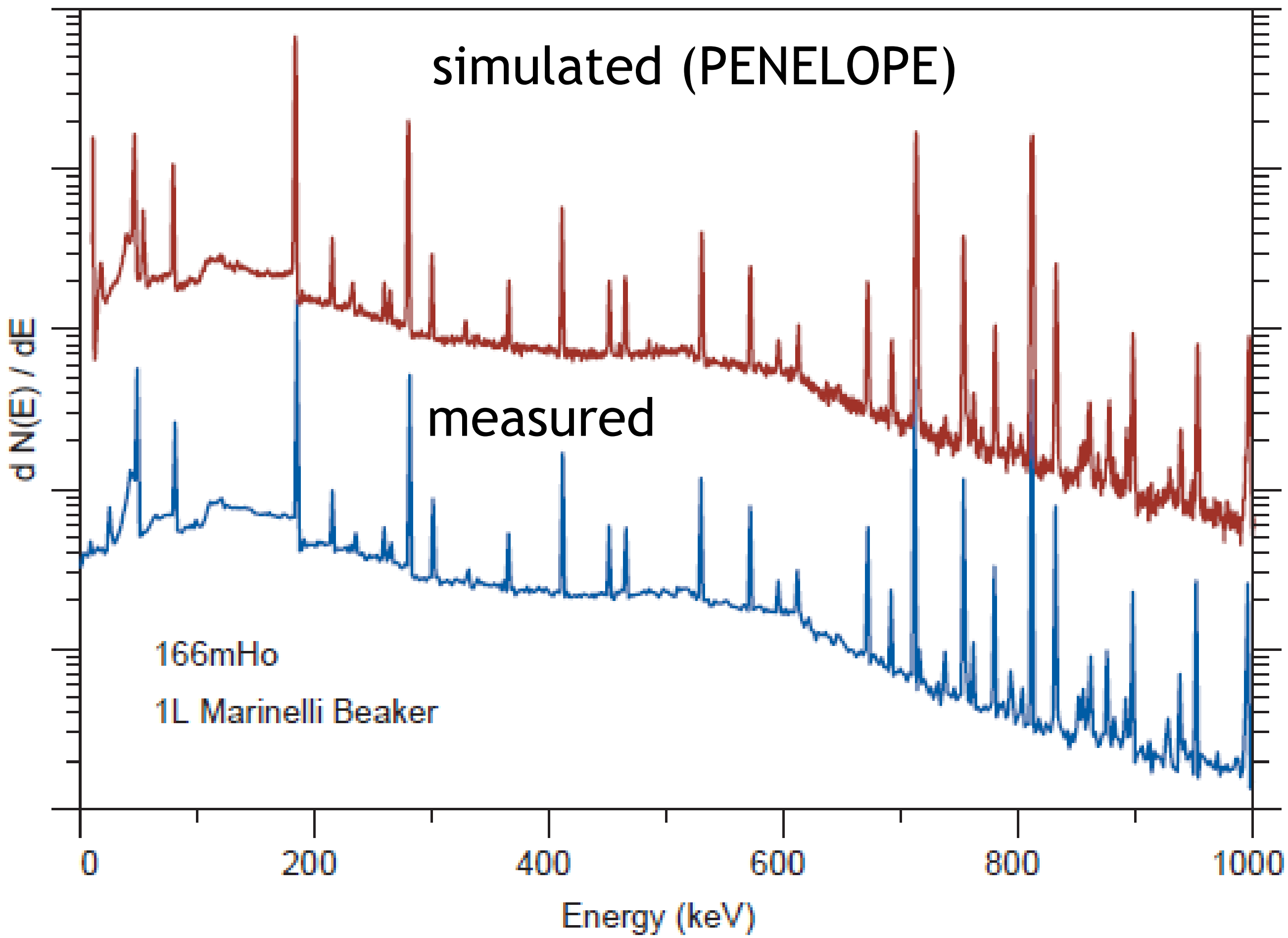




Example: gamma-ray spectrometry

- p-type HP Ge detector, Marinelli beaker (García-Toraño, *NIMA*, 2005)





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