Class II simulation of electron and proton transport: PENELOPE and PENH

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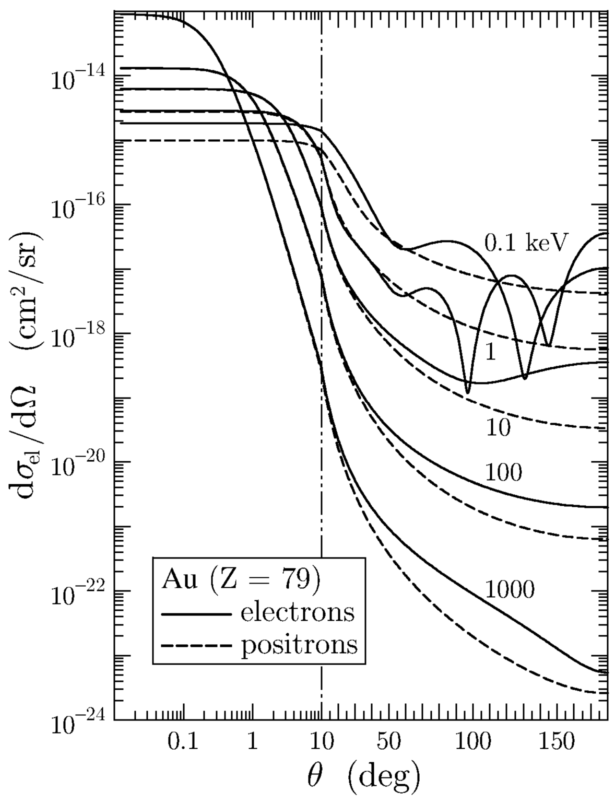
Why simulating charged particles is difficult?

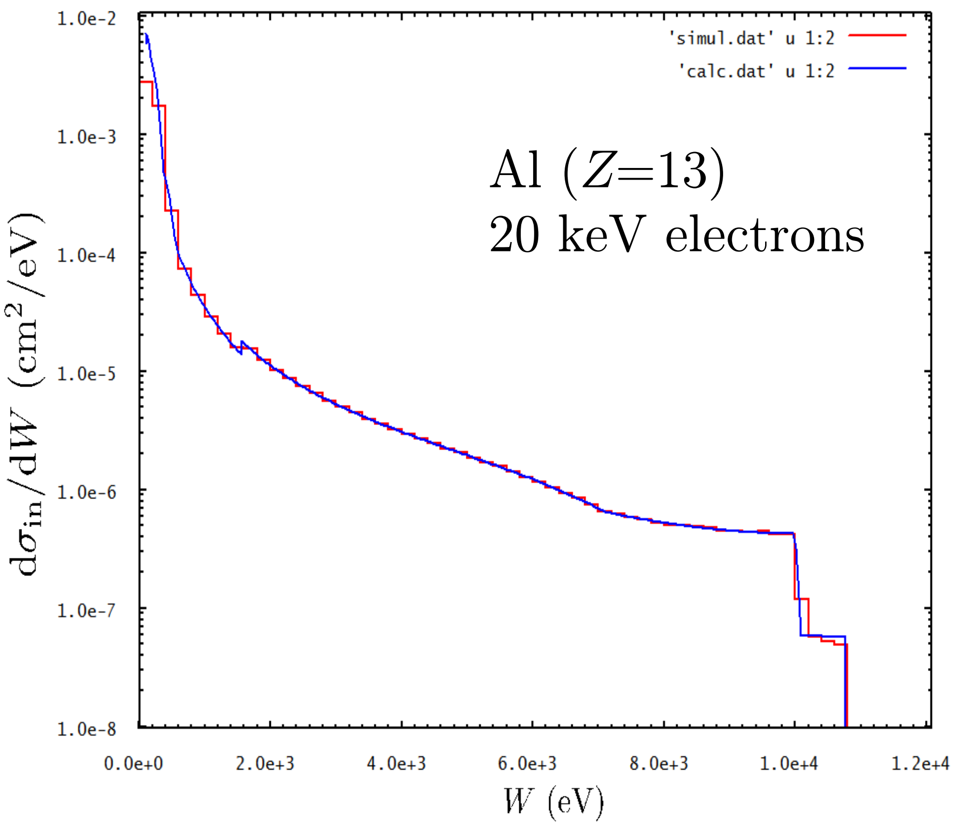
- Mostly because the transported particle undergoes many collisions in the course of its slowing down:

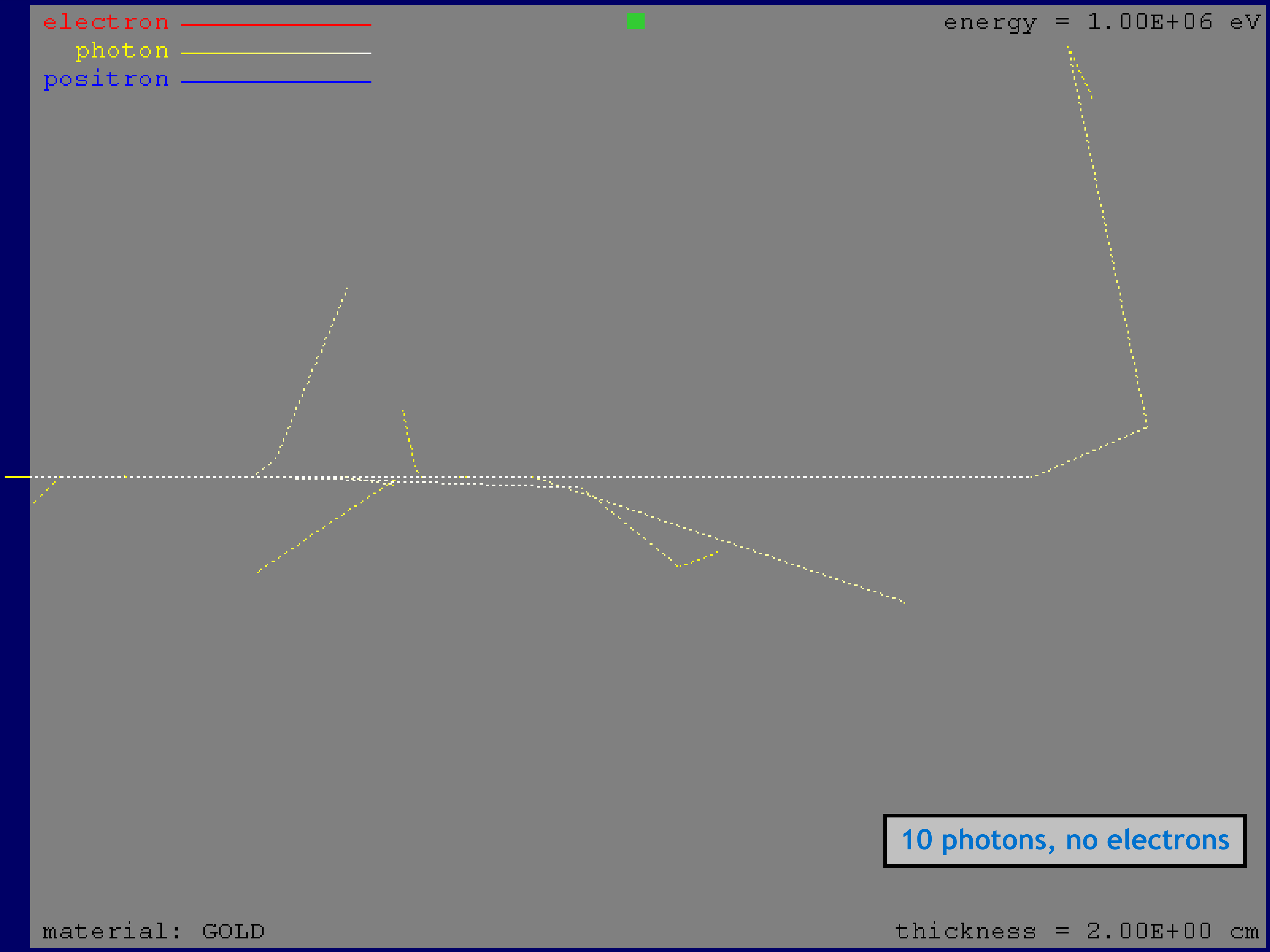
$$\langle \Delta E \rangle \sim 25 \text{ eV}$$

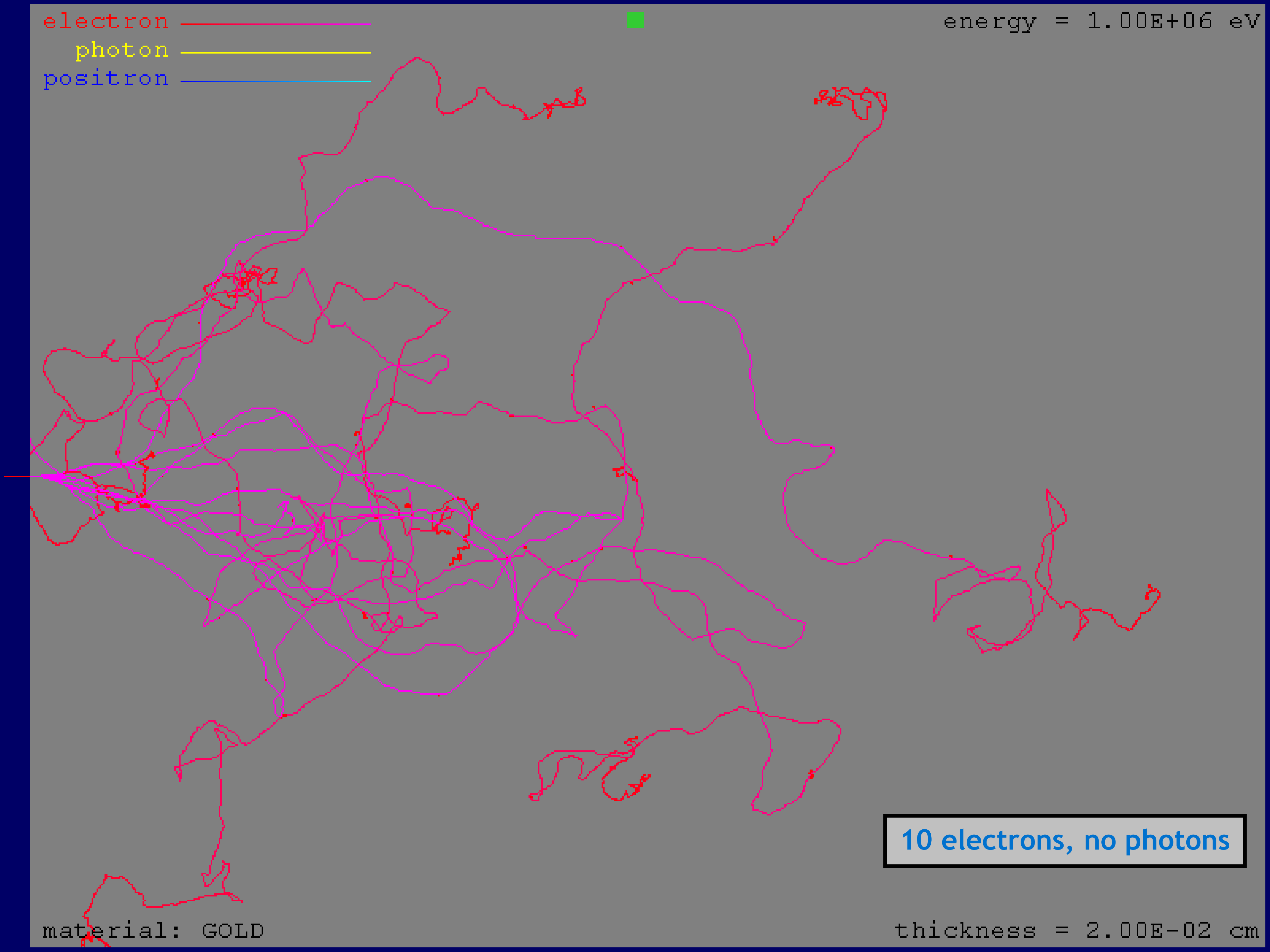
A 25 MeV electron will suffer about 10^6 collisions!

- … but most of them are "soft":






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

Possible simulation strategies

- **Detailed (analogue) simulation**, interaction by interaction
  - + Nominally exact
  - – Doable only for low energies, thin media

- **Class I (condensed) simulation**, complete grouping
  - + Works for high energies and/or thick media
  - – Difficulties to describe space displacements and interface crossings (requires switching to detailed simulation near interfaces)

- **Class II (mixed) simulation**
  - + Hard events are described "exactly" from their (restricted) DCSs
  - + Elastic, inelastic and bremsstrahlung are "tuned" independently
  - + Flexible (from detailed to class I)
  - – Slow when cut-offs are too small

- In PENELOPE and PENH we use strict class II simulation

Elastic collisions

- **Macroscopic quantities:**
  - Mean free path (determines the lengths of free flights)

$$\lambda_{\rm el}(E) = \left[\mathcal{N} \int \frac{{\rm d}\sigma_{\rm el}}{{\rm d}\Omega}\,{\rm d}\Omega\right]^{-1} \qquad \mathcal{N} \equiv \frac{N_{\rm A}\rho}{A_{\rm m}}$$

  - First and second transport mean free paths:

$$\lambda_{\rm el,1}(E) = \left[\mathcal{N} \int (1-\cos\theta) \frac{{\rm d}\sigma_{\rm el}}{{\rm d}\Omega}\,{\rm d}\Omega\right]^{-1}$$

$$\lambda_{\rm el,2}(E) = \left[\mathcal{N} \int \frac{3}{2}(1-\cos^2\theta) \frac{{\rm d}\sigma_{\rm el}}{{\rm d}\Omega}\,{\rm d}\Omega\right]^{-1}$$

Determine the first and second moments of the angular distribution after a given path length s

$$\boxed{\mu = \frac{1-\cos\theta}{2}}$$

$$\langle\mu\rangle = \frac{1}{2}\left[1-\exp\left(-s/\lambda_{\rm el,1}^{(\rm s)}\right)\right] \qquad \langle\mu^2\rangle = \langle\mu\rangle - \frac{1}{6}\left[1-\exp\left(-s/\lambda_{\rm el,2}^{(\rm s)}\right)\right]$$

Class II simulation of elastic collisions

- We set a (small) cut-off angle θ_c and consider:
  - **Hard collisions:** with $\theta > \theta_c$, only a few in each electron history
    Detailed simulation is inexpensive
  - **Soft collisions:** with $\theta < \theta_c$, a large number (on average) between each pair of hard interactions
    Class I simulation is appropriate

- Instead of defining the cutoff angle, we prefer to set the hard mean free path:

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

and determine θ_c from

$$\lambda_{\mathrm{el}}^{(\mathrm{h})}(E) = \left[\mathcal{N}\, 2\pi \int_{\theta_c}^{\pi} \frac{\mathrm{d}\sigma_{\mathrm{el}}}{\mathrm{d}\Omega} \sin\theta \,\mathrm{d}\theta\right]^{-1}$$

C_1 (< 0.2) limits the average angular deflection along a step
C_2 (< 0.2) limits the average fractional energy loss along a step

Simulation of hard collisions

- The DCS is stored in a dense logarithmic grid of ~200 energies. The random sampling of the scattering angle is performed by the inverse transform algorithm (RITA method)

- The DCS is sampled only for the energies E_i of the grid (allows pre-calculating the RITA sampling tables)

- For energies not in the table, the angular distribution is obtained by the method of weights,

$$p(E;\mu) = \left[\frac{\ln E_{i+1} - \ln E}{\ln E_{i+1} - \ln E_i}\right] p(E_i;\mu) + \left[\frac{\ln E - \ln E_i}{\ln E_{i+1} - \ln E_i}\right] p(E_{i+1};\mu)$$

  if $E \in (E_i, E_{i+1})$

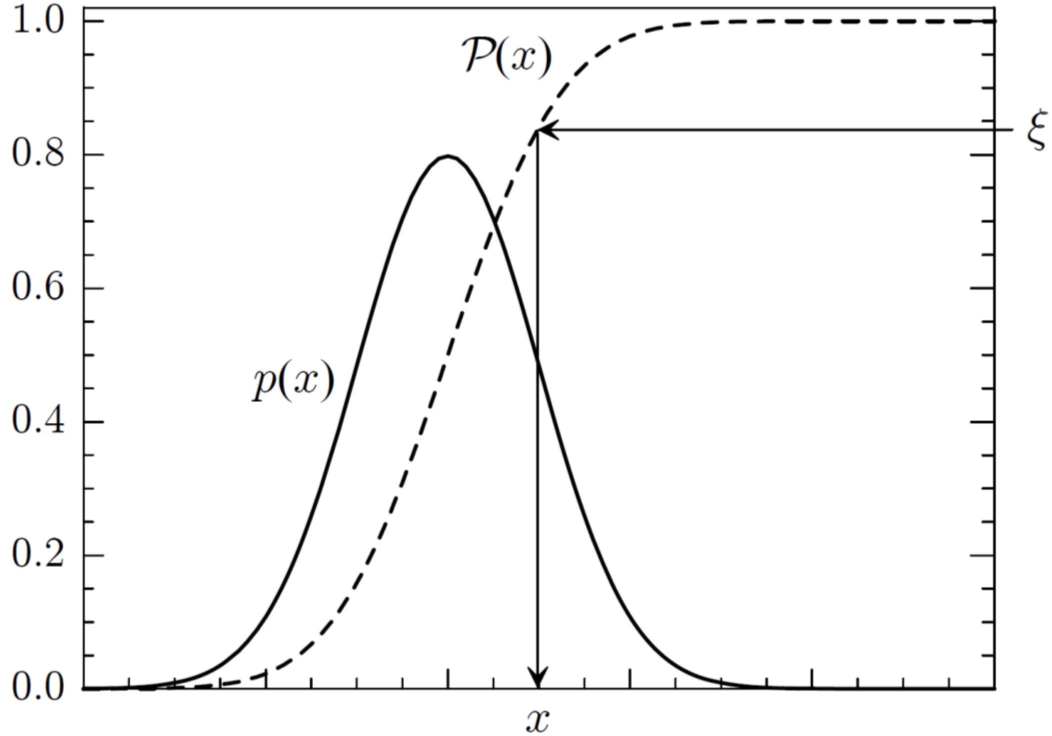
  Equivalent to linear interpolation of the DCS in $\ln E$

- The sampling of hard collisions (restricted to angles $\theta > \theta_c$) does not require manipulating the stored tables. The sampling is independent of the adopted cut-off!

Random sampling: inverse transform

- Cumulative distribution function $\mathcal{P}(x) \equiv \int_{-\infty}^{x} p(x')\,\mathrm{d}x'$
- x is generated as $x = \mathcal{P}^{-1}(\xi)$ or, equivalently, $\xi = \int_{x_{\min}}^{x} p(x')\,\mathrm{d}x'$

Graphically:



- Notice that we can restrict x by simply restricting ξ. The program uses energy-dependent cut-offs $\xi_c(E)$

Energy-loss interactions

- Inelastic collisions (simple GOS model for each electron shell):

$$\frac{\mathrm{d}^2\sigma_{\mathrm{in}}}{\mathrm{d}W\,\mathrm{d}\cos(\theta)} \qquad \frac{\mathrm{d}\sigma_{\mathrm{in}}}{\mathrm{d}W} = 2\pi \int_0^{\pi} \frac{\mathrm{d}^2\sigma_{\mathrm{in}}}{\mathrm{d}W\,\mathrm{d}\cos(\theta)} \sin\theta\,\mathrm{d}W$$

- Bremsstrahlung emission (Seltzer-Berger scaled cross section tables):

$$\frac{\mathrm{d}\sigma_{\mathrm{br}}}{\mathrm{d}W} = \frac{Z^2}{\beta^2}\frac{1}{W}\chi\left(Z, E, \frac{W}{E}\right)$$

- **Macroscopic quantities:**
  - Mean free paths:

$$\lambda_{\mathrm{in}}(E) = \left[\mathcal{N}\int_0^E W \frac{\mathrm{d}\sigma_{\mathrm{in}}}{\mathrm{d}W}\mathrm{d}W\right]^{-1} \qquad \lambda_{\mathrm{br}}(E) = \left[\mathcal{N}\int_{W_0}^E W \frac{\mathrm{d}\sigma_{\mathrm{br}}}{\mathrm{d}W}\mathrm{d}W\right]^{-1}$$

  - Stopping power (average energy loss per unit path length)

$$S(E) = \mathcal{N}\int_0^E W\left(\frac{\mathrm{d}\sigma_{\mathrm{in}}}{\mathrm{d}W} + \frac{\mathrm{d}\sigma_{\mathrm{br}}}{\mathrm{d}W}\right)\mathrm{d}W$$

  - Energy-straggling parameter (average increase in the variance of the energy-loss distribution per unit path length)

$$\Omega^2(E) = \mathcal{N}\int_0^E W^2\left(\frac{\mathrm{d}\sigma_{\mathrm{in}}}{\mathrm{d}W} + \frac{\mathrm{d}\sigma_{\mathrm{br}}}{\mathrm{d}W}\right)\mathrm{d}W$$

Class II simulation of energy-loss interactions

- We define cut-off energy losses W_{cc} and W_{cr} :
  - **Hard interactions:** with W > the cut-off (only a few, detailed simulation)
  - **Soft collisions:** with W < the cut-off (condensed simulation)

  Cut-off values of the order of 1 keV are usually appropriate (depending on the required energy resolution)

- Relevant quantities:
  - Mean free paths for hard interactions:

$$\lambda_{\mathrm{in}}(E) = \left[\mathcal{N} \int_{W_{\mathrm{cc}}}^{E} W \frac{\mathrm{d}\sigma_{\mathrm{in}}}{\mathrm{d}W} \mathrm{d}W\right]^{-1} \qquad \lambda_{\mathrm{br}}(E) = \left[\mathcal{N} \int_{W_{\mathrm{cr}}}^{E} W \frac{\mathrm{d}\sigma_{\mathrm{br}}}{\mathrm{d}W} \mathrm{d}W\right]^{-1}$$

  - Soft stopping power:

$$S_{\mathrm{s}}(E) = \mathcal{N} \int_0^{W_{\mathrm{cc}}} W \frac{\mathrm{d}\sigma_{\mathrm{in}}}{\mathrm{d}W} \mathrm{d}W + \mathcal{N} \int_0^{W_{\mathrm{cr}}} W \frac{\mathrm{d}\sigma_{\mathrm{br}}}{\mathrm{d}W} \mathrm{d}W$$

  - Soft energy-straggling parameter:

$$\Omega_{\mathrm{s}}^2(E) = \mathcal{N} \int_0^{W_{\mathrm{cc}}} W^2 \frac{\mathrm{d}\sigma_{\mathrm{in}}}{\mathrm{d}W} \mathrm{d}W + \mathcal{N} \int_0^{W_{\mathrm{cr}}} W^2 \frac{\mathrm{d}\sigma_{\mathrm{br}}}{\mathrm{d}W} \mathrm{d}W$$

  - … and the angular transport cross sections of soft inelastic collisions

Simulation of soft interactions

- The cumulative effect of soft events along a given path length s is described by the global polar angular deflection μ_{s} or θ_{s} and the total energy loss W_{s}
- These quantities are sampled from *artificial* distributions having the correct first and second moments.

$$\mu = \frac{1-\cos\theta}{2}$$

- **Angular deflection**

$$\frac{1}{\lambda^{(\mathrm{s})}_{\mathrm{el},\ell}(E)} = \mathcal{N}\int_0^{\mu_{\mathrm{c}}} \mathrm{d}\mu\, [1-P_\ell(\cos\theta)]\, \frac{\mathrm{d}\sigma_{\mathrm{el}}(E)}{\mathrm{d}\mu}$$

$$\frac{1}{\lambda^{(\mathrm{s})}_{\mathrm{in},\ell}(E)} = \mathcal{N}\int_0^{1} \mathrm{d}\mu\, [1-P_\ell(\cos\theta)] \int_0^{W_{\mathrm{cc}}} \mathrm{d}W\, \frac{\mathrm{d}^2\sigma_{\mathrm{in}}(E)}{\mathrm{d}W\,\mathrm{d}\mu}$$

$$\frac{1}{\lambda^{(\mathrm{s})}_{\mathrm{comb},\ell}(E)} = \frac{1}{\lambda^{(\mathrm{s})}_{\mathrm{el},\ell}(E)} + \frac{1}{\lambda^{(\mathrm{s})}_{\mathrm{in},\ell}(E)}$$

$$\langle\mu_{\mathrm{s}}\rangle = \frac{1}{2}\left[1-\exp(-s/\lambda^{(\mathrm{s})}_{\mathrm{comb},1})\right] \qquad \langle\mu_{\mathrm{s}}^2\rangle = \langle\mu_{\mathrm{s}}\rangle - \frac{1}{6}\left[1-\exp(-s/\lambda^{(\mathrm{s})}_{\mathrm{comb},2})\right]$$

Exact moments for pure elastic scattering. A correction is required to account for soft energy losses along the step

- **Energy loss:** Because possible energy transfers in individual soft events are bounded, we can account for the variation of the parameters along the step, assuming they vary linearly with E

$$\langle W_{\rm s}\rangle = S_{\rm s}(E_0)\, s \left\{1 - \frac{1}{2}\left[\frac{{\rm d}\ln S_{\rm s}(E)}{{\rm d}E}\right]_{E=E_0} S_{\rm s}(E_0)\, s\right\}$$

$$\mathrm{var}(W_{\rm s}) = \Omega_{\rm s}^2(E_0)\, s \left\{1 - \left[\frac{1}{2}\frac{{\rm d}\ln \Omega_{\rm s}^2(E)}{{\rm d}E} + \frac{{\rm d}\ln S_{\rm s}(E)}{{\rm d}E}\right]_{E=E_0} S_{\rm s}(E_0)\, s\right\} = \sigma^2$$

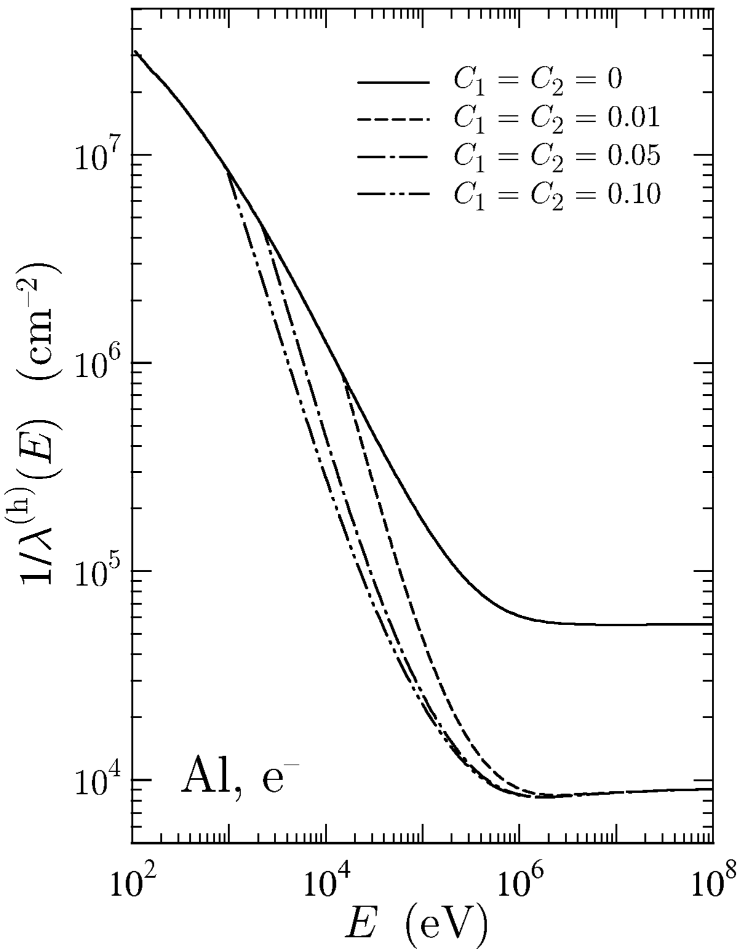
For steps that are long enough, the distribution of soft energy losses is approx. Gaussian (central limit theorem). We use a Gaussian truncated at 3σ to have a well defined maximum loss

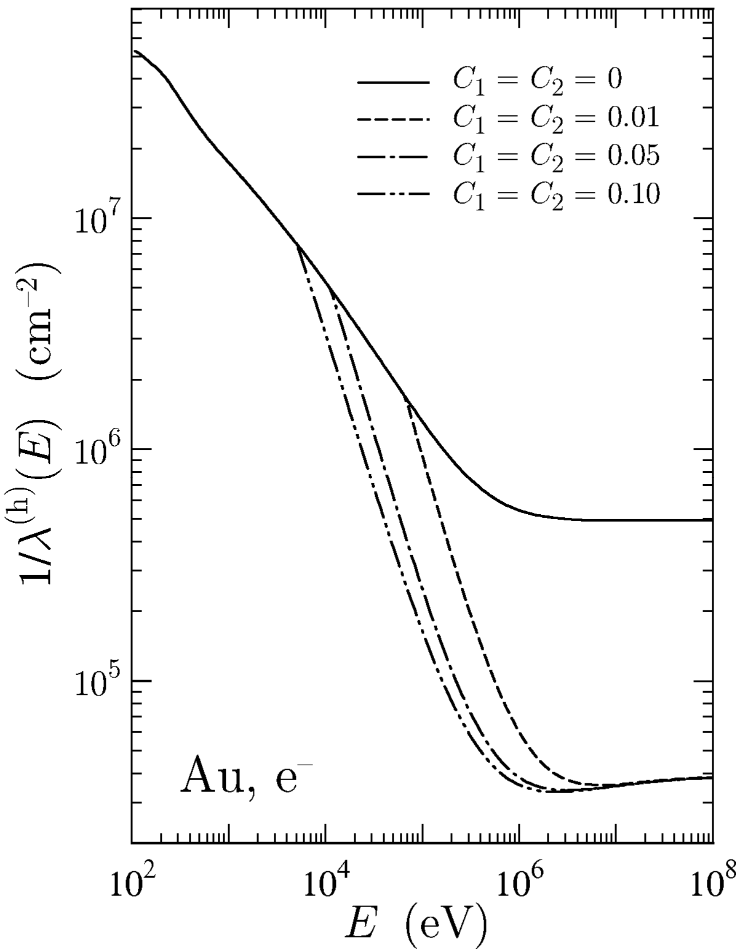
$$P_{\rm I}(W_{\rm s}) = \begin{cases} \exp\left[-\dfrac{(W_{\rm s} - \langle W_{\rm s}\rangle)^2}{2(1.015387\,\sigma)^2}\right] & \text{if } |W_{\rm s} - \langle W_{\rm s}\rangle| < 3\,\sigma \\ 0 & \text{otherwise} \end{cases}$$

or a suitable *artificial* distribution with the correct first and second moments

- Having a well defined maximum loss, we can account for the variation with E of the mean free paths for hard events

Variation of the hard mfp with energy



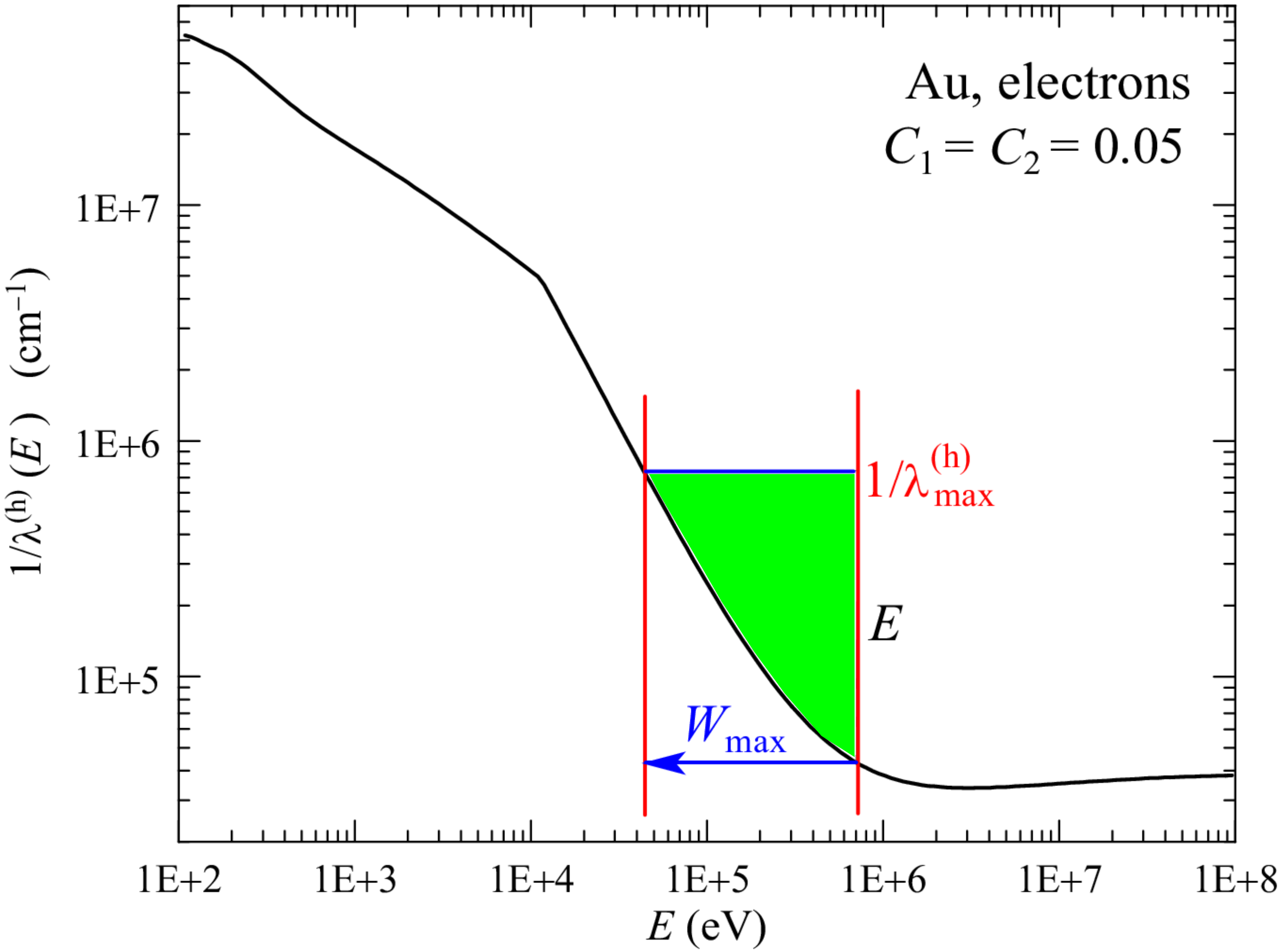


Both with $W_{cc} = W_{cr} =$ 100 eV

- The usual sampling formula for the path length $s = -\lambda_T^{(h)} \ln \xi$ is NOT valid

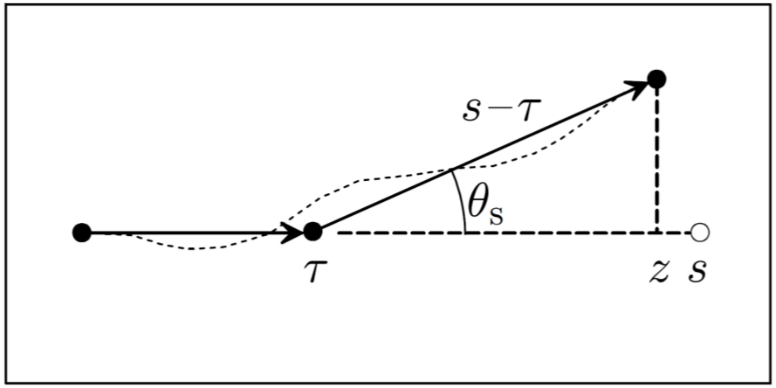
Path length to the next hard interaction

- The variation of the mfp with energy is accounted for by introducing delta interactions (to get a constant mfp in the covering energy interval)



The random hinge method

- To determine the space displacement after a step (and the position of the next hard interaction) we use the following algorithm



1.- Sample the length s of the step to the next hard interaction

2.- Sample the soft energy loss W_s along the step

3.- Move the electron a random distance $\tau = \xi s$

4.- Sample the deflection angle θ_s due to soft elastic and inelastic collisions and change the direction of motion

5.- Move the electron the remaining distance $s - \tau$

The energy W_s may be deposited either at the hinge or uniformly along the step, *i.e.*, as in the CSDA with stopping power $S_s = W_s/s$

Simulation algorithm

1.- Set the initial state variables (or new material)
2.- Sample the step length
3.- Move to the hinge
4.- If the particle crosses an interface go to step 2
6.- Change the direction of flight (and optionally the energy)
7.- Move to the hard event at the end of the step
8.- If the particle crosses an interface go to step 2
9.- Simulate the hard interaction or the delta interaction
10.- Go to 2

The particle is absorbed when its energy becomes less than the adopted cut-off

- A great advantage of class II schemes is that the history of a particle is a sequence of free flights with alternating hard interactions and hinges
- The same program can perform detailed simulation (no hinges). This allows for strictly checking the stability of the results under variations of the simulation parameters

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

Stability study

- **Example:** 500 keV electrons in Al. s = 200 μm

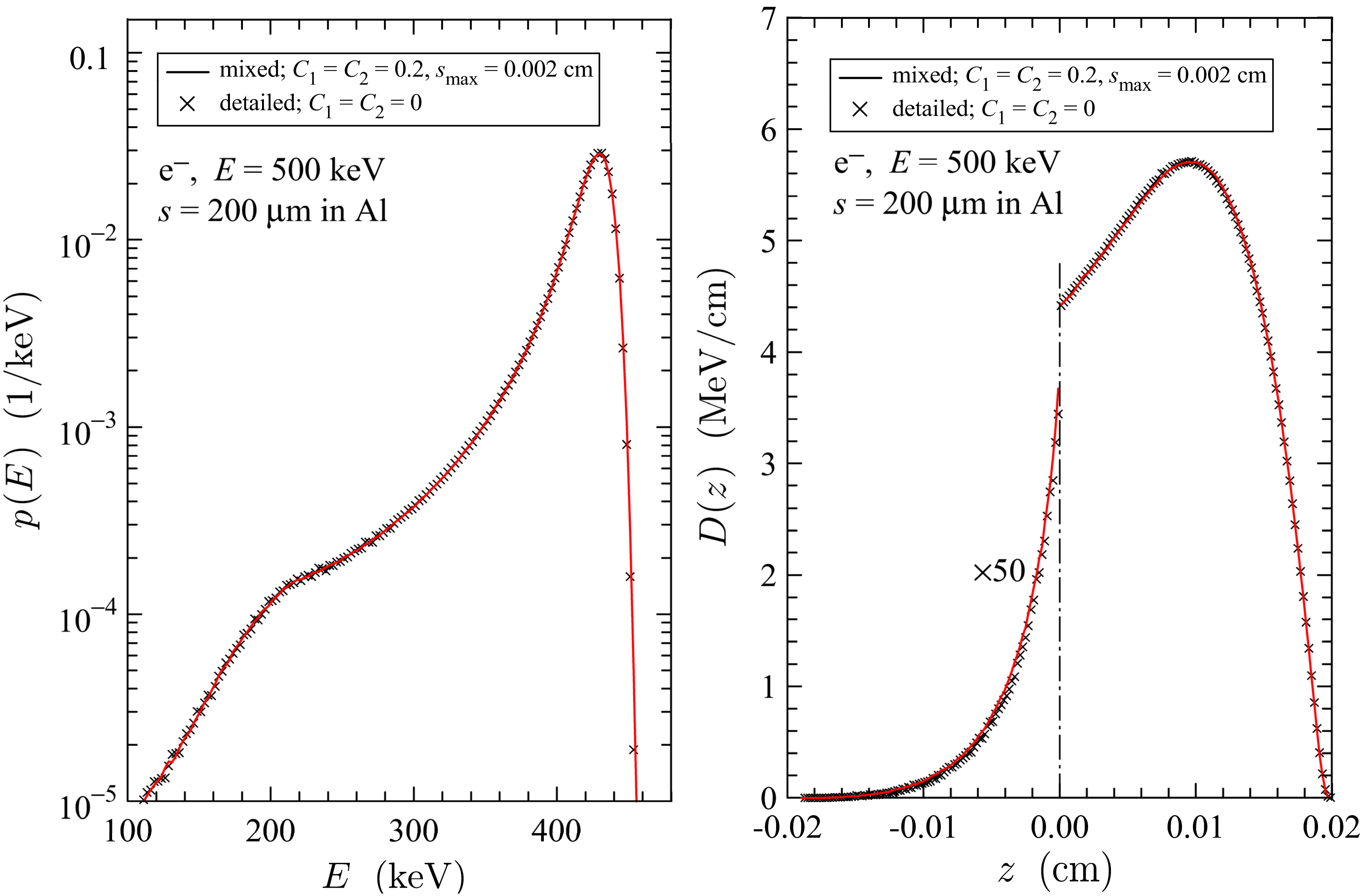
- **Detailed simulation:** $C_1 = C_2 = 0$; W_{cc} = 0 eV
  W_{cr} = -10 eV (soft bremsstrahlung disregarded)

Average numbers of interactions: elastic 1297
inelastic 1181
bremsstrahlung 0.03

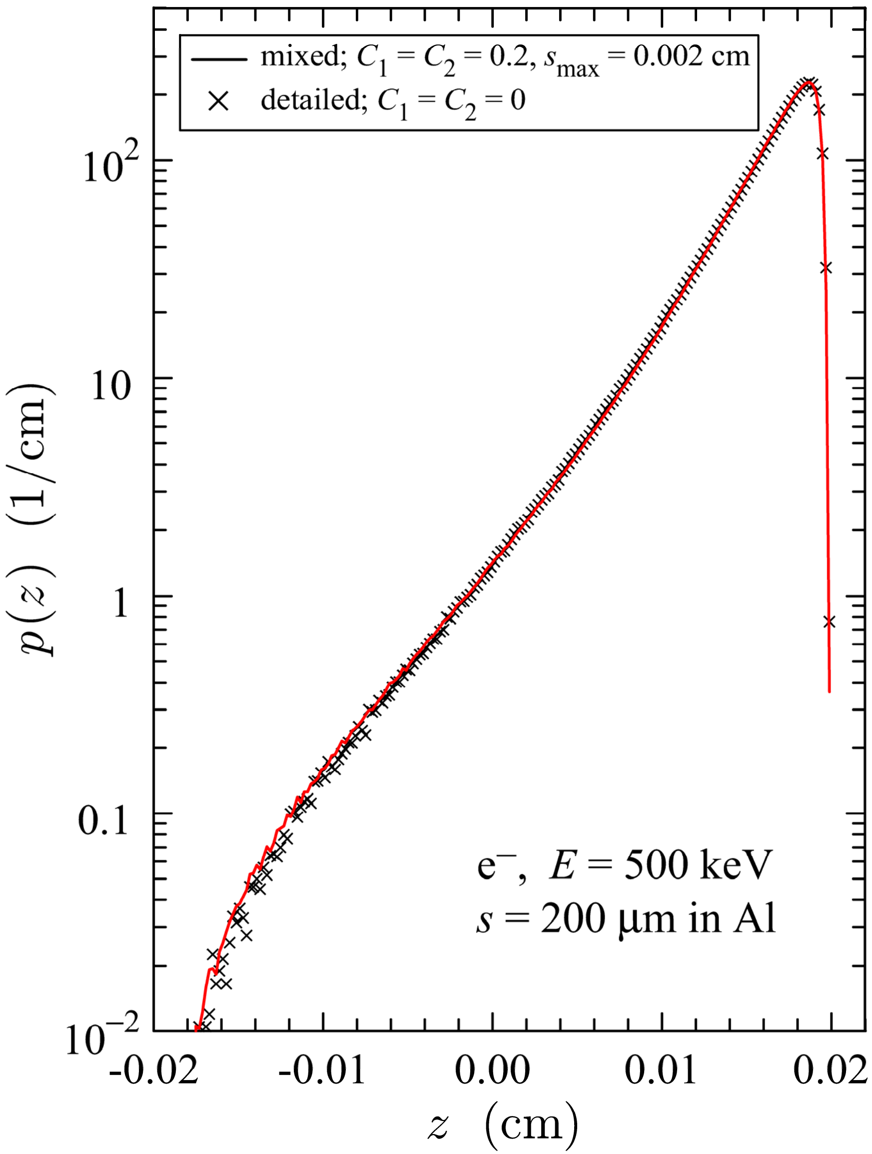
- **Class II simulation:** $C_1 = C_2 = 0.2$ (extreme value)
  W_{cc} = 1 keV; s_{max} = 20 μm
  W_{cr} = -10 eV (soft bremsstrahlung disregarded)

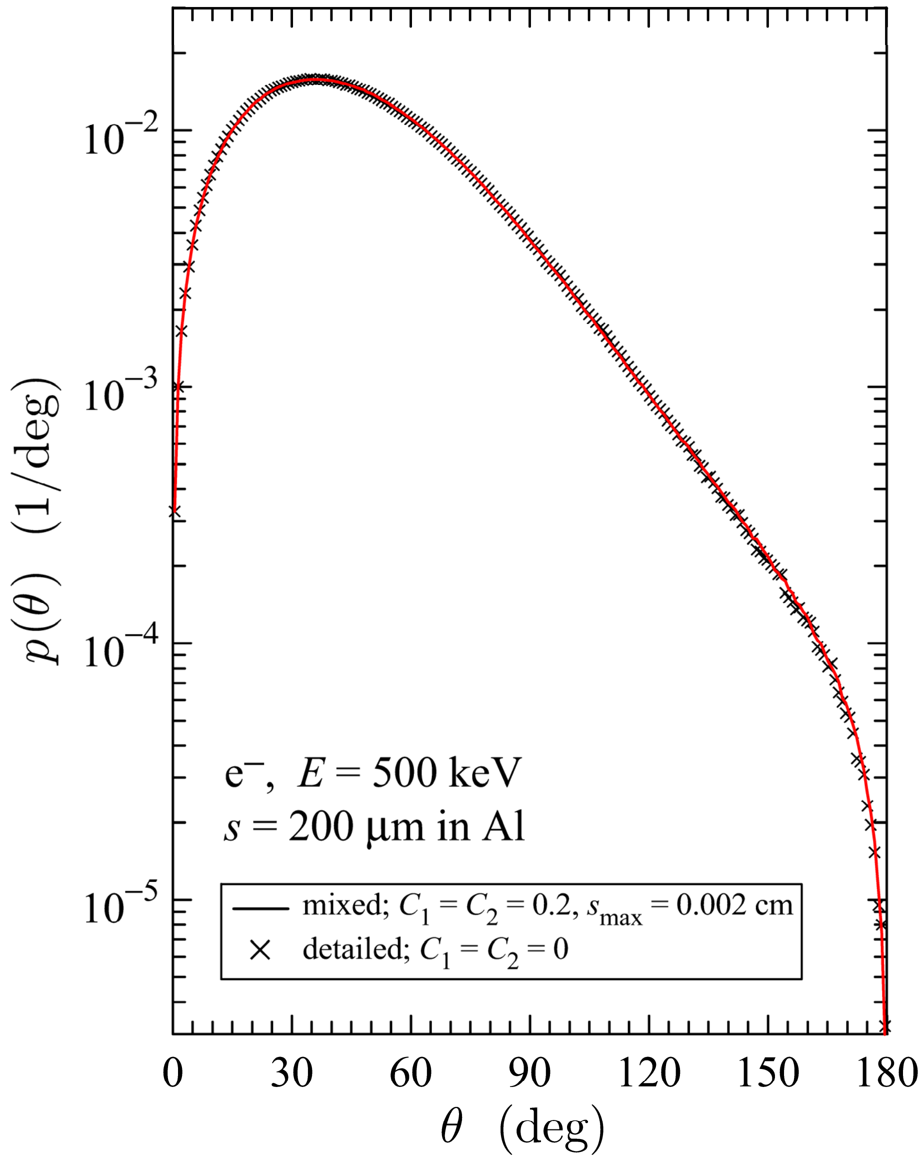
Average numbers of interactions: hard elastic 4.7
hard inelastic 3.9
hard bremsstrahlung . . 0.03
delta interactions 6.0
hinges 15

About 75 times faster (not favorable conditions)



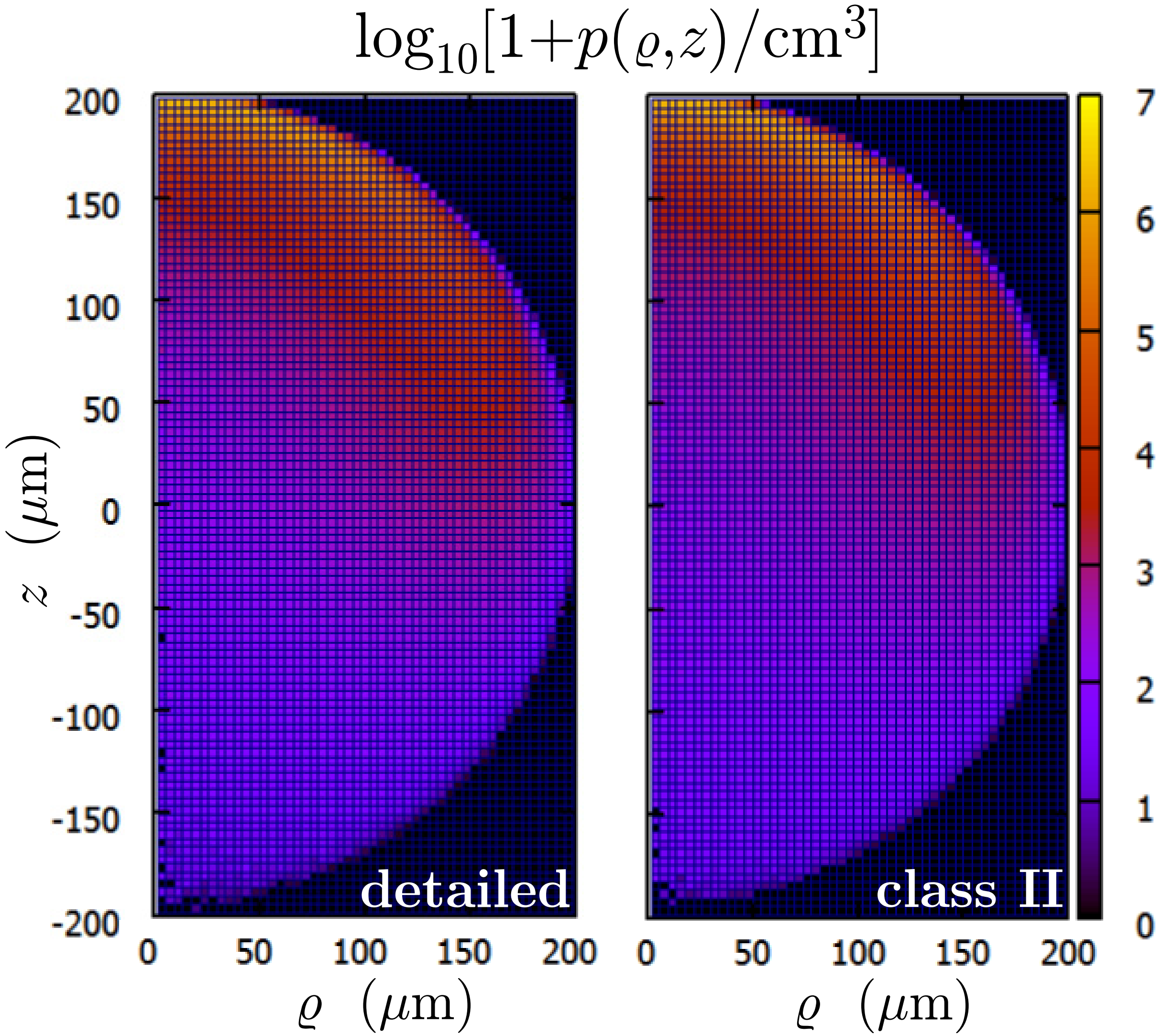
crosses: detailed; solid lines: class II





crosses: detailed; solid lines: class II

Spatial distribution of final positions



$\varrho = \sqrt{x^2 + y^2}$