



Barcelona, Parc Güell

Transport and interaction of electromagnetic radiation

Francesc Salvat



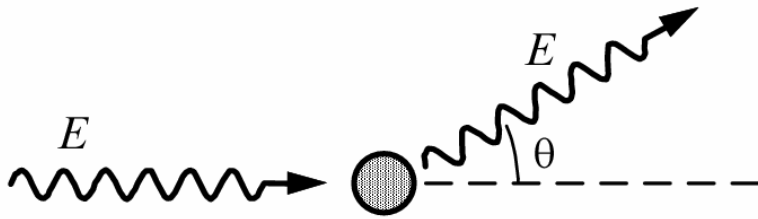
UNIVERSITAT DE BARCELONA



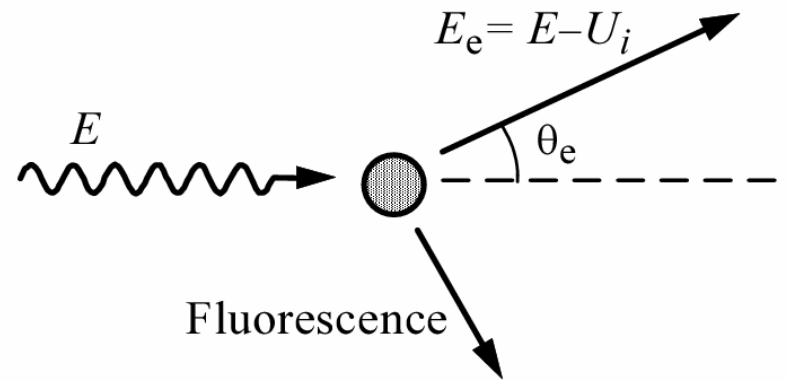
● *Outline:*

- Interactions of electrons and photons
- Detailed (analogue) simulation
- Electron and positron transport
- Applications

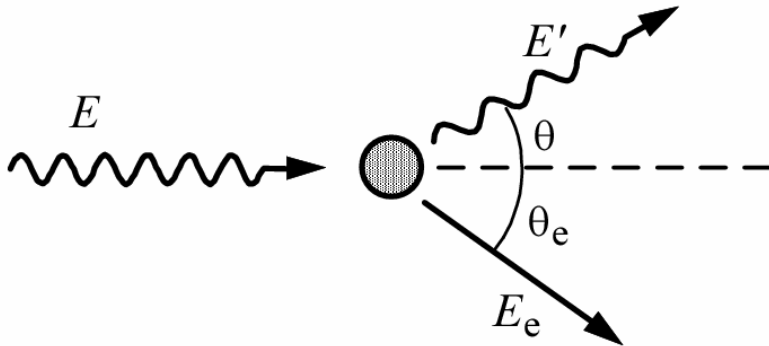
● Photon interactions



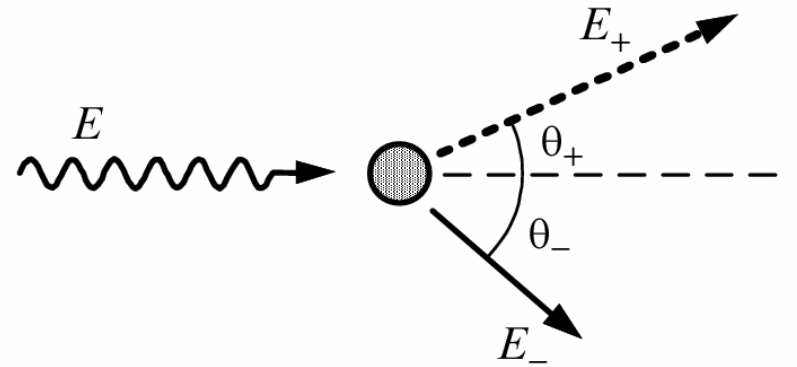
Rayleigh scattering



Photoelectric absorption

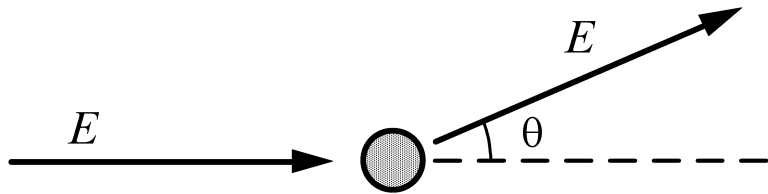


Compton scattering

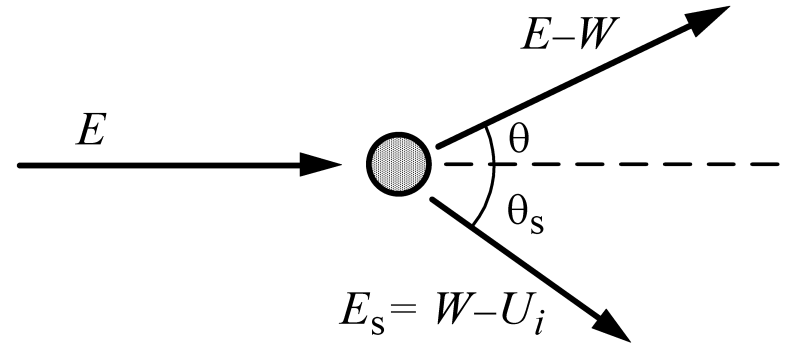


Pair production

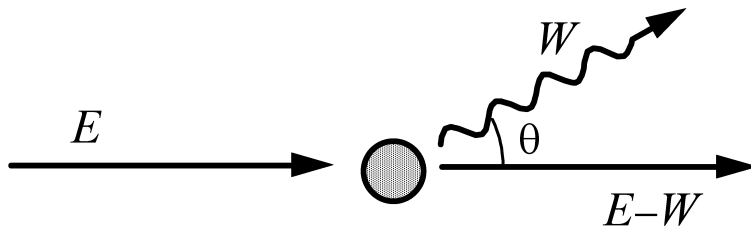
● Electron and positron interactions



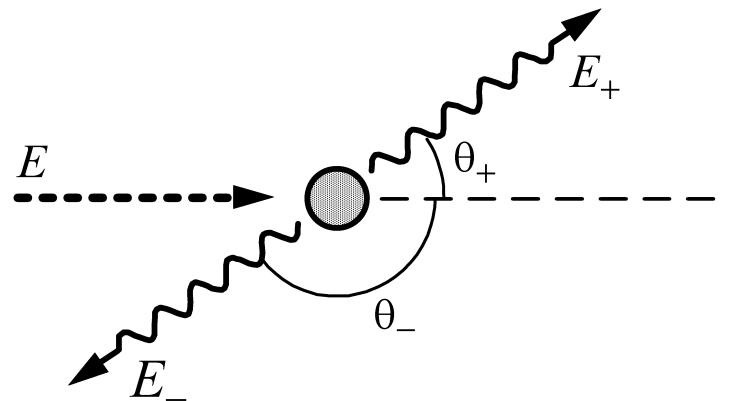
Elastic scattering



Inelastic scattering



Bremsstrahlung emission



Positron annihilation

● Simulation of $e^\pm - \gamma$ transport

Basic problem: Given a radiation source in a material structure, determine the radiation flux and the space distribution of deposited energy (particle penetration and slowing down, secondary particles)

Notice: 1) the interaction events are **stochastic** and so is the transport process

2) the problem involves multiple variables:

- kind of particle
- position coordinates (3)
- energy (1)
- direction of motion (2)

⇒ a problem well suited for Monte Carlo simulation

- 1954: E. Hayward and J. Hubbell Monte Carlo of photons
- 1963: M. Berger Monte Carlo of charged particles

● Radiation transport physics

● Basic assumptions in MC:

- ◆ The medium is homogeneous, isotropic and amorphous with known composition and density
(random scattering medium) $\mathcal{N} = N_A \rho / A_m$
- ◆ Collisions (interactions) are with single atoms
Not valid at low energies (diffraction and coherence effects)
- ◆ All physics is contained in the **atomic** cross sections
- ◆ Interactions “localize” the particles (as in a cloud chamber)
- ◆ Individual particle histories are generated as a succession of “free flights and collisions” (trajectory model)

The required information reduces to the DCSs for the relevant interaction mechanisms

The reliability of the results is determined by the adopted DCSs

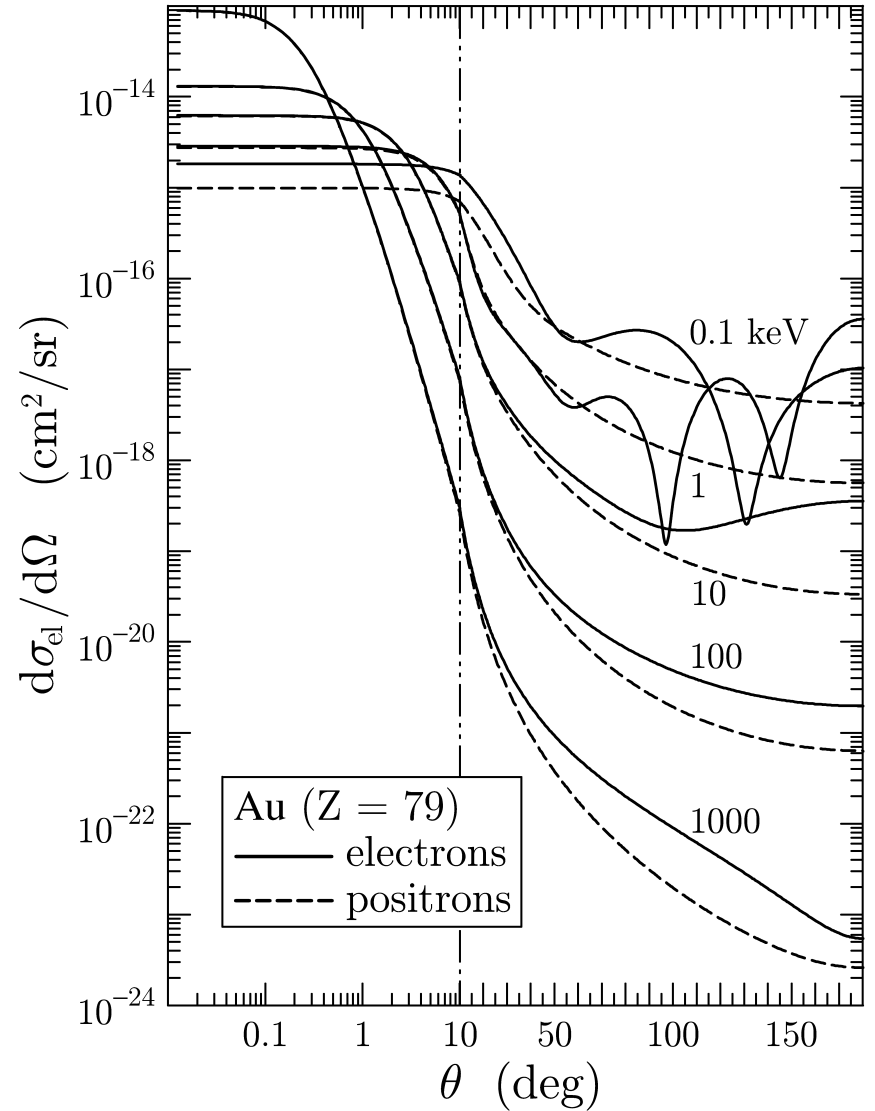
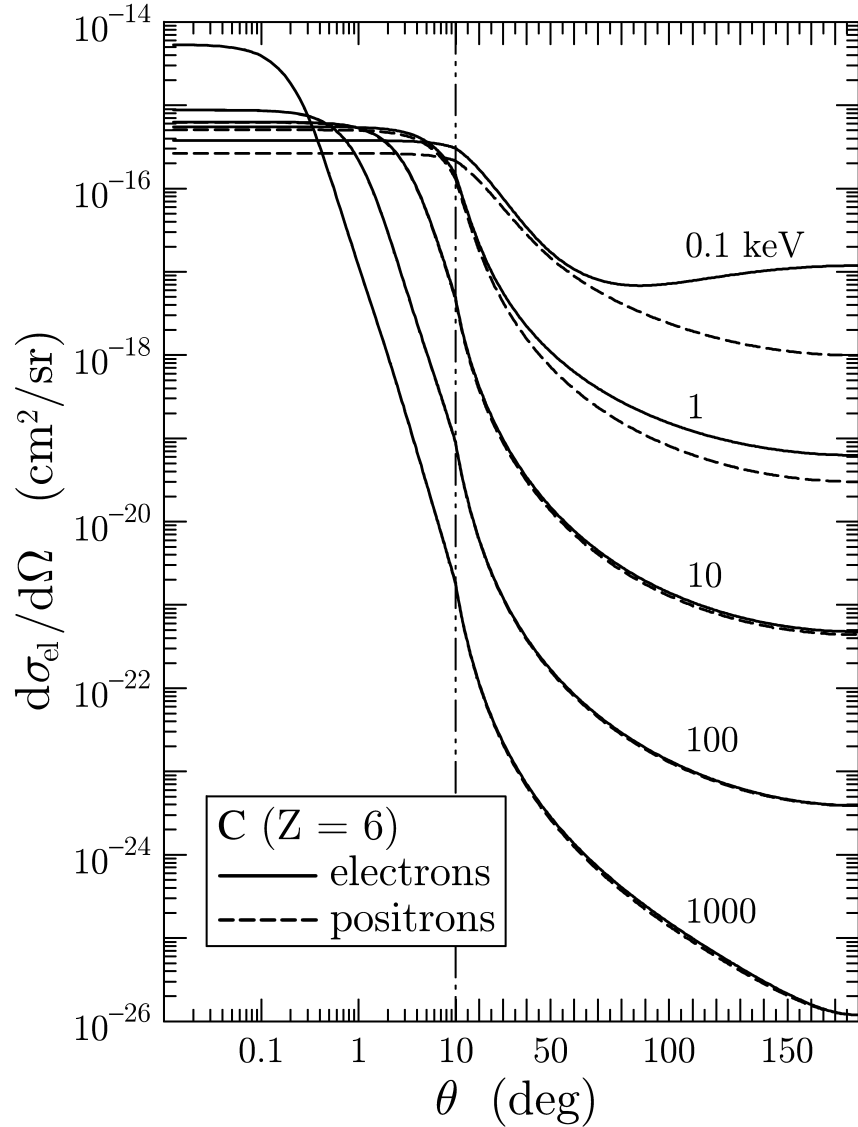
● Sources of interaction data

First-principles calculations, analytical approxs., empirical formulas, ...

● Numerical databases

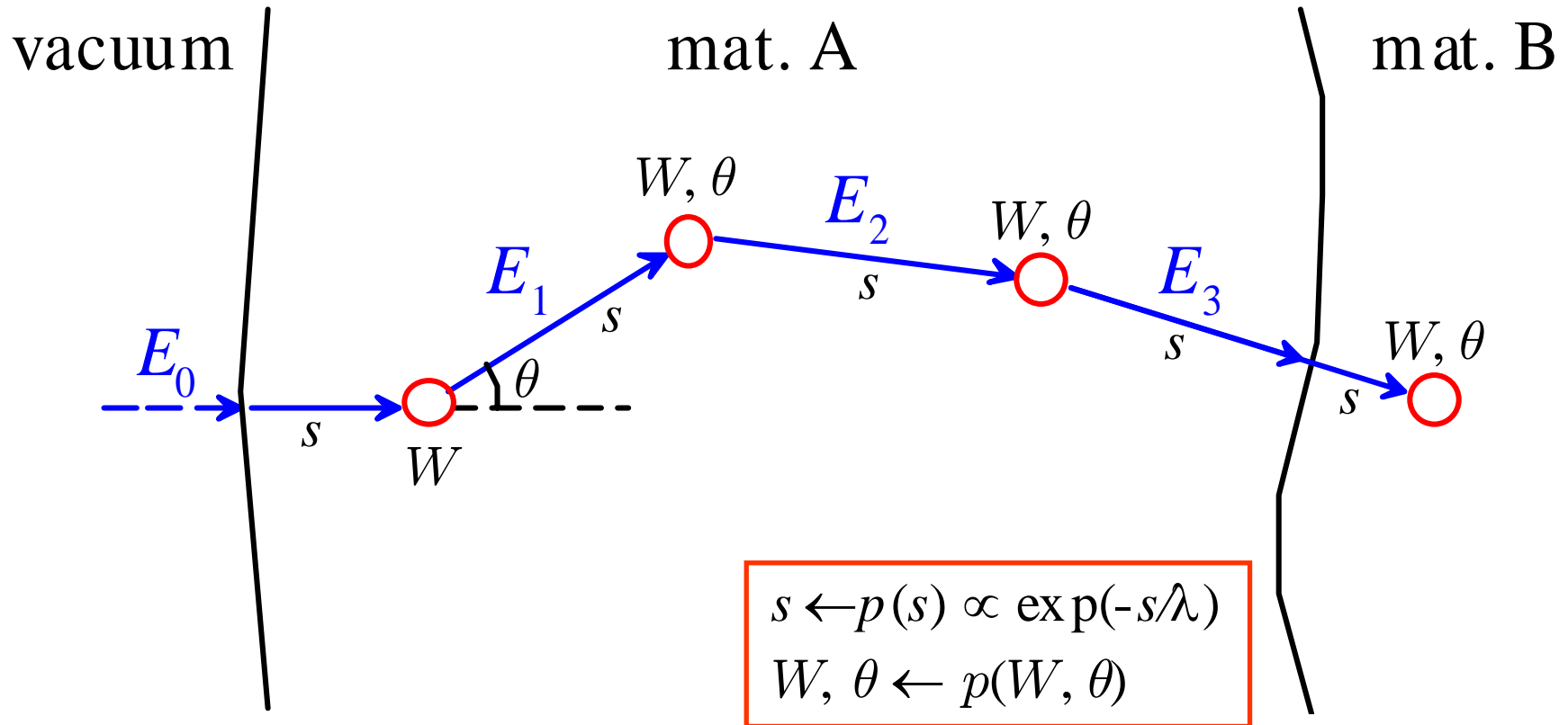
- Stopping powers of electrons and positron (ICRU)
 - Photoelectric, pair production total cross sections (Hubbell and Berger, XCOM; Cullen et al., EPDL)
 - Compton cross sections (impulse approximation, ANDT)
 - Atomic relaxation data (Cullen et al., EADL)
 - Bremsstrahlung emission: scaled DCSs and shape functions (Seltzer and Berger; Kissel et al., ANDT)
 - Elastic scattering of electrons and positrons (NIST, ICRU, UB)
 - Ionization cross sections (NIST, UB)
-
- Numerical data are usually generated from **approximate** theories
 - Databases provide only partial information
 - On average, the interaction models currently used are accurate to within a few percent...
 - **Do not trust calculations claimed to be more accurate than that!**

● Example: elastic scattering DCSs



● Detailed (analogue) simulation

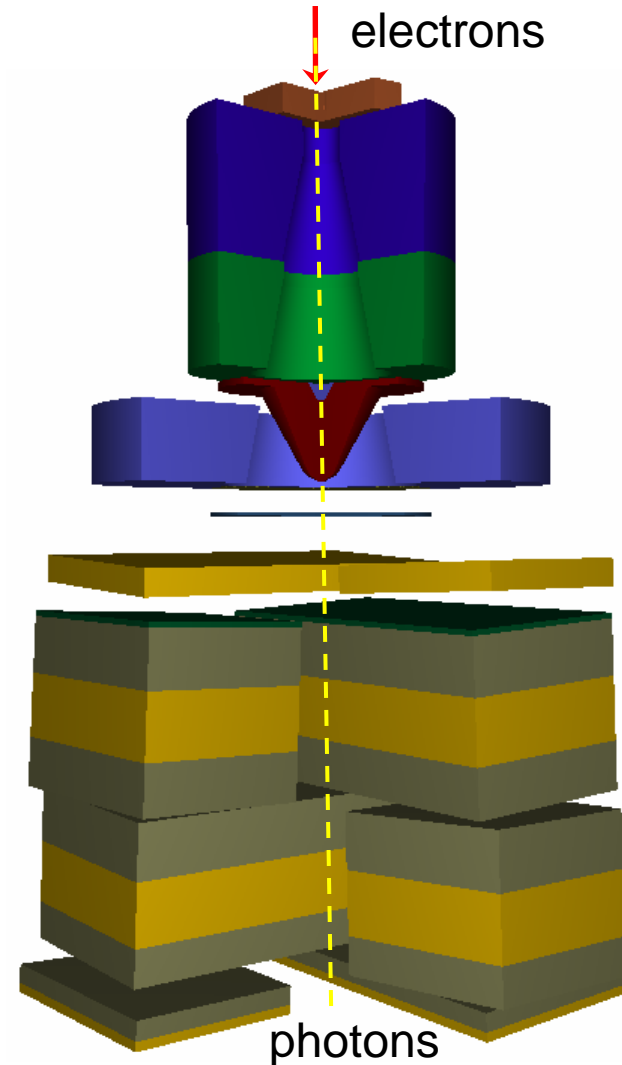
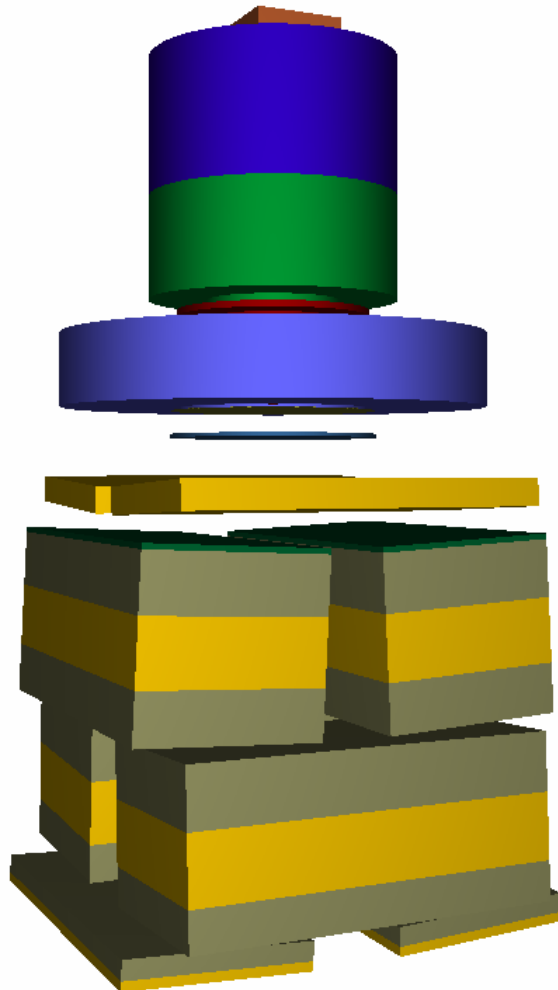
- All interaction events are simulated in chronological succession:



- The method is nominally exact (for energies higher than ~ 1 keV)
- Feasible only for **photons** and **low-energy electrons and positrons**
- High-energy electrons and positrons are more difficult...

● Geometry packages

Geometry (almost) completely decoupled from physics.
Combinatorial or quadric geometries



● Why is electron/positron simulation difficult?

Mostly because a high-energy electron/positron suffers many collisions in the course of its slowing down:

$$\langle \Delta E \rangle_{1 \text{ coll.}} \approx 30 \text{ eV}$$

Example: A 30 MeV electron interacts ~1 million times!

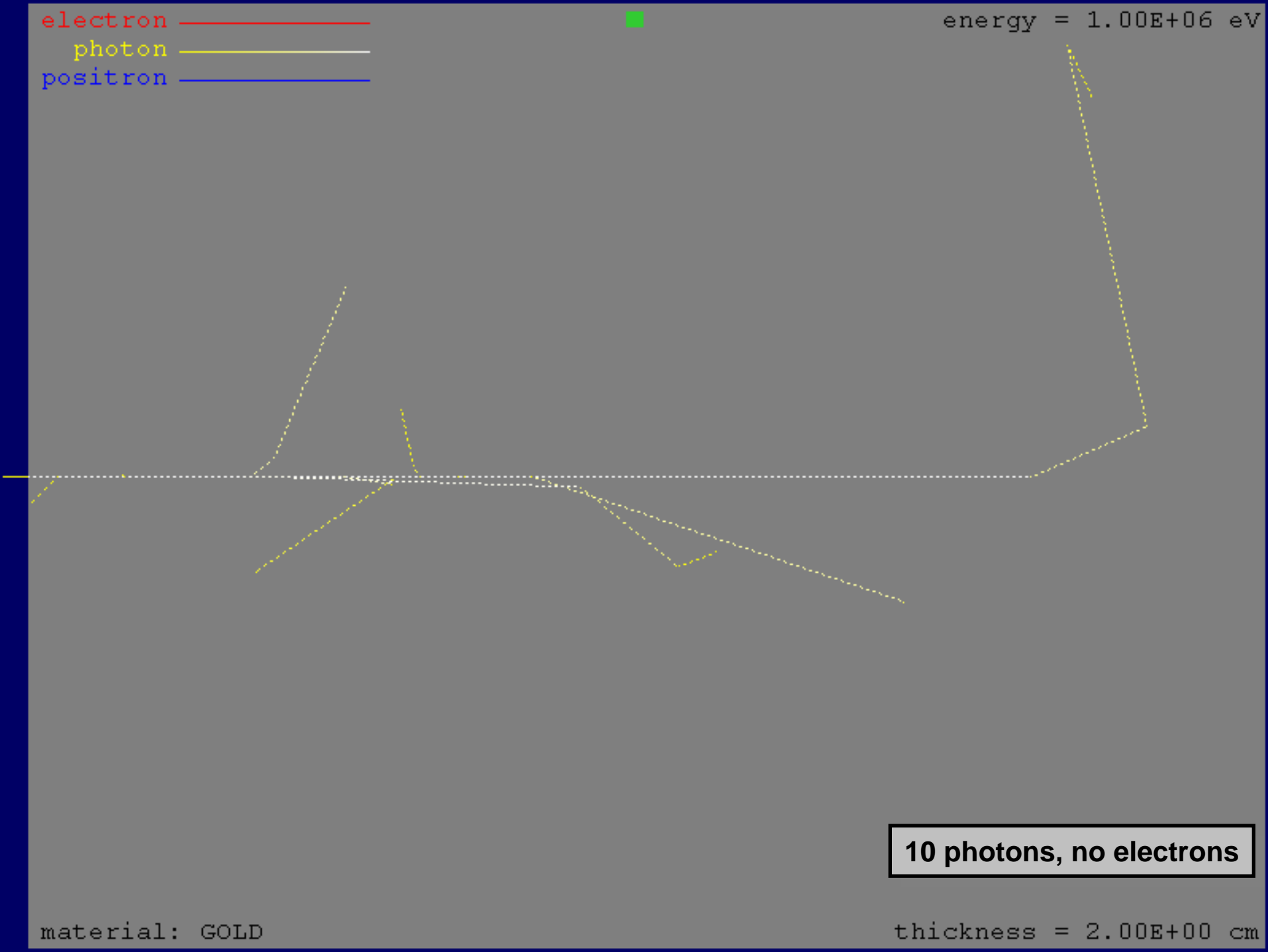


An image is worth one thousand words...

electron ———
photon ———
positron ———



energy = 1.00E+06 eV



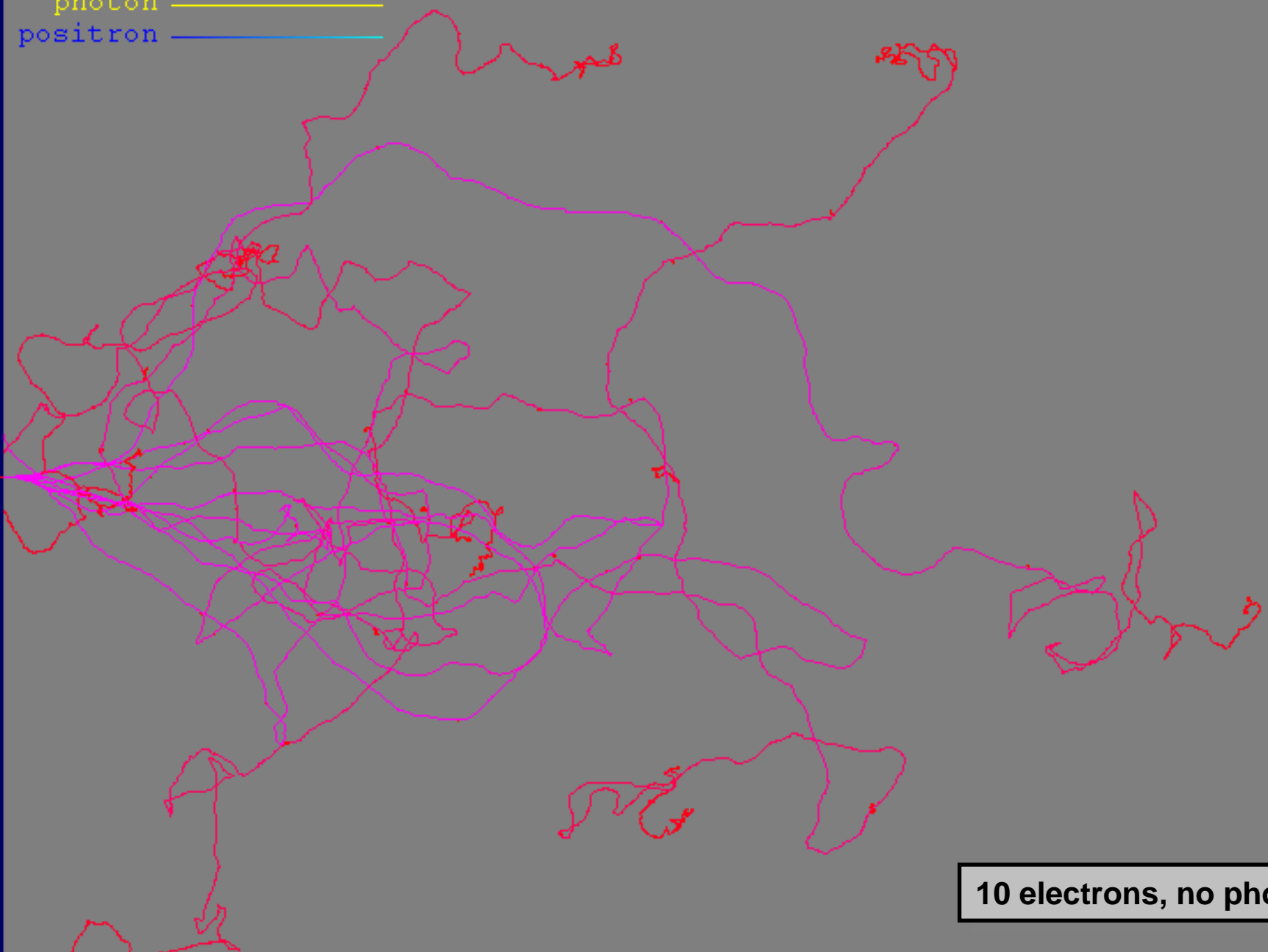
10 photons, no electrons

material: GOLD

thickness = 2.00E+00 cm

electron ———
photon ———
positron ———

energy = 1.00E+06 eV



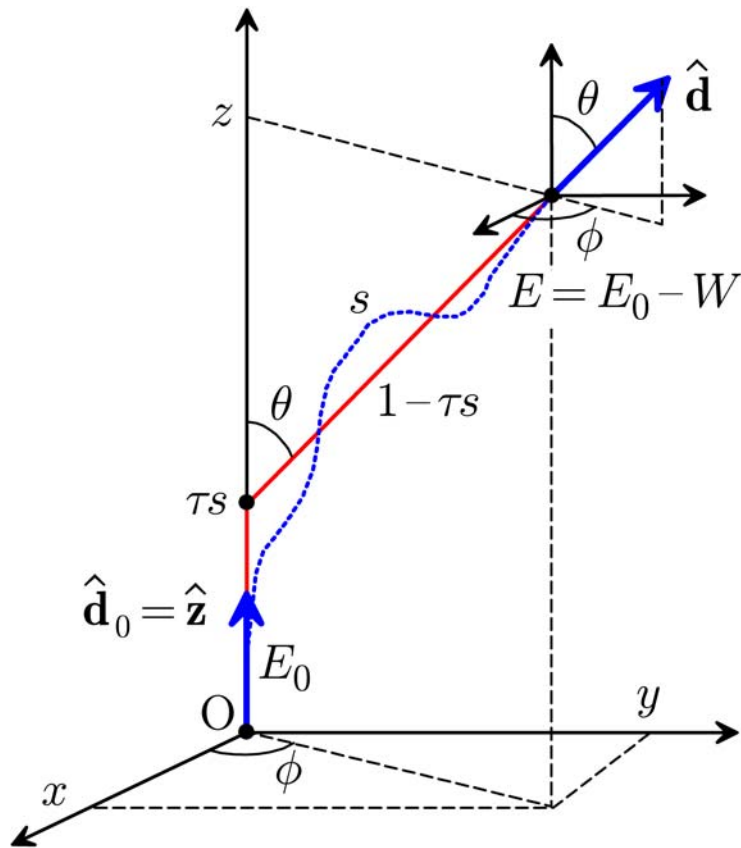
10 electrons, no photons

material: GOLD

thickness = 2.00E-02 cm

● Condensed (class I) simulation algorithms

Basic idea: Simulate the (many) interactions in a path segment of a given length s by a single computational step using multiple-scattering *approximate* theories



● Energy loss:

◆ Theories of Landau, Blunk-Leisegang, Vavilov. $p(E_0, s; W)$

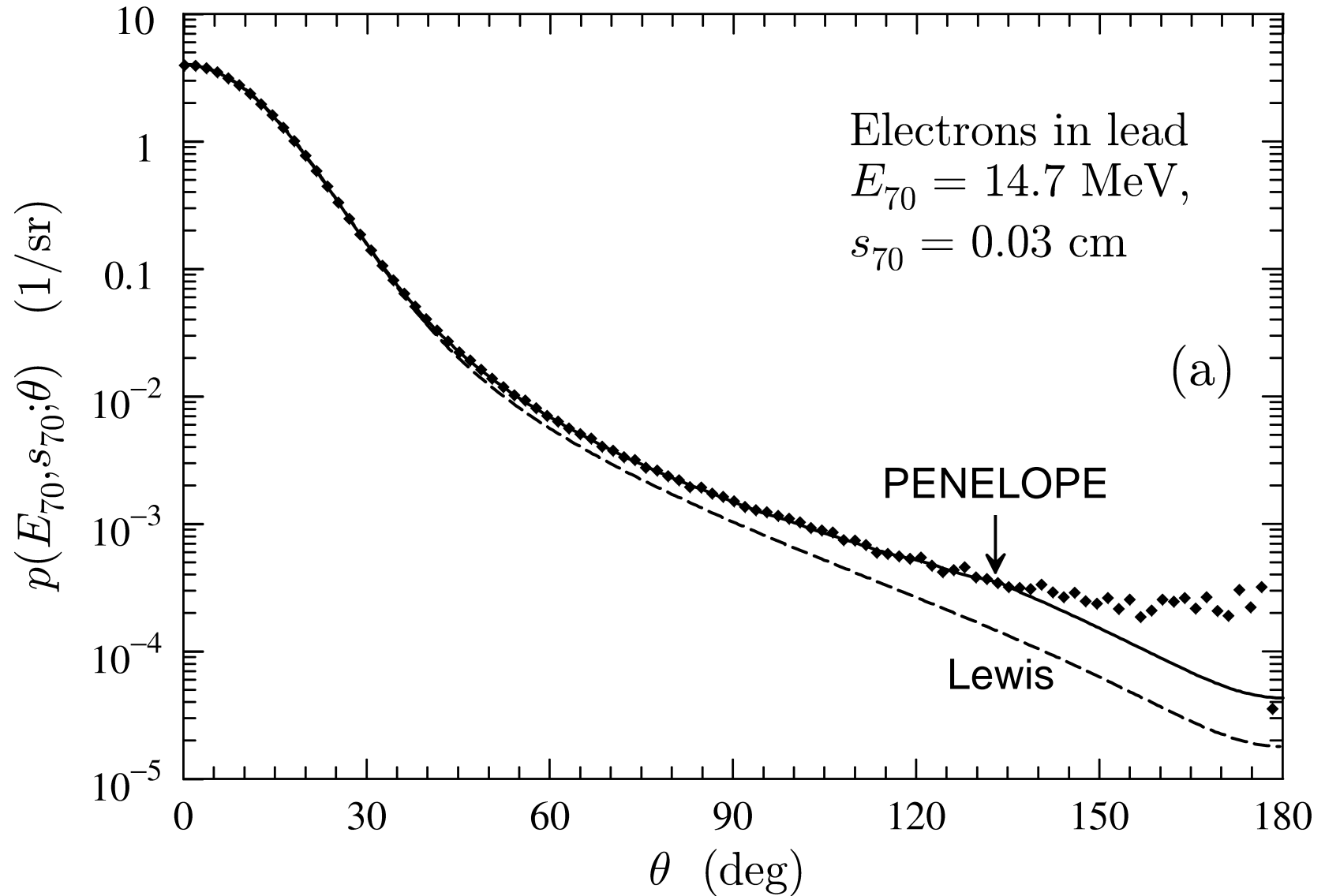
● Angular deflection:

◆ Goudsmit-Saunderson: neglects energy-loss along the step. “Exact” Legendre expansion of $p(E_0, s; \theta)$

◆ Lewis: energy-loss accounted within the CSDA. “Exact” Legendre expansion of $p(E_0, s; \theta)$ and a few space moments, $\langle z \rangle$, $\langle x^2 + y^2 \rangle$, $\langle z \cos \theta \rangle$

Other details of the space distribution are not known

● Example of multiple scattering distribution



● Limitations of condensed algorithms

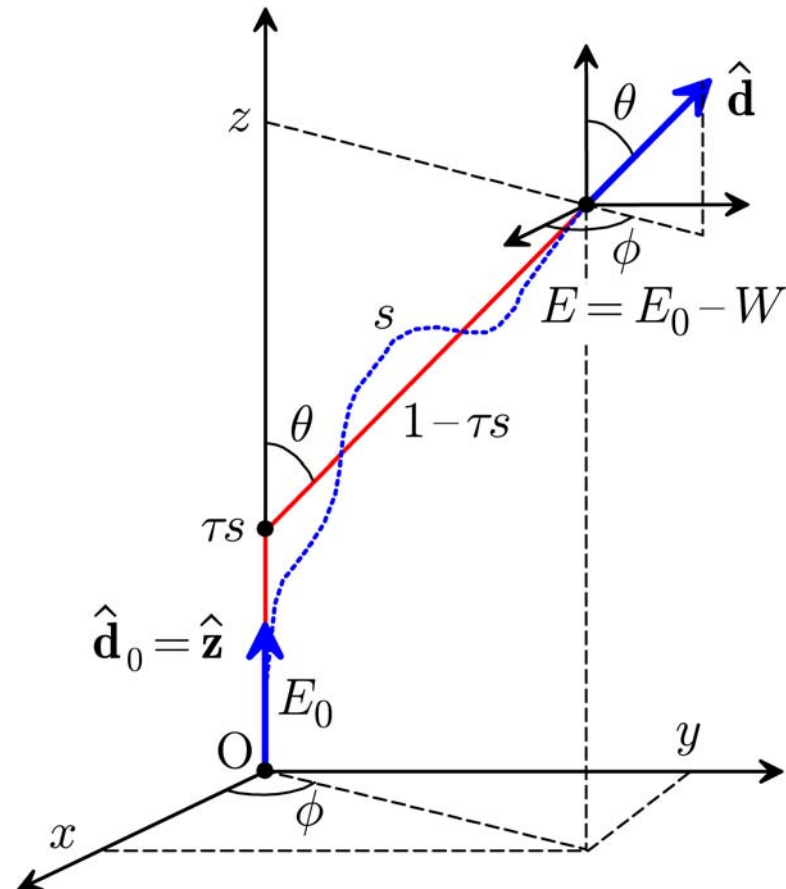
- Energy loss and angular distributions contain approximations
- Multiple scattering distributions are tabulated for **fixed** path lengths (or energy losses) \Rightarrow difficulties with interface crossings
- Very limited information on space distributions available: we do not know **where** the electron is at the end of the step

● Random-hinge method

Reproduces Lewis' moments

$$\langle z \rangle, \langle x^2 + y^2 \rangle, \langle z \cos \theta \rangle$$

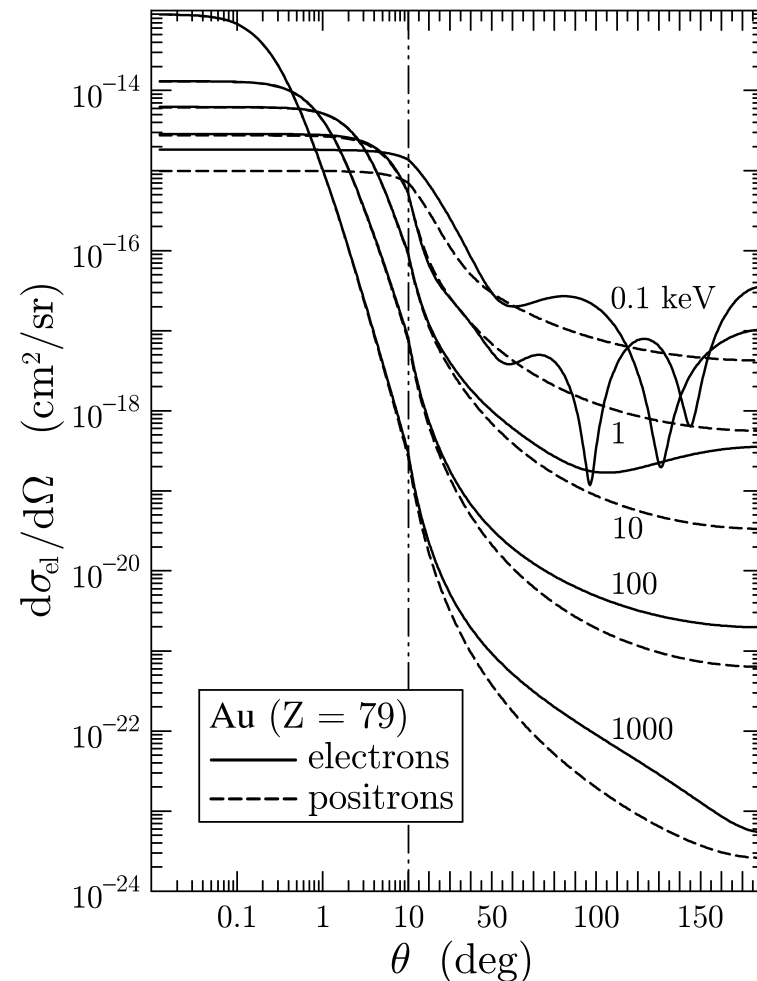
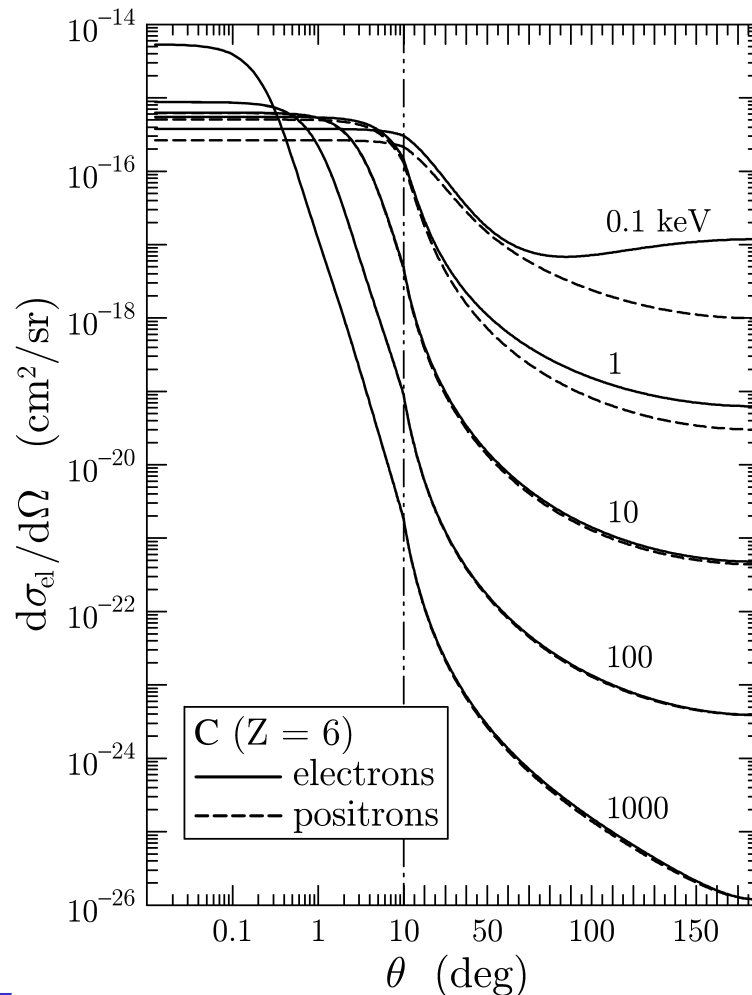
Step-end points fill the “transport” sphere



Mixed (class II) simulation algorithms

Basic idea: The majority of interactions produce very small angular deflections and/or energy losses

Example: elastic scattering



● Mixed (class II) simulation algorithms

Basic idea: The majority of interactions produce very small angular deflections and/or energy losses

We can **define** (small) angle and energy-loss cutoffs (θ_c, W_c) and consider:

- **Hard collisions:** with $\theta > \theta_c$ or $W > W_c$, only a few in each electron history
Detailed simulation is inexpensive
- **Soft collisions:** with $\theta < \theta_c$ and $W < W_c$, a large number (on average) between each pair of hard interactions
Condensed (class I) simulation is accurate

● Advantages of mixed algorithms

- Hard interactions are simulated “exactly”
- Accurate (and easy) description of interface crossings
- Very stable with respect to the cutoffs (fast)

● General-purpose Monte Carlo codes

- **ETRAN** (Berger and Seltzer, NIST, 1978)
- **MCNP5** (Los Alamos; 1990 – MCNP4)
- **EGS4** (Nelson, Hirayama and Rogers; SLAC 1985)
- **EGSnrc** (Kawrakow and Rogers; NRC 2003)
- **GEANT4** (Pia et al., CERN, 2005)
- **FLUKA** (Ferrari et al., CERN, 2005)
- **EGS5** (Hirayama et al., SLAC-KEK, 2005)
- **PENELOPE** (Salvat et al., UB, 1996-2005)

● The code system PENELOPE

PENetration and **E**nergy **LO**ss of **P**ositrons
and **E**lectrons (... and photons)

A general-purpose Monte Carlo code for the simulation of coupled electron-photon transport in arbitrary geometries

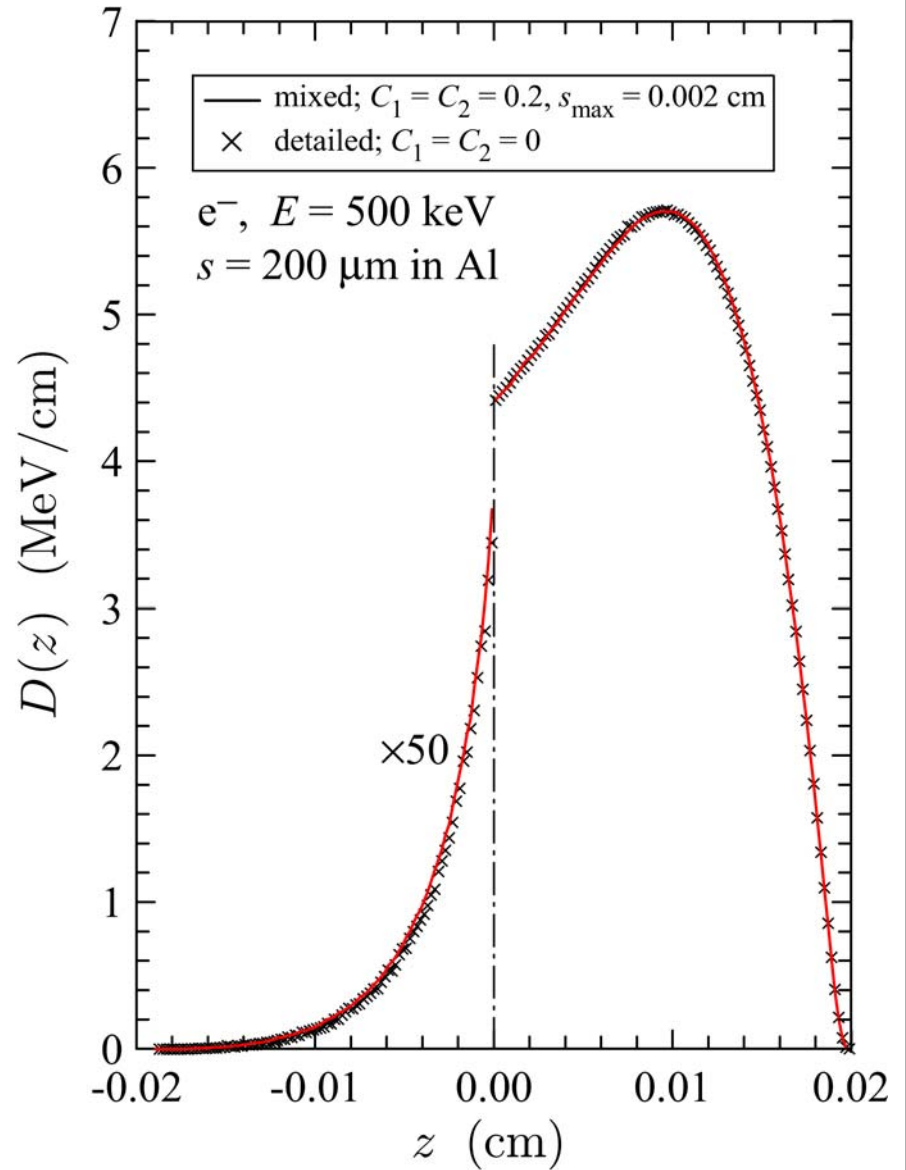
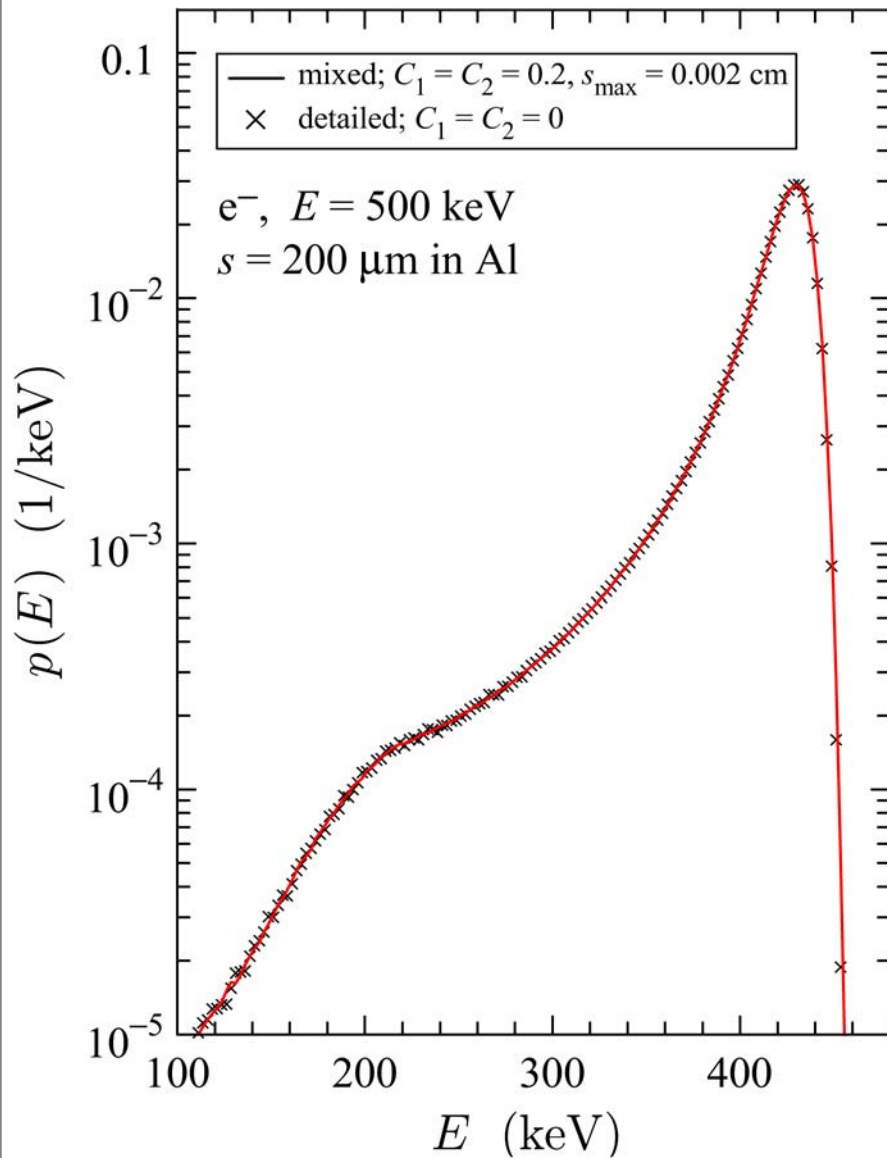
Distributed by the OECD-NEA Data Bank (Paris)

(~600 registered users, thoroughly checked... in specific energy ranges)

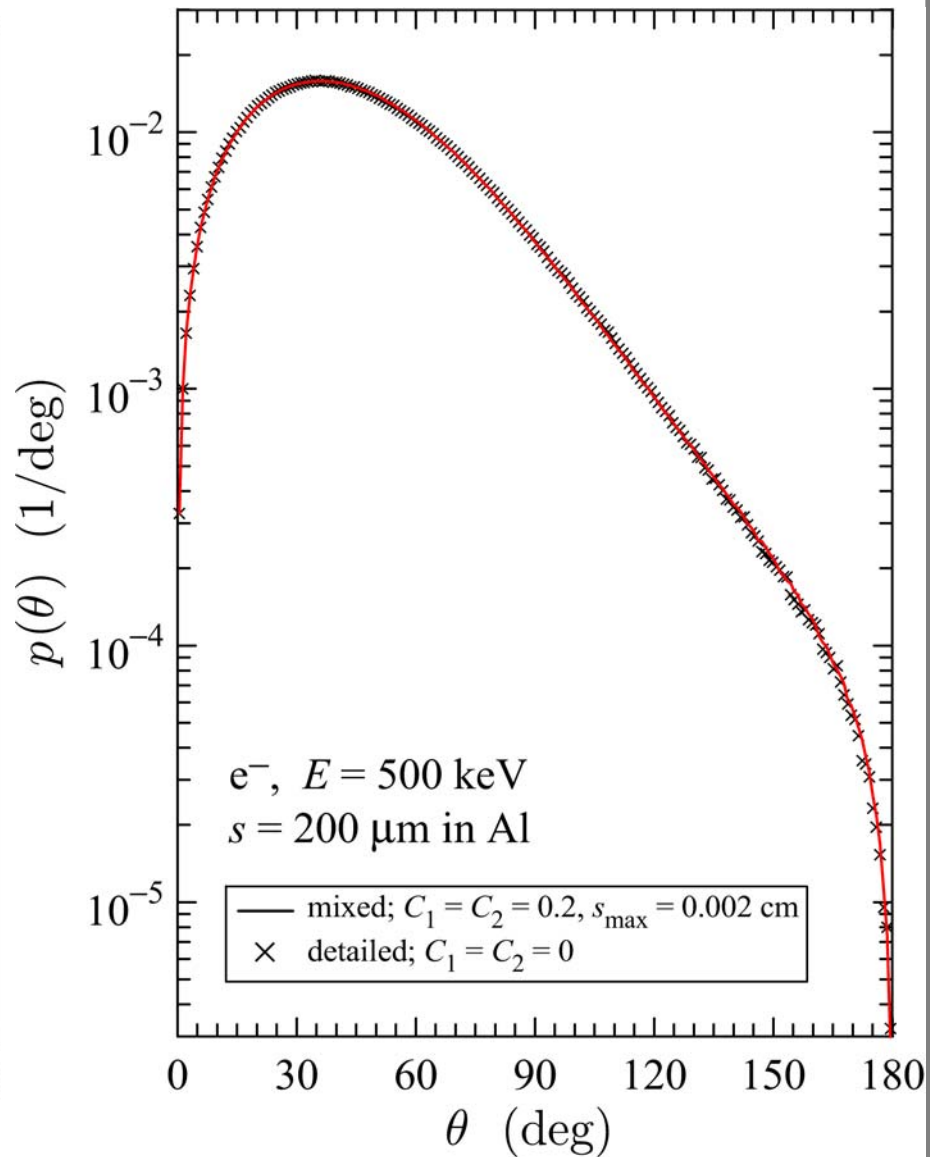
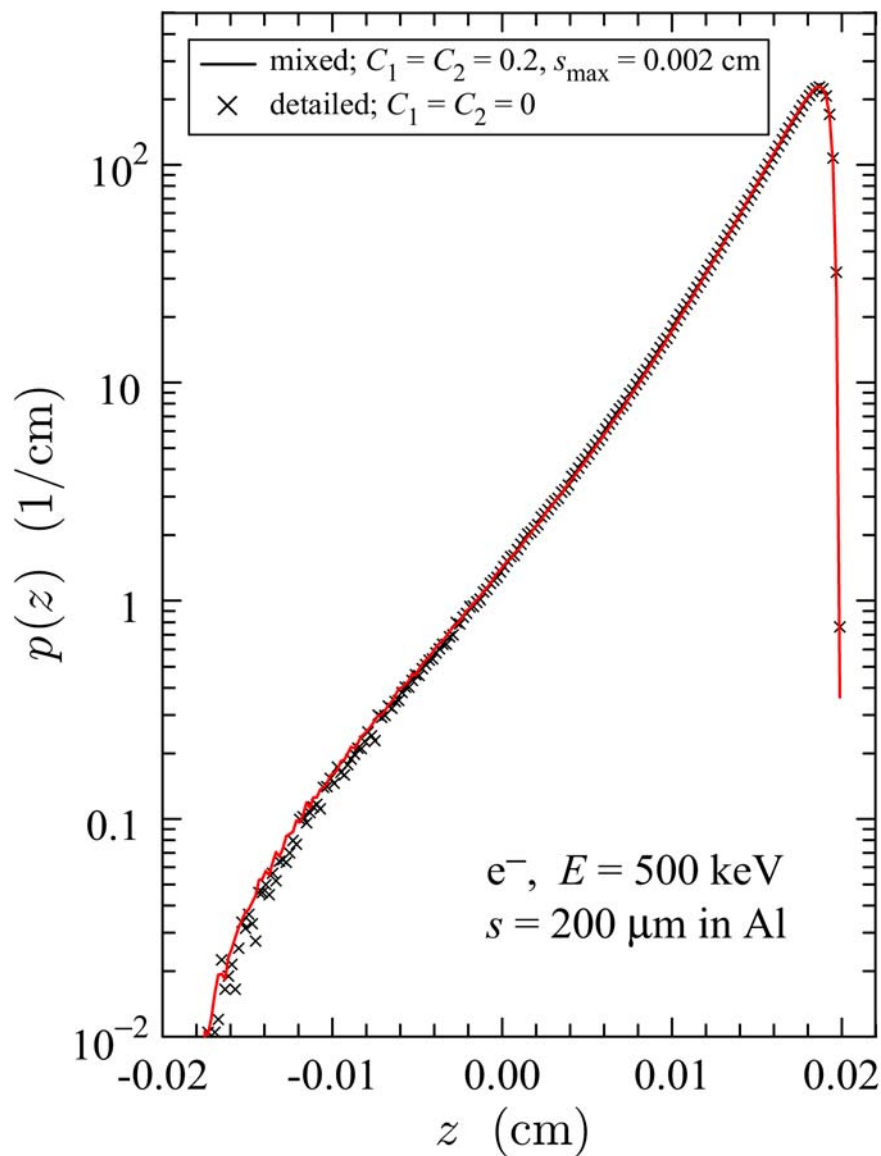
<http://www.nea.fr/lists/penelope.html>

● *Main features*

- ◆ All kinds of interactions (except nuclear reactions) in the energy range
 from 50 eV to 10^9 eV (covered by the database)
- ◆ Implements the most accurate physical models available (limited only by the required generality)
- ◆ Simulates electrons and positrons (tunable class II scheme) and photons (detailed, interaction by interaction)
- ◆ Simulates fluorescent radiation from K, L and M-shells
- ◆ Includes a flexible geometry package (constructive quadric geometry)
- ◆ Electron and positron transport in external magnetic and electric fields (in matter)



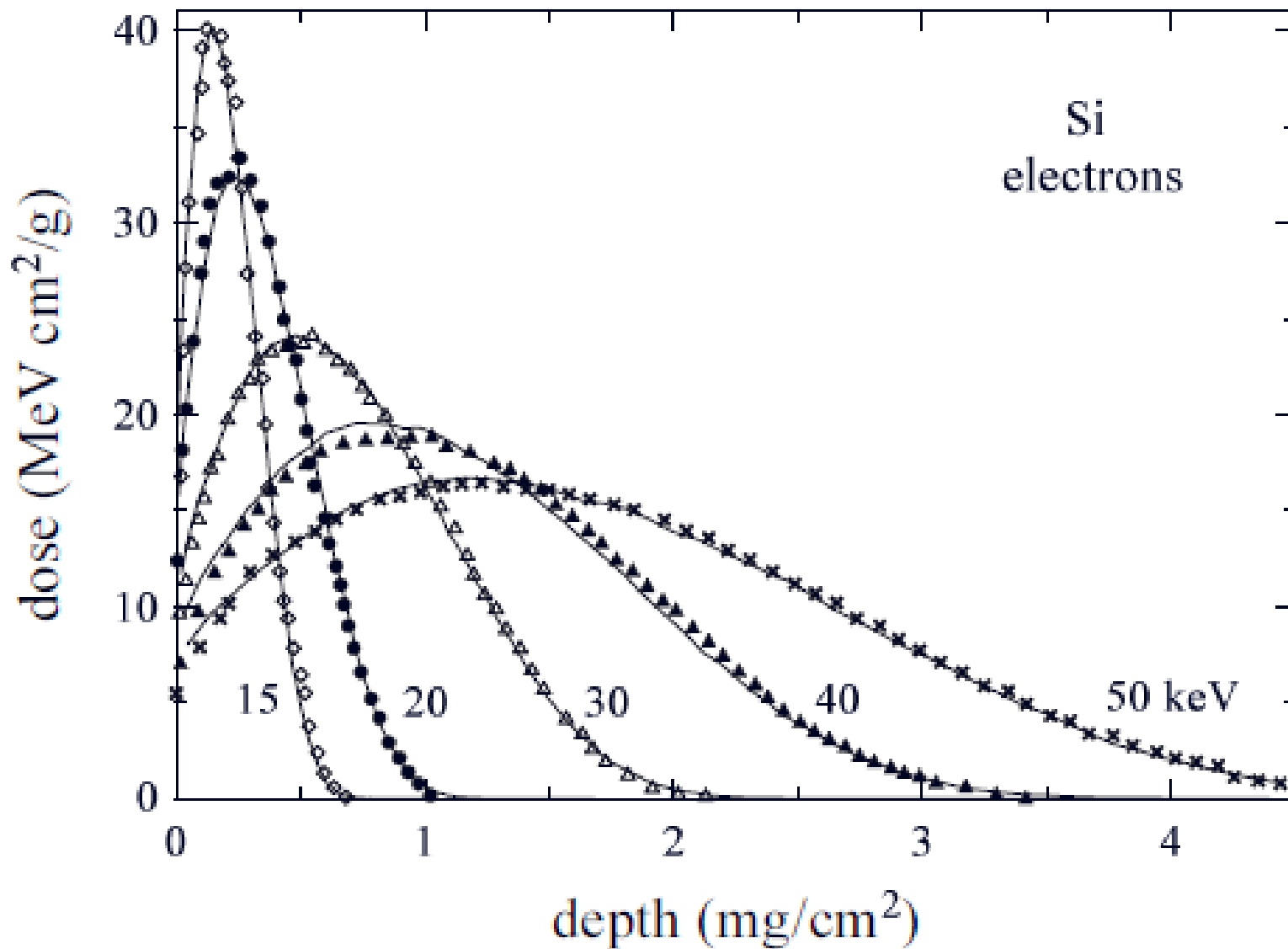
crosses: detailed simulation
 solid lines: mixed simulation



crosses: detailed simulation
 solid lines: mixed simulation

● *Simulation vs. experiment*

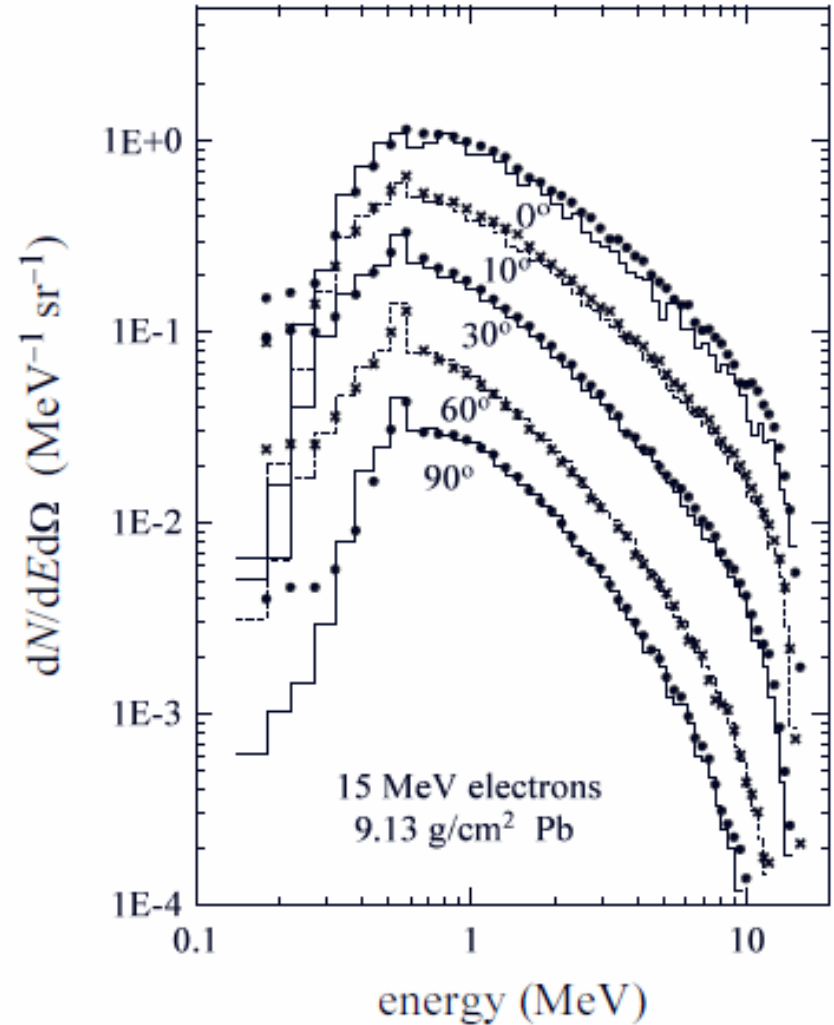
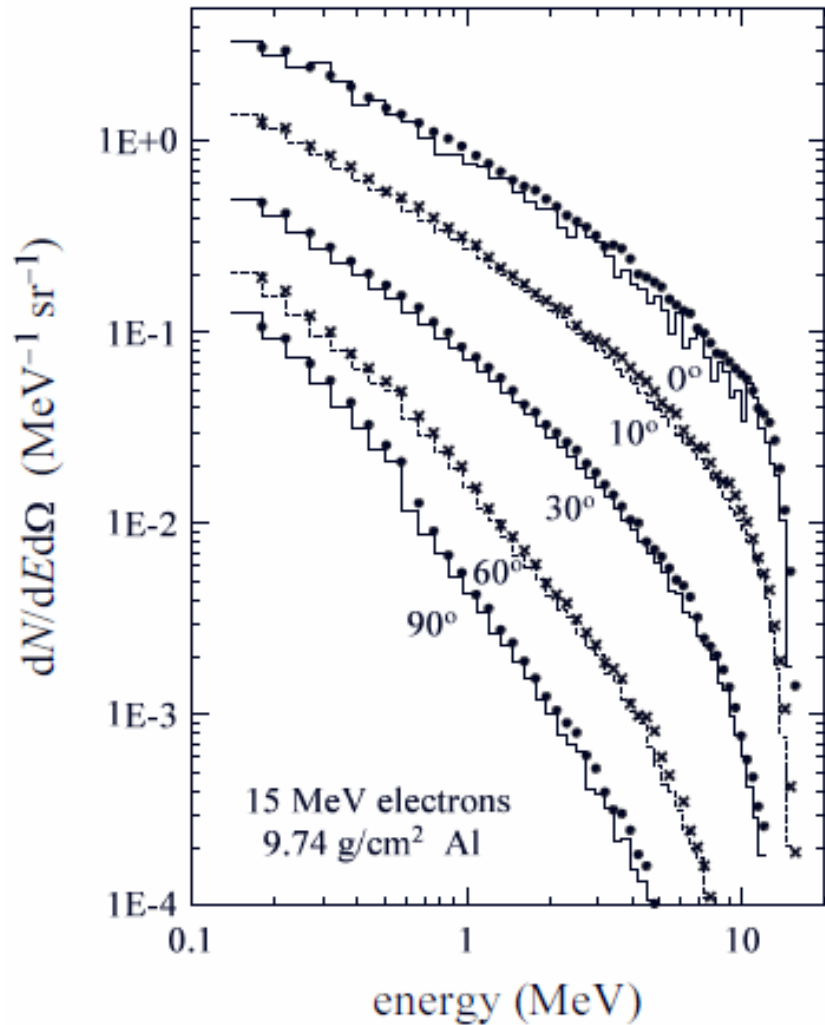
(Sempau et al, NIMB 2003)



● Simulation vs. experiment

(Sempau et al, NIMB 2003)

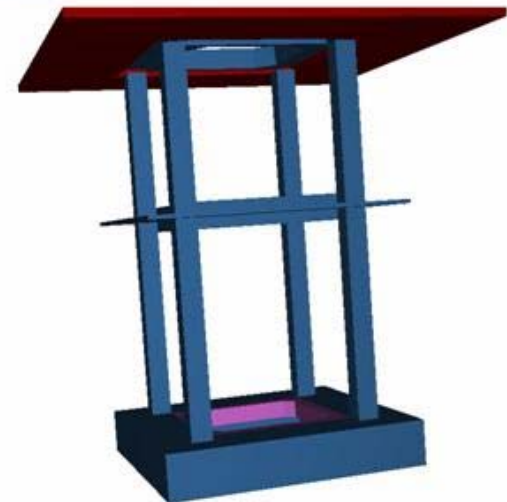
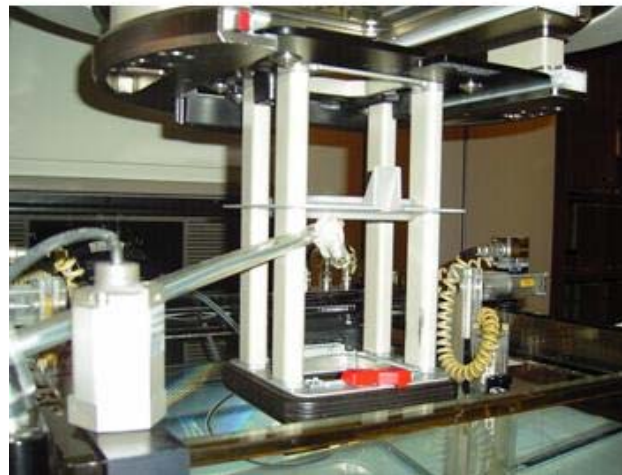
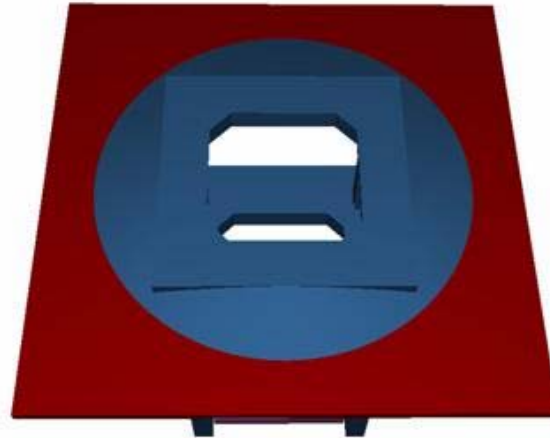
Bremsstrahlung emission



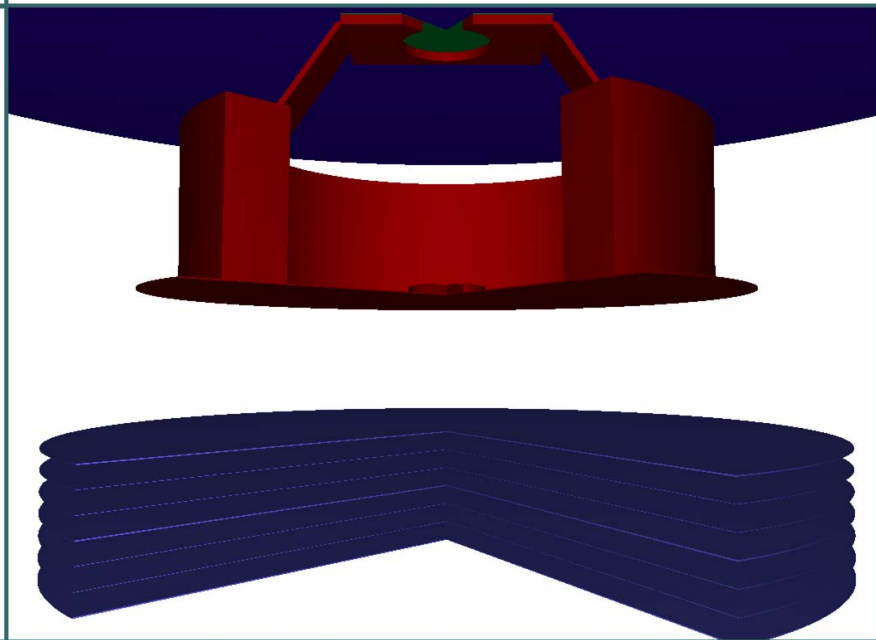
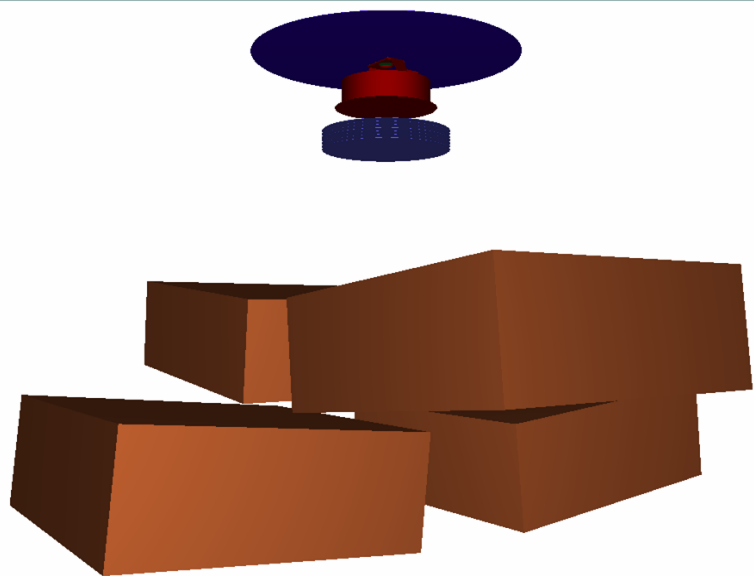
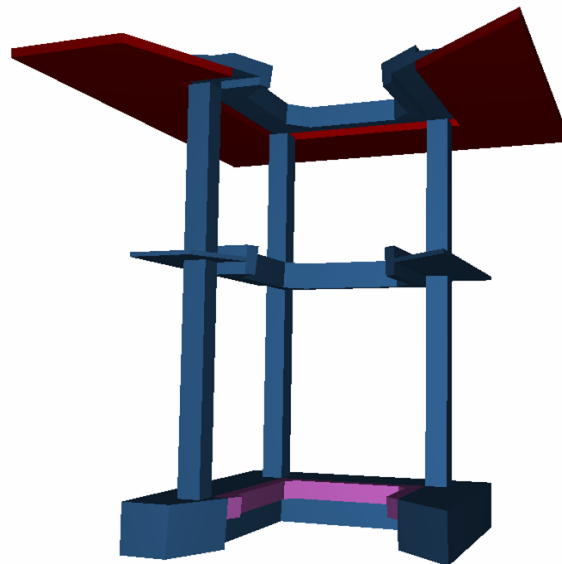
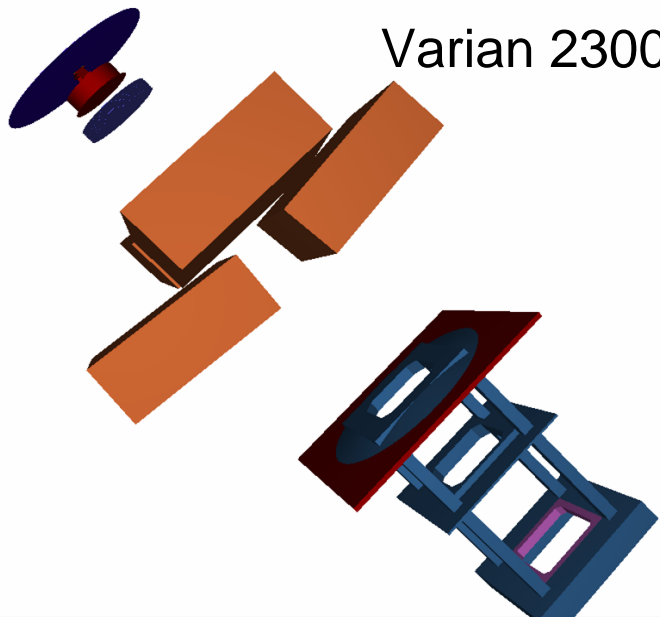
- **Application examples**

- **Modelling medical electron accelerators**

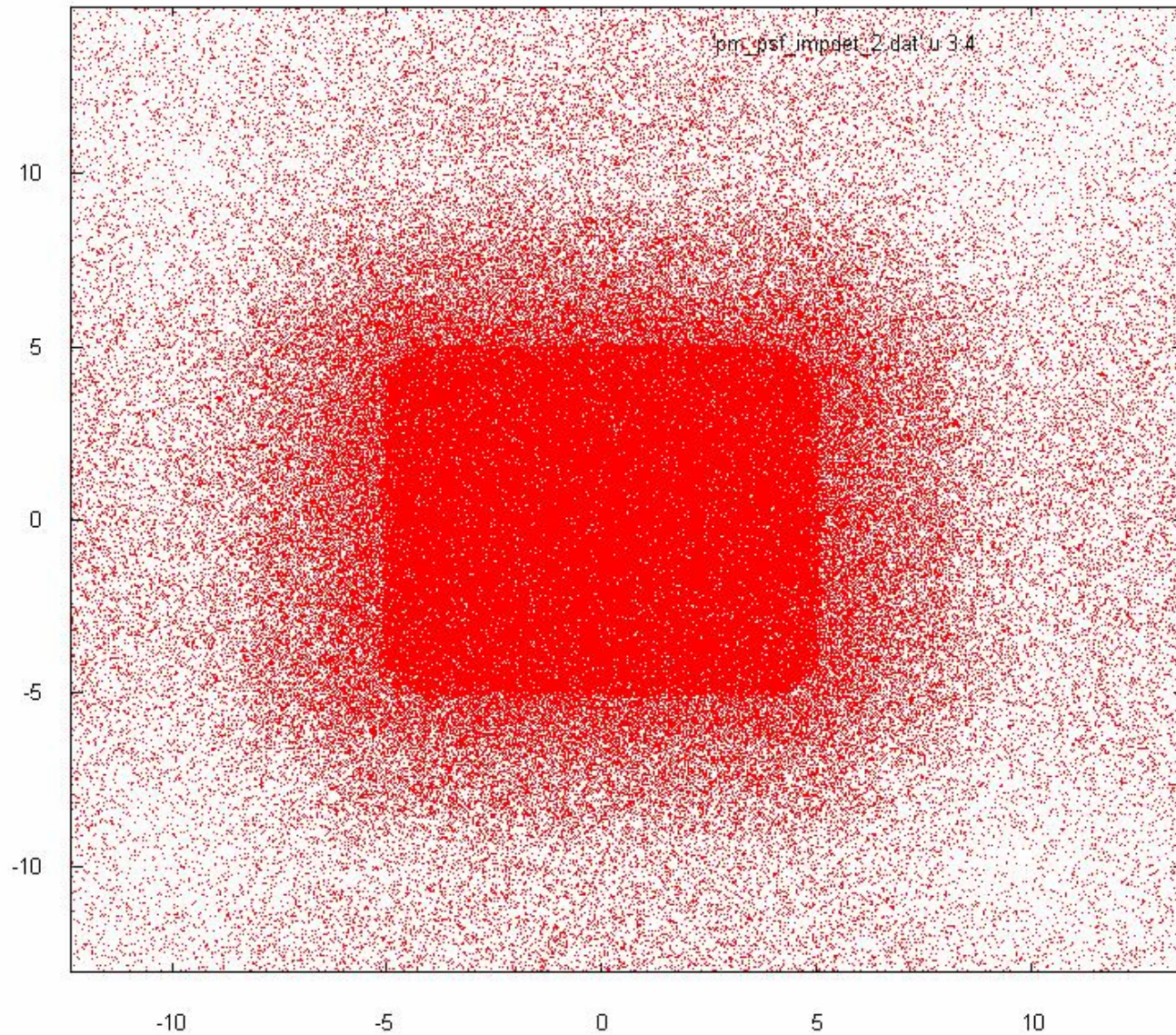
Varian 2300 C/D



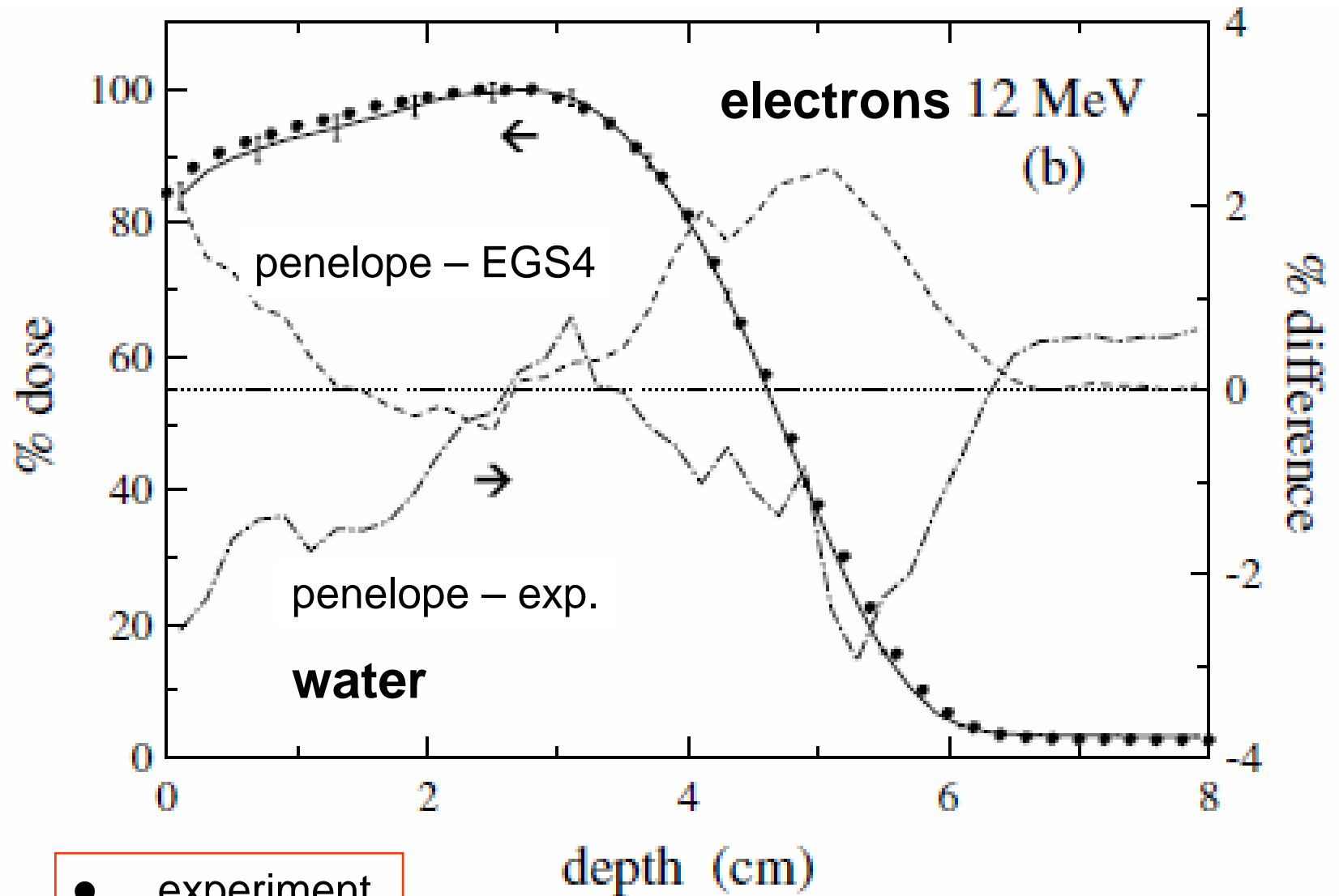
Varian 2300 C/D



● Photons in phase-space file. 10x10 cm field



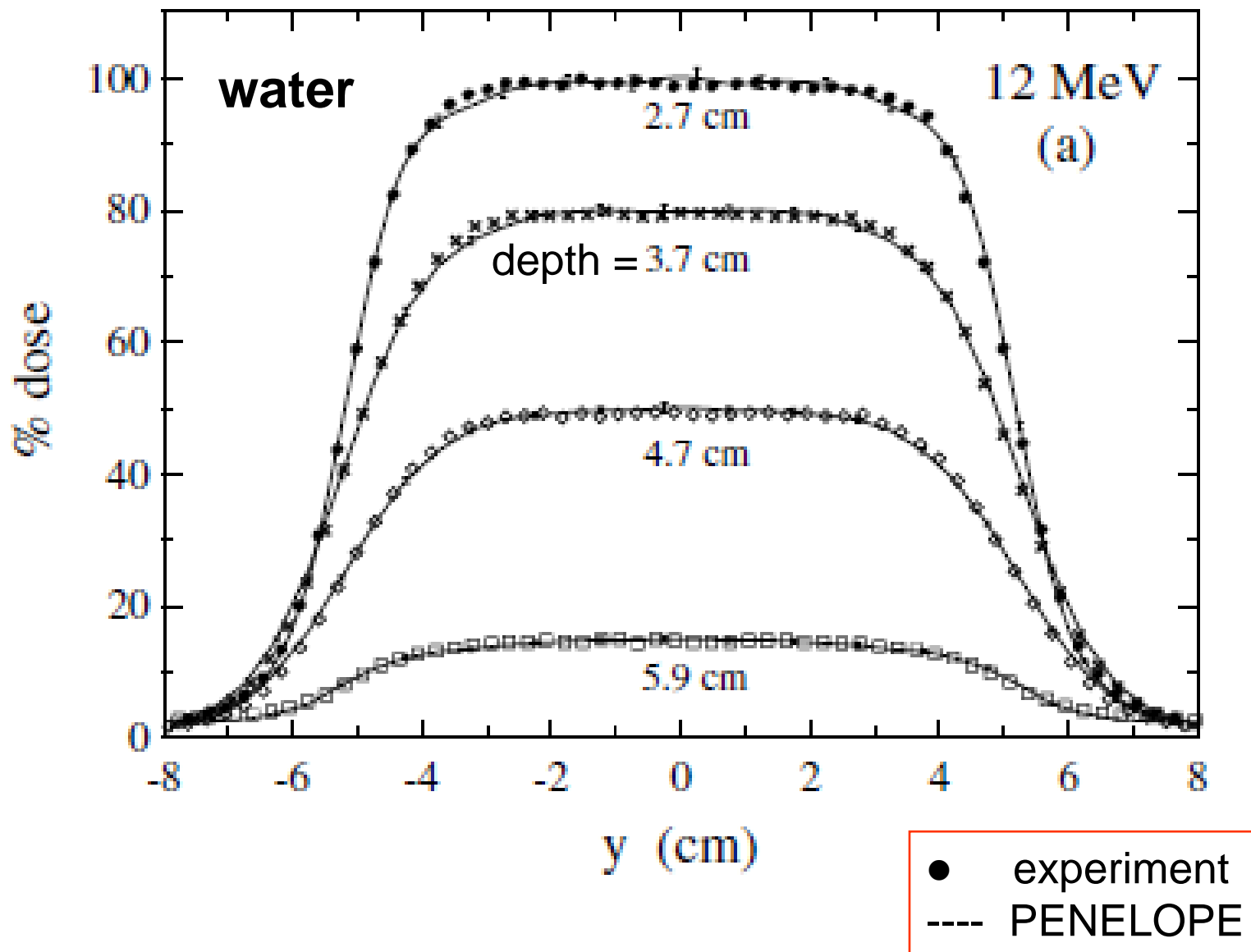
● Depth-dose distribution from a Siemens KDS



- experiment
- PENELOPE

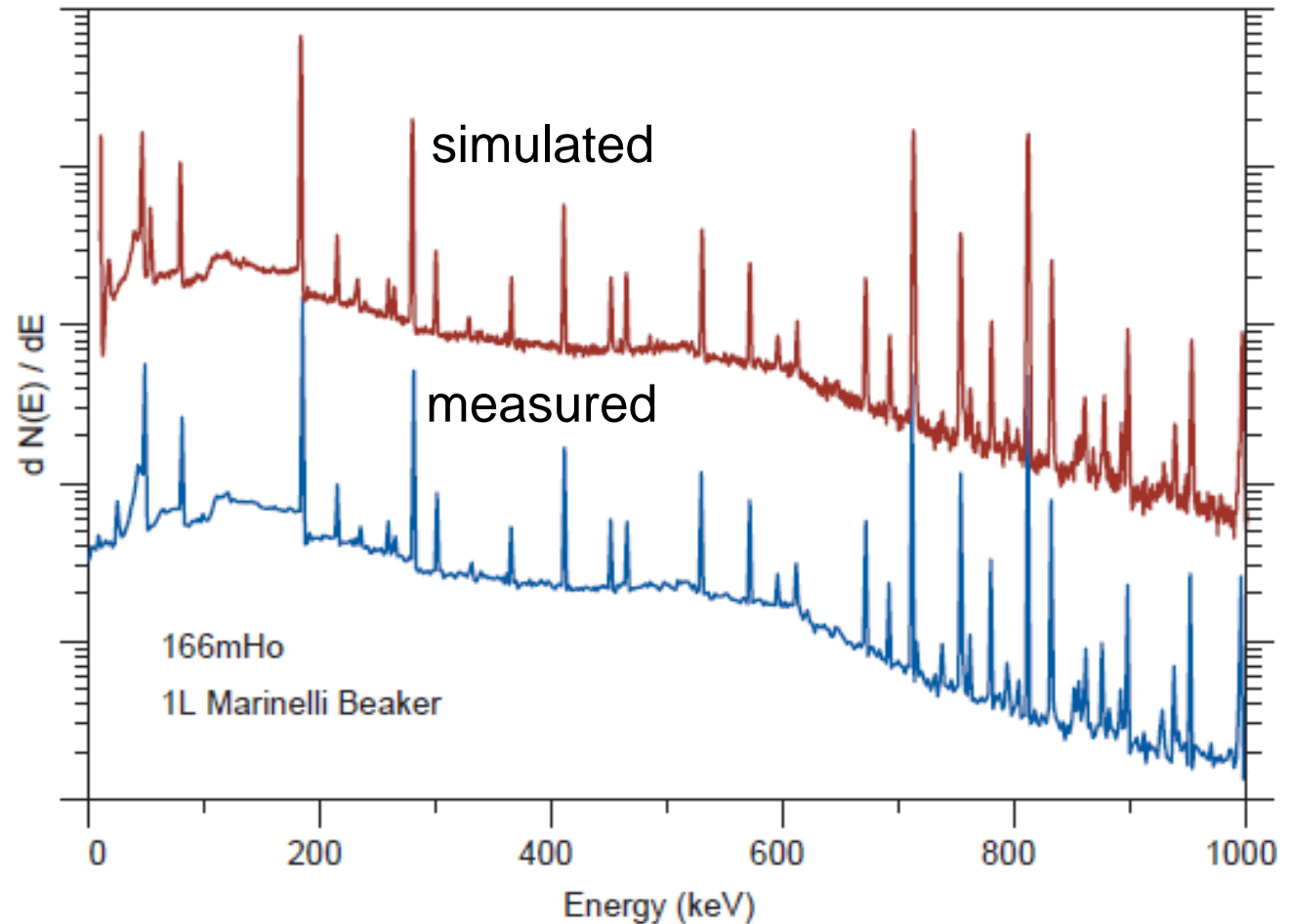
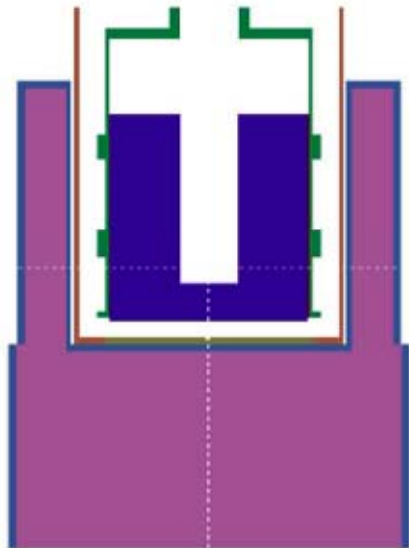
Sempau et al., PMB 2001

● Lateral dose profiles from a Siemens KDS



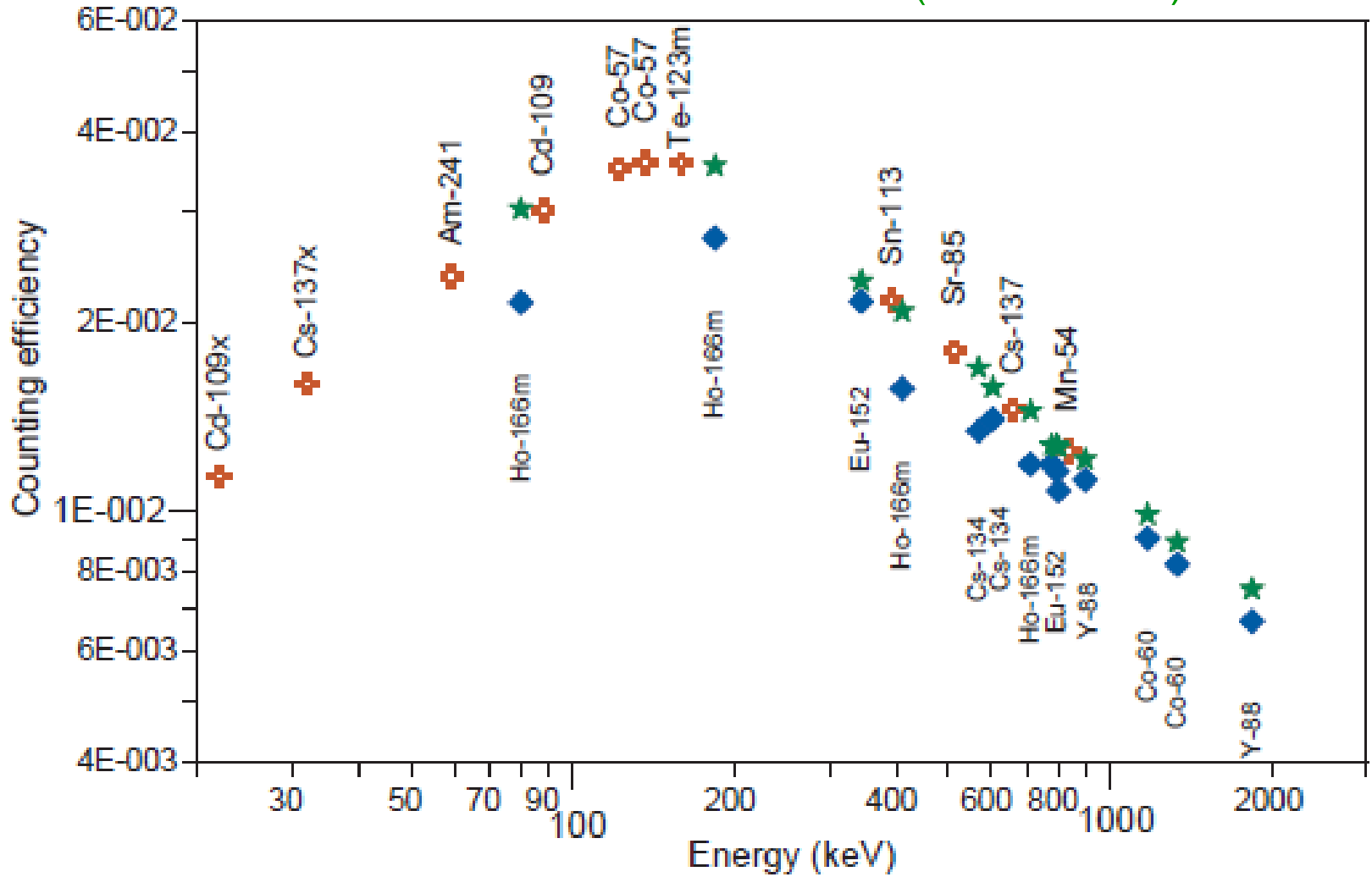
● Example. Gamma-ray spectrometry

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

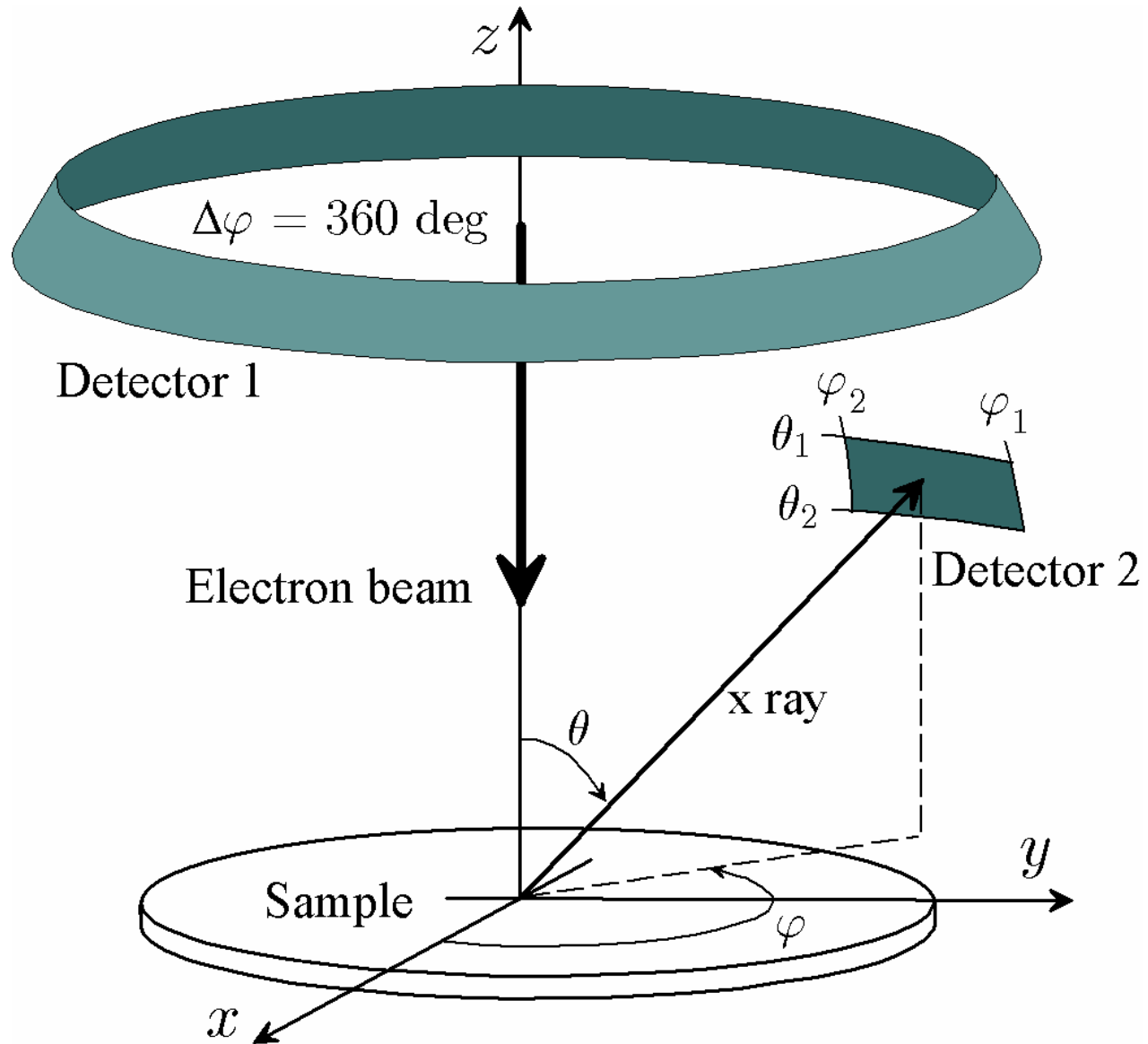


● Detection efficiencies.

- ✚ not affected by coincidences
- ◆ affected by coincidence-summing
- ★ simulation (PENELOPE)

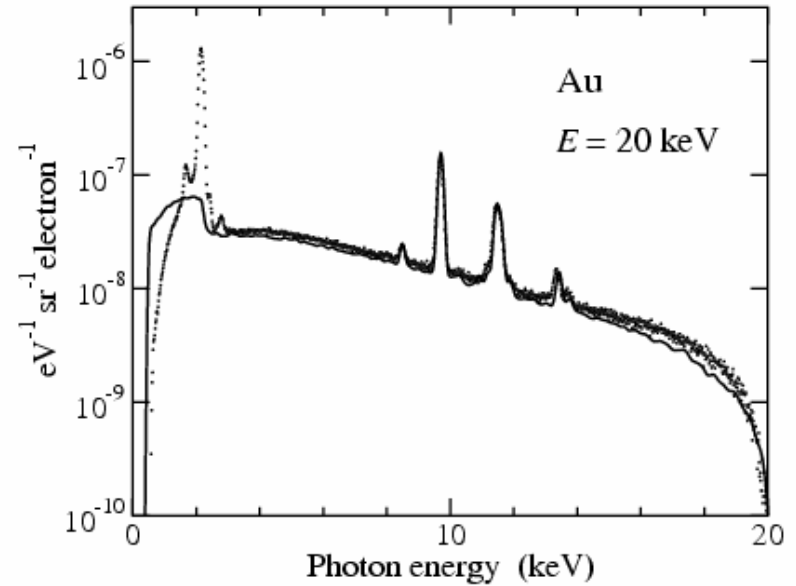
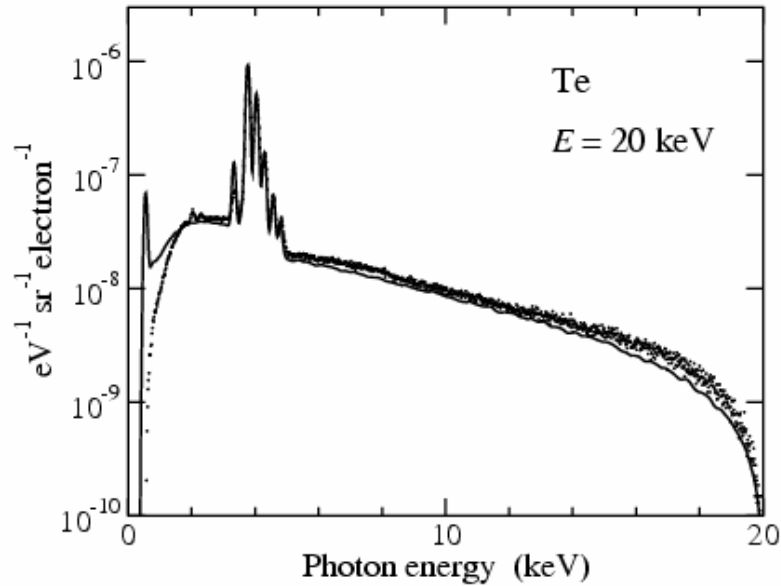
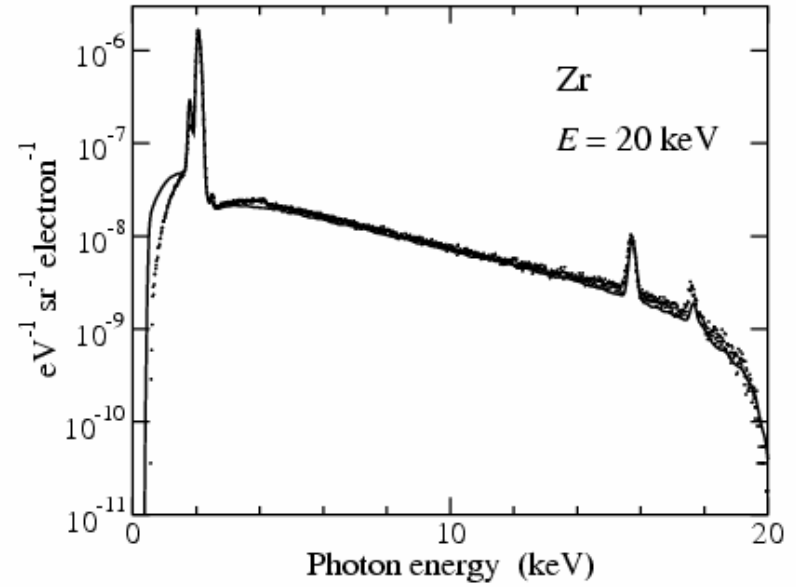
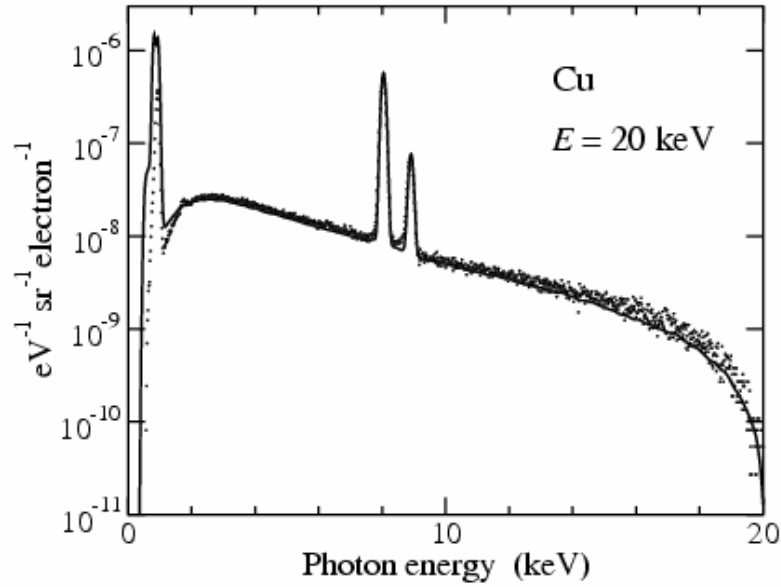


● X-ray microanalysis



● X-ray microanalysis

(experiment vs. simulation)



● Topics of current interest, development

- Fast simulation algorithms for radiotherapy treatment planning
Class I (condensed) algorithms with MC multiple-scattering distributions
- Low-energy electron and photon transport
Need of more reliable cross sections (aggregation effects)
- Quantification in electron probe microanalysis, x-ray fluorescence, Auger spectroscopy. Design of low-energy x-ray tubes
- Measurements of ionisation cross sections, brems in solids
(MC used to correct for multiple-scattering effects)
- Radiation metrology standards.
Design and characterization of radiation detectors.
Radiation protection (shielding and dosimetry)



Barcelona, Parc Güell