Electromagnetic interactions and transport of charged particles (e^-, e^+, muons, charged hadrons, ions)

Review interactions of leptons and photons

Transport of charged particles

Transport and delta-ray-production thresholds

EM process overview

- **Elastic scattering on screened electrostatic potential of target atoms (Coulomb scattering):**
  - Single scattering
  - Condensed multiple Coulomb scattering
- **Collisions of charged particles with target electrons:**
  - Continuous energy loss along a particle step: stopping power (dE/dx) description + fluctuations
  - Discrete energy losses (delta ray production)
- **Radiative losses (Bremsstrahlung)**
- **Ions:**
  - Corrections in the stopping power: effective charge, Mott correction, etc.
  - Additional EM processes: direct e-/e+ pair production, electromagnetic dissociation.
- **Muons:** +Pair production, photonuclear reaction, muon capture.
- **Positrons**: +annihilation in flight
- **Photons**: Rayleigh+Compton scattering, photo-absorption, pair production, photonuclear reactions, muon pair production.

Photon and $e^{\pm}$ interactions in FLUKA

Photon and e± interactions in FLUKA

- FLUKA's e± and γ physics package (EMF) is already enabled with most **`DEFAULT`**, except: EET-TRAN, NEUTRONS, SHIELDING. To deactivate:

  EMF : OFF ▼

  (Note: If EMF is disabled, the energy of electrons/positrons/photons are deposited on the spot)

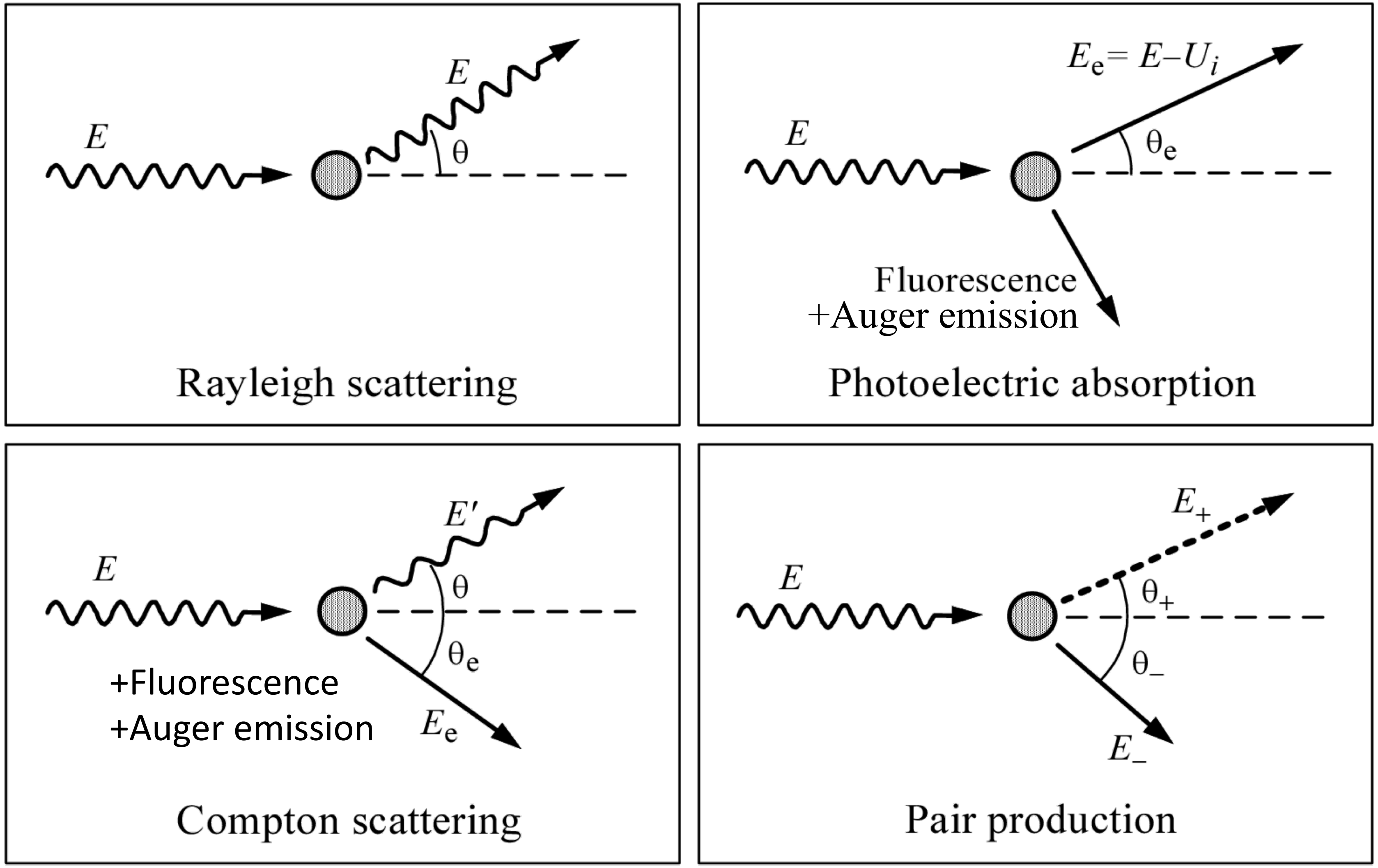
- Energy range: e± : 1 keV - 1000 TeV, γ : 100 eV - 1000 TeV

- Up-to-date γ cross sections from the EPDL database

- Energy conservation is ensured within computer precision

- Full coupling between hadronic (incl. low-energy neutrons) and electromagnetic shower

Photon interactions overview



+photo-nuclear processes

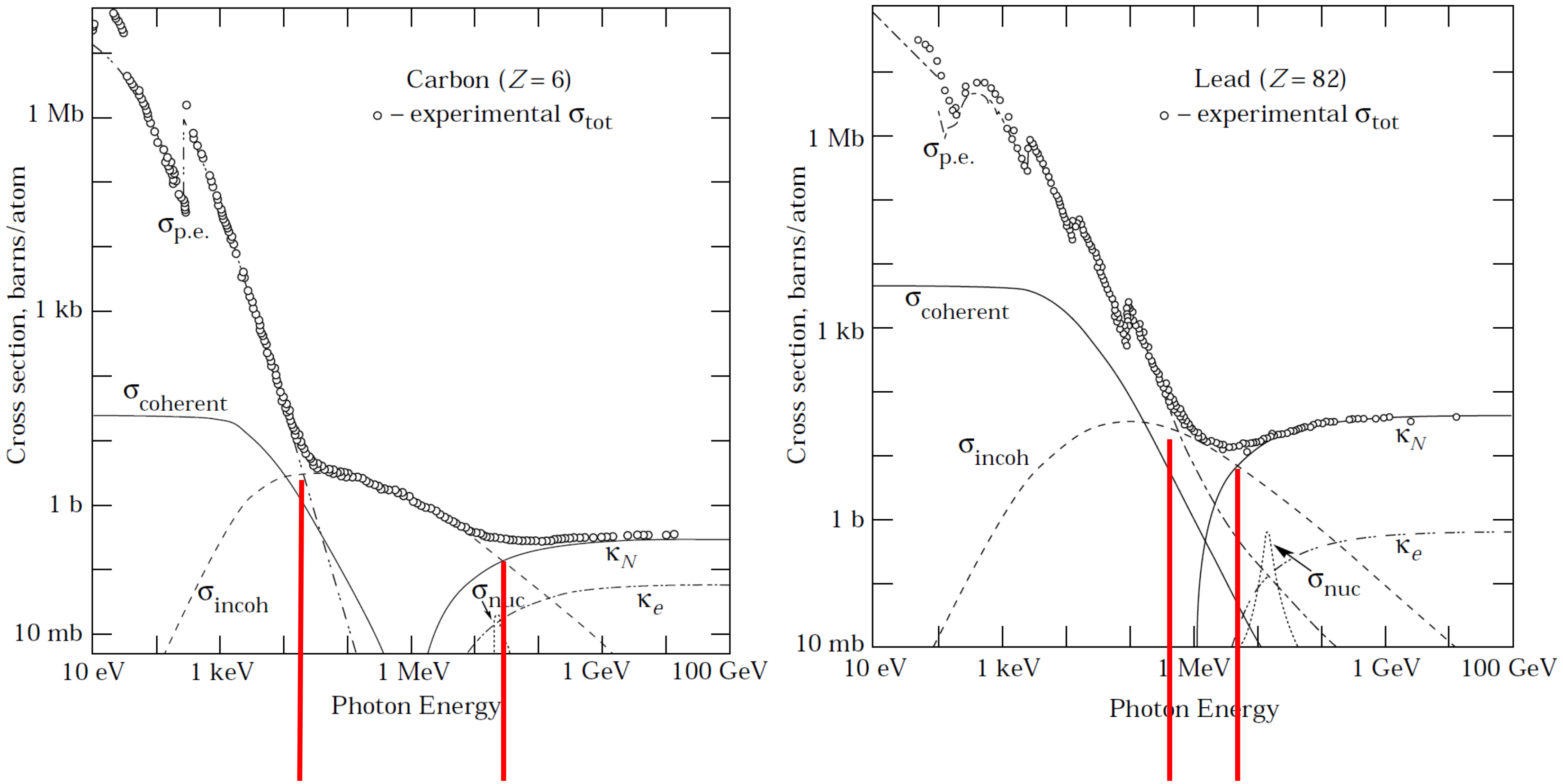
+photo-muon production

TERMINOLOGY:
absorption/emission,
not “photon scattering” (!)

(Figures kindly shared by the PENELOPE authors)

Photon interaction cross sections overview

- Interaction cross sections on a single free atom
- Aggregation effects (relevant at very low energies) not accounted for
- Rayleigh (coherent) scattering somewhat suppressed, but it gives photon shower broadening at low energies



Photoelectric dominated | Compton dominated | Pair dominated

Photoelectric dominated | Compton dominated | Pair dominated

$\sigma \propto Z^5$ | $\sigma \propto Z$ | $\sigma \propto Z^2$

e^{-+} interaction overview

- Ionization losses (see block on ionization and transport below):
  - Delta-ray production respectively modelled via the Møller and Bhabha cross sections
- Bremsstrahlung production
  - Differential cross sections from the Berger and Seltzer (NIST) database
  - Consideration of Landau-Pomeranchuk-Migdal effect and soft photon suppression (Ter-Mikaelyan polarization effect)
- Positron annihilation
  - Both at rest and in flight
  - For annihilation at rest, account for mutual polarization of the two emitted photons.
- Electro-nuclear interactions

FLUKA card summary

EMF : transport of electrons, positrons, and photons on/off

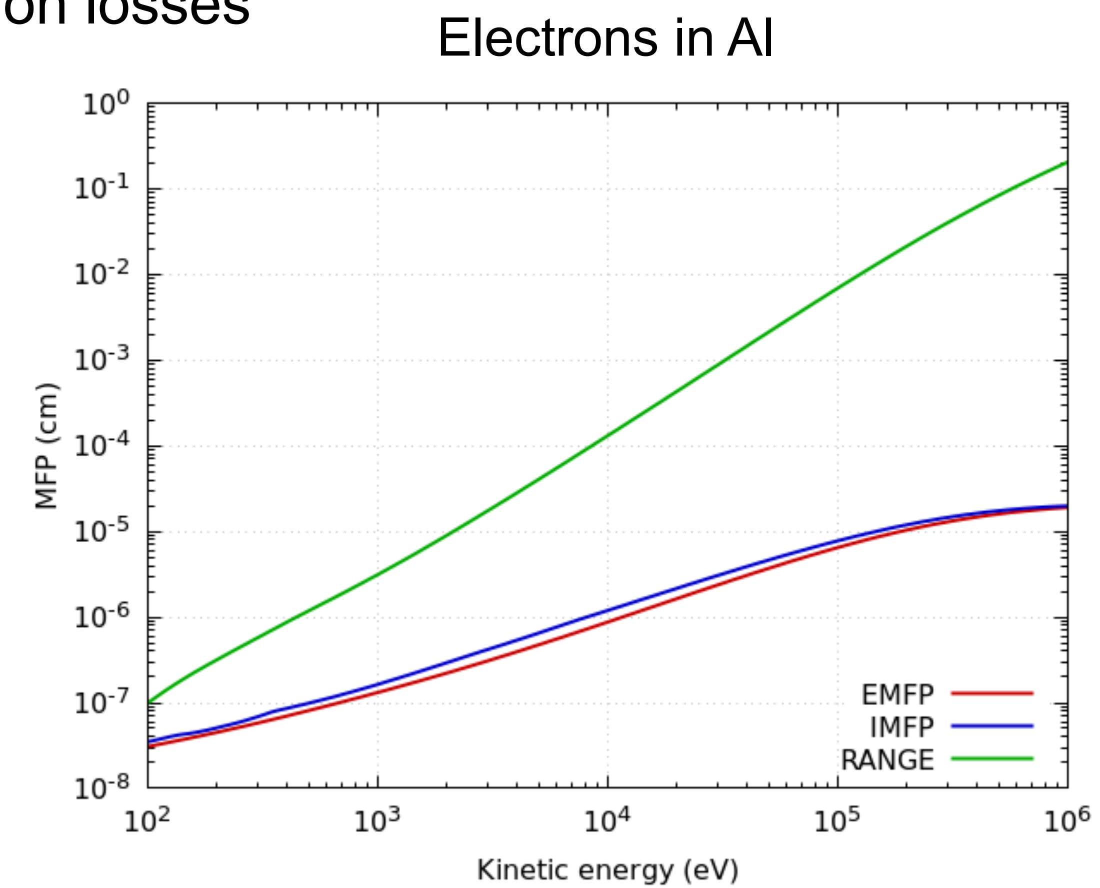
Ionization and transport - Overview

- We will briefly discuss the following interaction mechanisms of charged projectiles traversing a material:
  - Ionization losses: energy loss in collisions with target electrons
  - Elastic collisions with the (screened) Coulomb potential of atoms (multiple Coulomb scattering)

- In addition, we address here the concept of **transport thresholds**

Estimate number of events in detailed MC simulations

- **EMFP**: mean free path between consecutive Coulomb scattering
- **IMFP**: mean free path between consecutive ionization losses
- **RANGE**: estimated distance traveled to rest



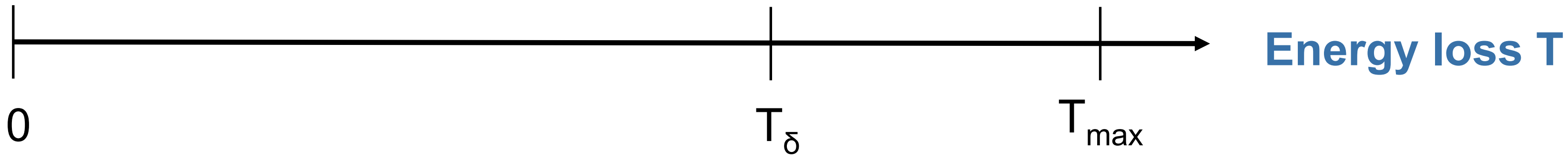
- Estimate number of ionization losses:
  - N=RANGE/IMFP
  - E.g. for a 1-MeV electron, **$N \sim 10^4$**
- Estimate number of Coulomb losses:
  - N=RANGE/EMFP
  - E.g. for a 1-MeV electron, **$N \sim 10^4$**
- **Too many to simulate explicitly!**
- A more practical approach is necessary to keep CPU time within acceptable bounds.

Condensed simulation of ionization losses

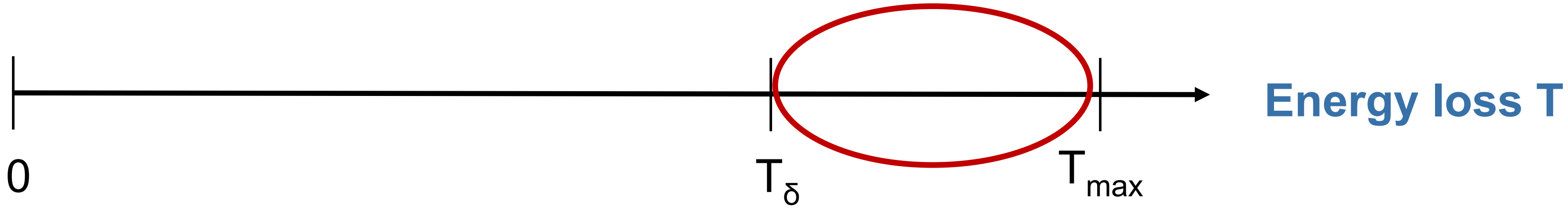
- Algorithm adopted in FLUKA:
  - Sample ionization losses (and generated delta ray) **explicitly** when **energy transfer is large**
  - Account for the combined effect of many **small ionization losses along the step** (without explicitly simulating the generated delta rays)

Ionization energy losses in FLUKA

- Two different treatments: **small** vs **large** energy losses:

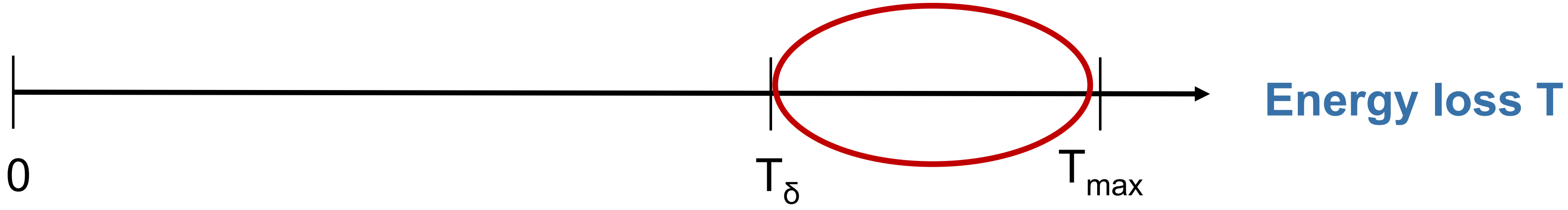


Large ionization energy losses (detailed sampling)



- Large energy loss $T > T_\delta$ transferred to a target electron
- Invested in setting in motion this knock-on electron (δ ray)
- δ rays are typically energetic and can transport energy away from their point of origin, so it makes sense to sample their production and transport explicitly (discrete losses)
- Differential cross sections: Moller (e-), Bhabha (e+), generic spin-0, spin-1/2…

Delta-ray production threshold



- FLUKA sets default values, which can be overridden (rule of thumb below):
  - Electrons and positrons: **EMFCUT** card with SDUM=PROD-CUT
    FUDGEM (see below)

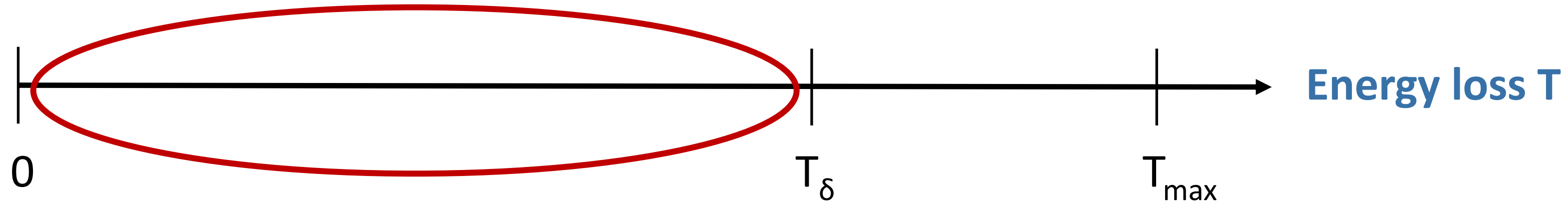
```
EMFCUT   Type: PROD-CUT ▾
      e-e+ Threshold: Kinetic ▾ e-e+ Ekin: 1e-05 γ: 1e-6
Fudgem: 1e-5 Mat: ALUMINUM ▾ to Mat: ALUMINUM ▾ Step:
```

  - Charged hadrons, muons, and ions: **DELTARAY** card

```
DELTARAY   E thres: 1e-5 # Log dp/dx:  Log width dp/dx:
Print: NOPRINT ▾ Mat: ALUMINUM ▾ to Mat: ALUMINUM ▾ Step:
```

- Probability of explicit delta-ray production depends on T_δ, the **delta-ray production threshold**

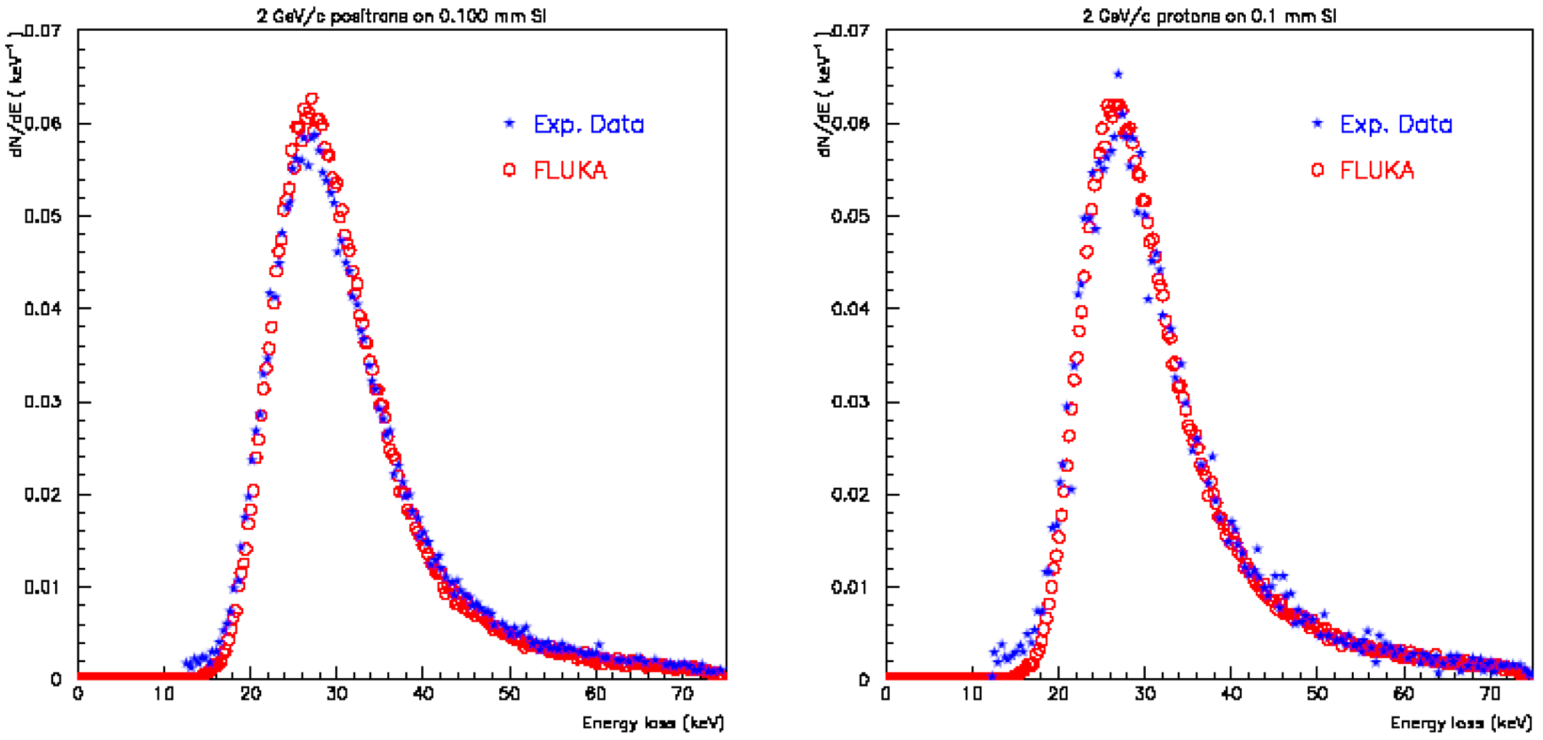
Small energy losses (condensed description)



- Ionization loss cross sections go like $1/T^2$, so
  - Small losses are dominant.
  - Expensive CPU-wise to simulate them all
- We account for the aggregate effect of small losses ($T<T_\delta$) along particle step:
  - Determine average energy loss per unit path length up to T_δ (restricted stopping power)
  - This is a random variable: fluctuations applied on top
- Energy is deposited along the step (not carried away by delta rays)

Energy loss distributions

- Experimental (blue dots) vs simulated (red dots) energy loss distributions for 2 GeV/c positrons (left) and protons (right) traversing 100 um of Si.



- J. Bak et al, NPB 288, 681 (1987)

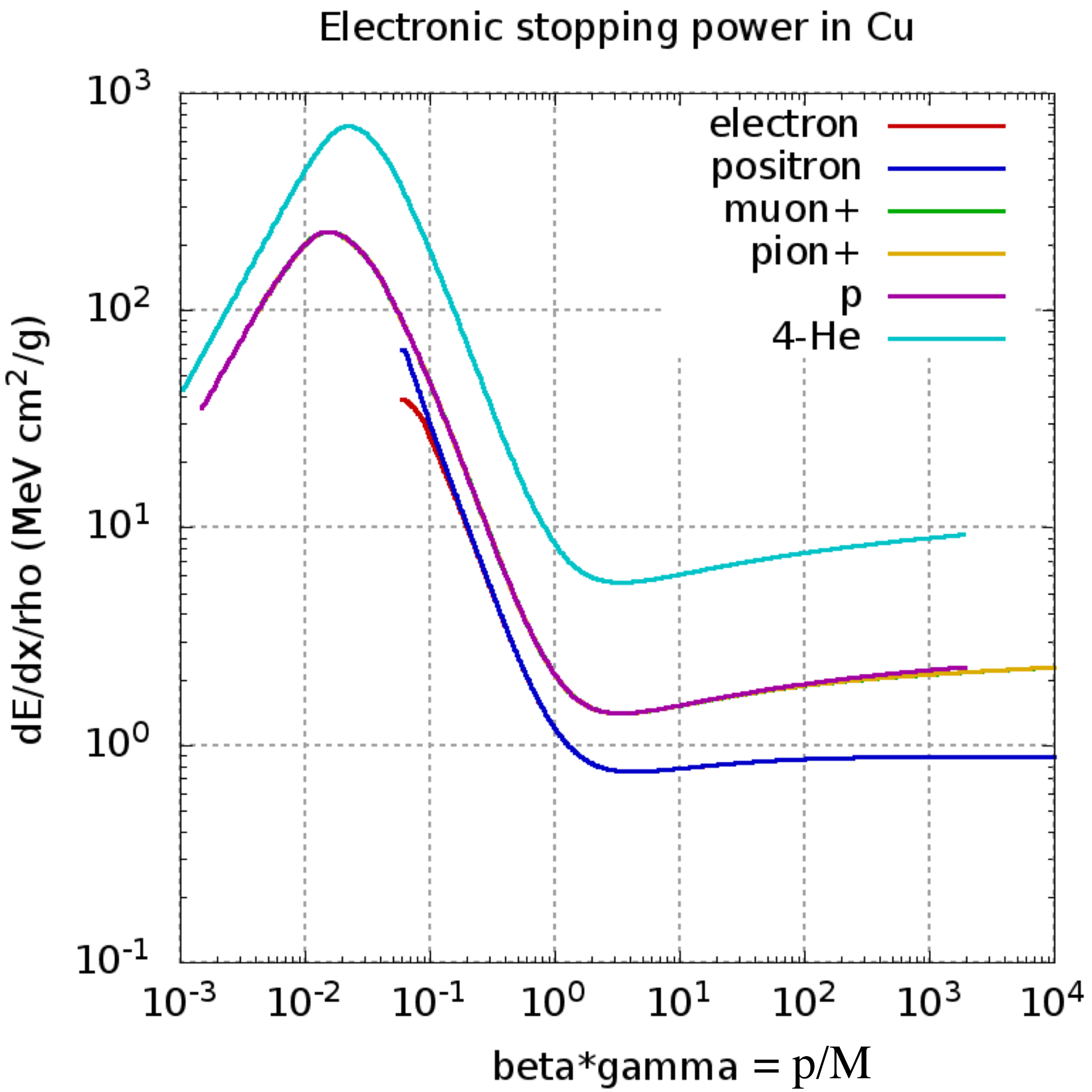
Printing the electronic stopping power

- Electrons and positrons: **EMFFIX** and SDUM=PRINT

- Charged particles: **DELTARAY** and SDUM=PRINT

- If requested, the stopping power is printed in the .out file (requires minimal scripting to extract and plot)

Electronic stopping power overview



Z_{alpha}=2

$Z_{mu,pi,p}$=1

|Z|=1

Radiative stopping power

Electrons

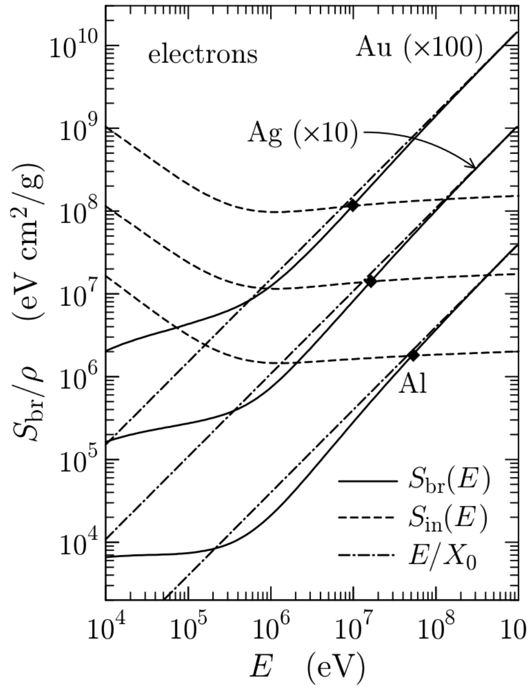
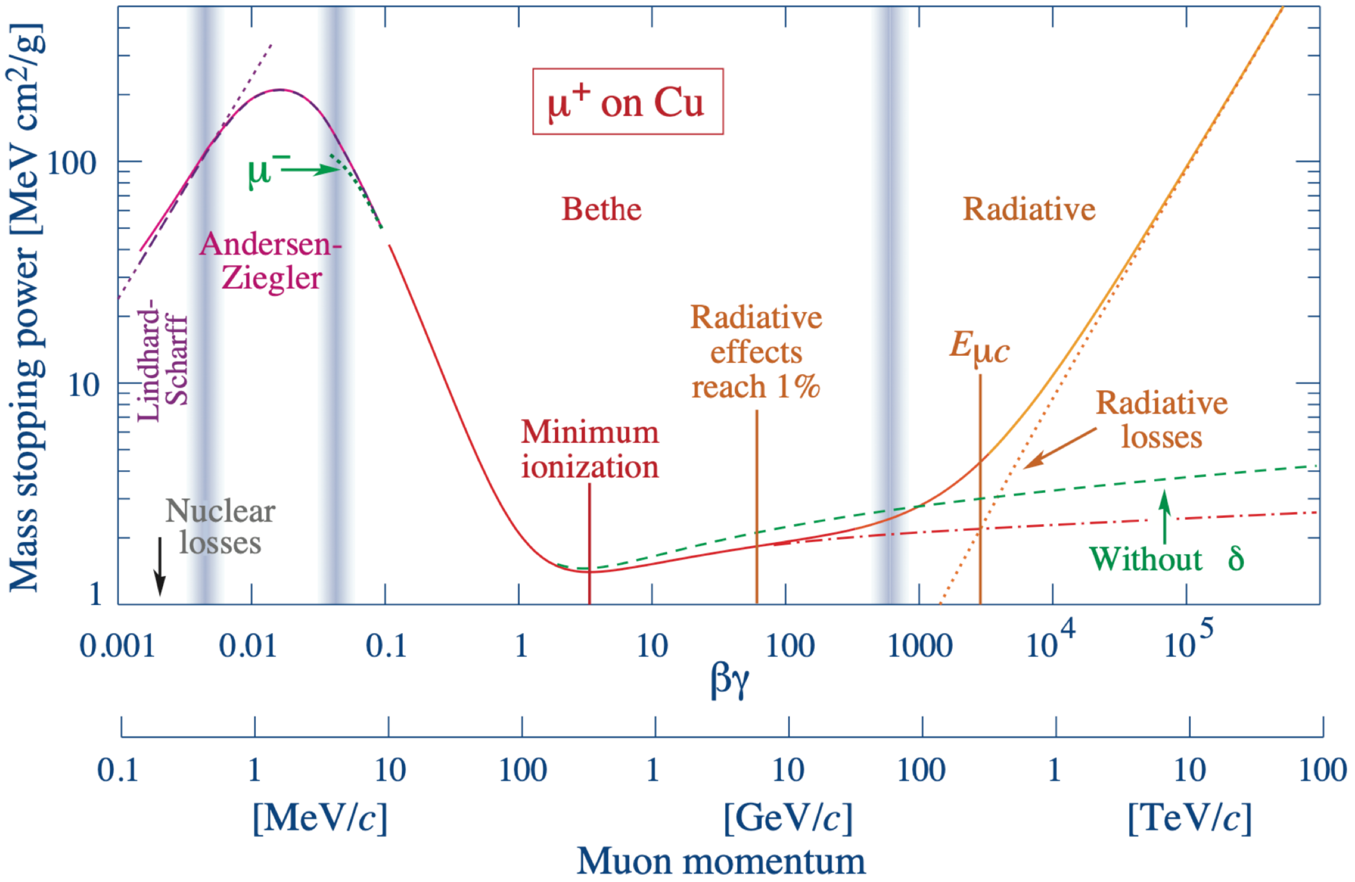


Figure 3.15: Radiative and collision stopping powers for electrons in aluminium, silver (×10) and gold (×100) as functions of the kinetic energy (solid and dashed curves, respectively). Dot-dashed lines represent the high-energy approximation given by Eq. (3.160). Diamonds indicate the critical energy E_{crit} at which the radiative stopping power starts dominating for each material.

Muons in Cu



Depth-dose distribution of ^{238}U in steel

- All charged particles share the **same** approach.

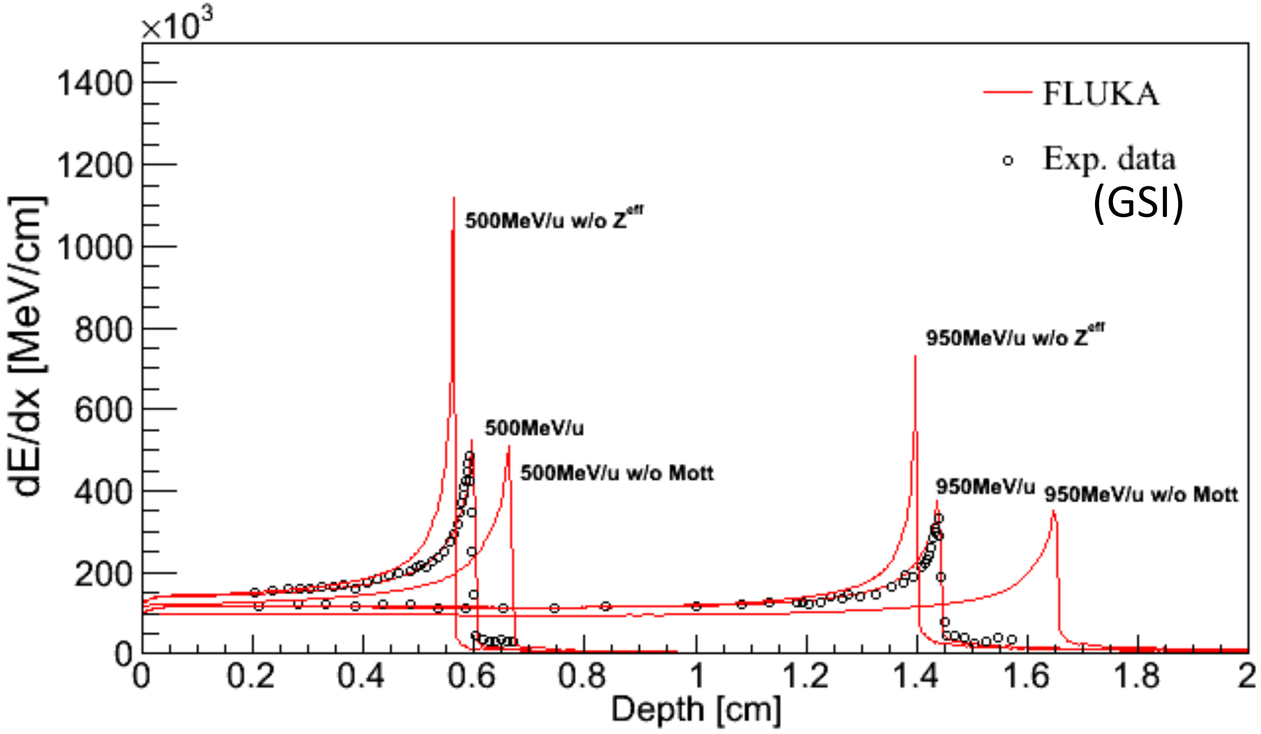
- Heavy ions require the following refinements:

  Effective charge
  (up-to-date parametrizations for Z>1)

  Mott cross section

  Nuclear form factor of projectile ion in delta-ray production

  Direct e-/e+ production



Ref: *U.I. Uggerhøj,*
[Mat. Fys. Medd. Dan. Vid. Selsk., vol. 52, 699-729 (2006)]

Summary

- We have discussed two separate treatments for ionization energy losses in FLUKA: discrete vs continuous
- Discrete losses (above delta production threshold) sampled explicitly
- Continuous losses described effectively along particle step
- Dedicated effort for ions leads to good agreement with experiments

FLUKA card summary

EMFCUT : set delta ray production threshold for electrons and positrons

EMFFIX : print stopping power for electrons and positrons

DELTARAY : set delta ray production threshold for muons and charged hadrons
+ print stopping power for charged hadrons and muons

Multiple Coulomb scattering

The problem

- Charged particles are elastically scattered from (screened) electrostatic potential of atoms
- This type of interactions governs the broadening of charged-particle showers in materials
- Elastic collisions are also frequent
- It is impractical to sample elastic scattering events individually
- Multiple scattering theory: effective scheme to describe effect of many deflections along a particle step

- Formally: after a step length, what does the angular distribution look like?

The Moliere distribution

- In FLUKA we use an algorithm based on the Moliere multiple-scattering theory
- Basic assumptions:
  - Differential cross section in an individual collision: screened Rutherford

$$\frac{d\sigma_{mol}}{d\Omega} = \left[\frac{z^2 Z^2 e^4}{4c^4\beta^2 E^2 \sin^4\frac{1}{2}\theta}\right]\left[\frac{(1-\cos\theta)^2}{(1-\cos\theta+\frac{1}{2}\chi_a^2)^2}\right]$$

  - Solve the transport equation within the small-angle approximation.
  - Analytical manipulations → **minimum applicable step length (energy-dependent)**

- Distribution of angles after step t:

$$F_{Mol}(\theta,t)\mathrm{d}\Omega = 2\pi\chi\mathrm{d}\chi\left[2\,\mathrm{e}^{-\chi^2} + \frac{1}{B}f_1(\chi) + \frac{1}{B^2}f_2(\chi) + \ldots\right]\left[\frac{\sin\theta}{\theta}\right]^{\frac{1}{2}}$$

$$f_n(\chi) = \frac{1}{n!}\int_0^\infty u\,\mathrm{d}u\,J_0(\chi u)\,\mathrm{e}^{-u^2/4}\left(\frac{u^2}{4}\ln\frac{u^2}{4}\right)^n$$

- At every step t, we sample aggregate deflection from F_{Mol}

Model performance in demanding circumstances

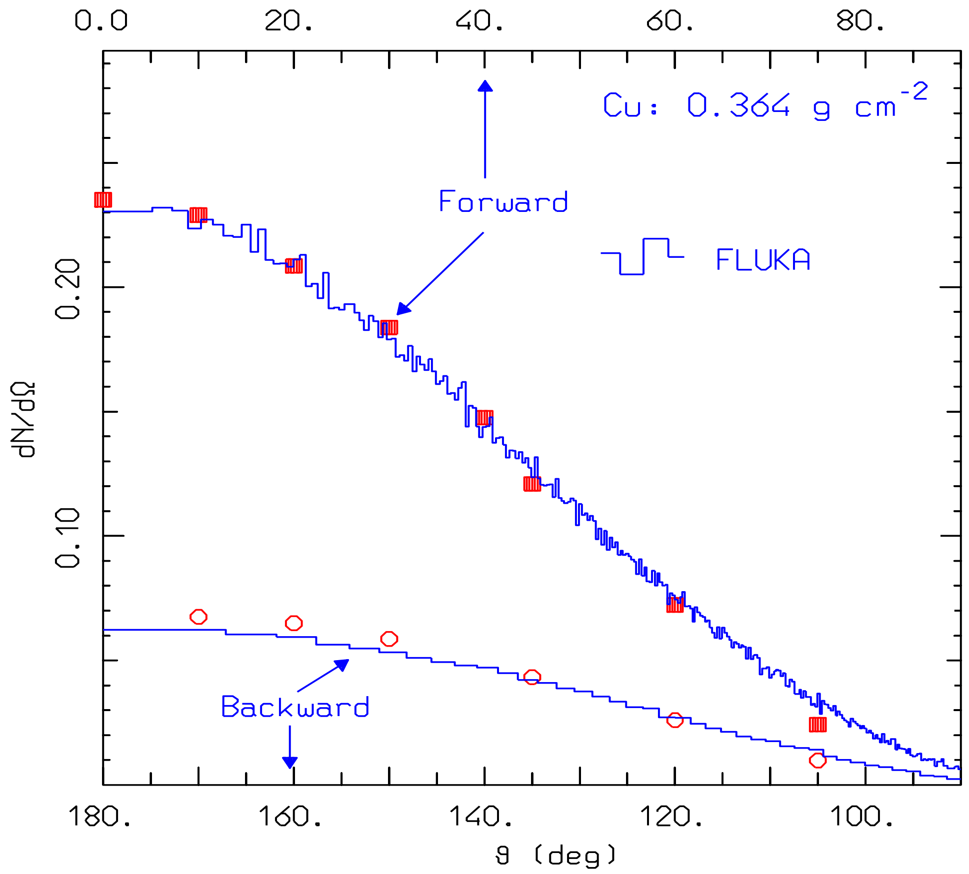
- As a result of the modelling effort, even demanding situations like electron backscattering can be modelled, in most cases without resorting to single scattering (not bad for an algorithm based on the Moliere theory!)

- E.g.: 1.75 MeV electrons on 0.364 g/cm^2 Cu foil

- Transmitted (forward scattered) and backscattered electron angular distributions.

- Dots: experimental data
  Curves: FLUKA

- Same algorithm for charged hadrons and muons (!)



User control of multiple-Coulomb-scattering algorithm

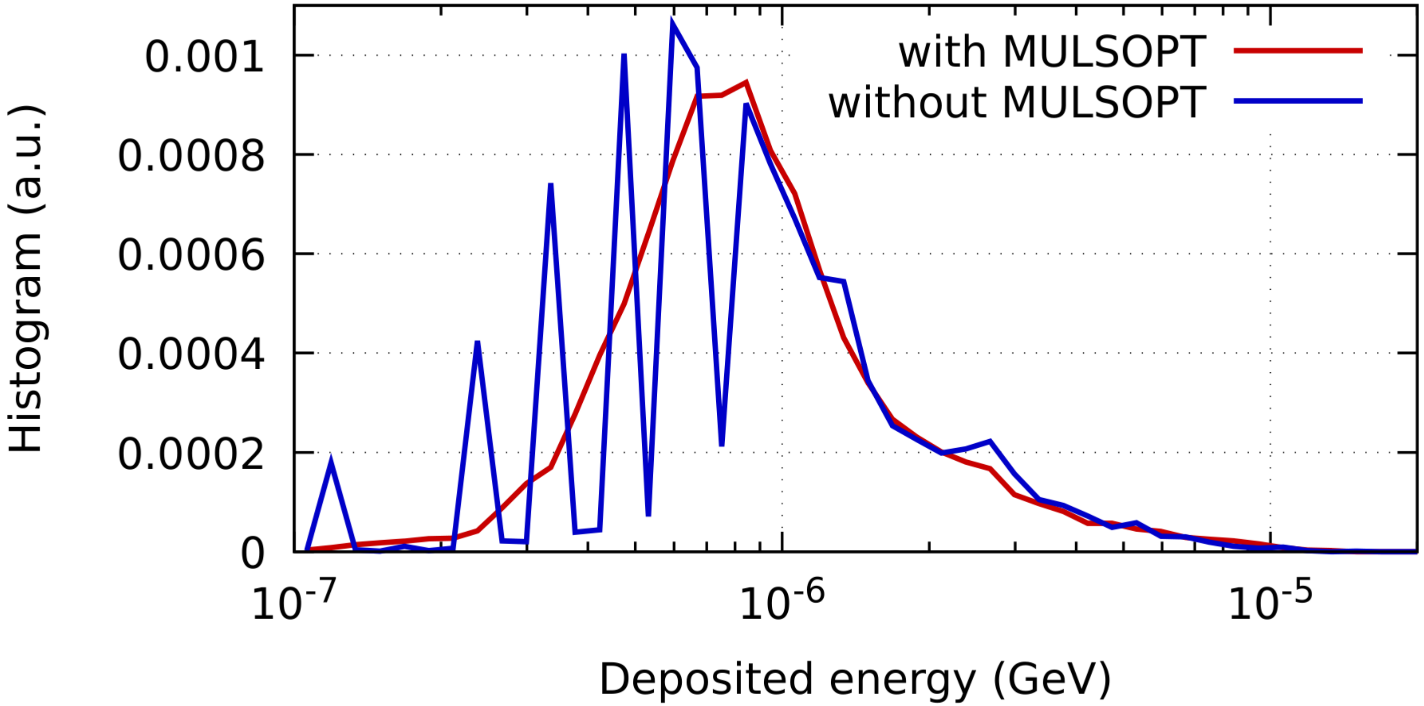
- There are situations where the Moliere theory is not applicable:
  - Transport in residual gas
  - Interactions in thin geometries like wires or slabs (few elastic collisions)
  - Electron spectroscopies at sub-10-keV energies
  - Micro-dosimetry
- One can request to switch single scattering on via the **MULSOPT** card
- The scope of this card is large. We focus on a few aspects only:

MULSOPT Type: GLOBEMF ▾ Min step: Stretching: ▾
Optimal: Single scat: On ▾ E<Moliere: On ▾ # scatterings: 2

  - "Single scat": switch on single scattering at boundaries or for too short steps
  - "E<Moliere": resort to single scattering for energies too low for Moliere theory to apply
  - "# of scatterings": number of single scattering events approaching boundary
- Likewise for charged hadrons and muons, with SDUM=GLOBHAD

Dosimetry in micrometric volumes

- Energy deposition by a 100-MeV p beam in a 1 um^3 Si detector volume immersed in a 10 um^3 Si volume
- Spikes due to non-applicability of Moliere theory. Mitigated switching to single-scattering (**`MULSOPT`**) and restricting maximum step size
- Steps in scored quantities can be further mitigated by shortening step sizes (**`FLUKAFIX`**, **`EMFFIX`**, **`STEPSIZE`**)

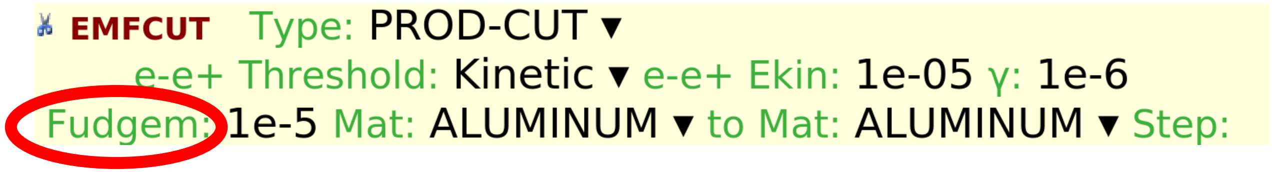


The FUDGEM parameter (avoid a FLUKA stop!)

```
*** Atomic electron contribution to mcs for material XXXXX set to 0, are you sure? ***
*** if so, re-enter it as 1.0e-05 and run again, if not check the manual for the ***
*** EMFCUT card, PROD-CUT, WHAT(3), execution stopped meanwhile ***
```

The FUDGEM parameter (avoid a FLUKA stop!)

- Setting delta-ray production threshold there's a mysterious parameter called FUDGEM:



- Collisions with atomic electrons also contribute to angular deflection
- (Simplified) way to account for them: enhance Z^2 in Rutherford cross-section as $Z^2+Z=Z(Z+1)$
- For low delta-ray production threshold T_δ we could inadvertently incur a double counting in the average projectile deflection due to collisions with atomic electrons:
  - Once when explicitly generating delta-rays
  - Again in Coulomb scattering (via the +1 above, essentially)
- For high T_δ no problem: effect accounted via multiple Coulomb scattering
- The main idea: Z(Z+FUDGEM):
  - For T_δ much larger than ~30 keV, FUDGEM=1
  - For smaller T_δ linearly interpolate such that for T_δ~1 keV, FUDGEM=1e-5 (zero)

FLUKA card summary

EMFCUT : careful with FUDGEM

MULSOPT : request single scattering, fine-tune MCS parameters

More on thresholds
(heads-up for the exercise)

The transport threshold

- In a MC simulation, particles are tracked until they either
  - Leave the simulation geometry
  - Their energy drops below a predefined value, the **transport threshold**

- Every **`DEFAULTS`** defines values for transport and delta-ray-production thresholds

- One should not blindly rely on the default values. They depend on
  - the dimensions of your geometry
  - the granularity of your scoring grids

Setting transport thresholds

- For electrons, positrons and photons:

```
EMFCUT    Type: transport ▾
      e-e+ Threshold: Kinetic ▾ e-e+ Ekin: 1e-05 γ: 1e-6
       Reg: TARGET ▾ to Reg:  ▾ Step:
```

- For charged hadrons, muons, and ions:

```
PART-THR    Type: Energy ▾ E: 1e-05
      Part: PROTON ▾ to Part: PROTON ▾ Step:
```

CAREFUL: if you set from particle to particle, you may inadvertently kill low-energy neutrons (can be transported down to 10^{-14} GeV)

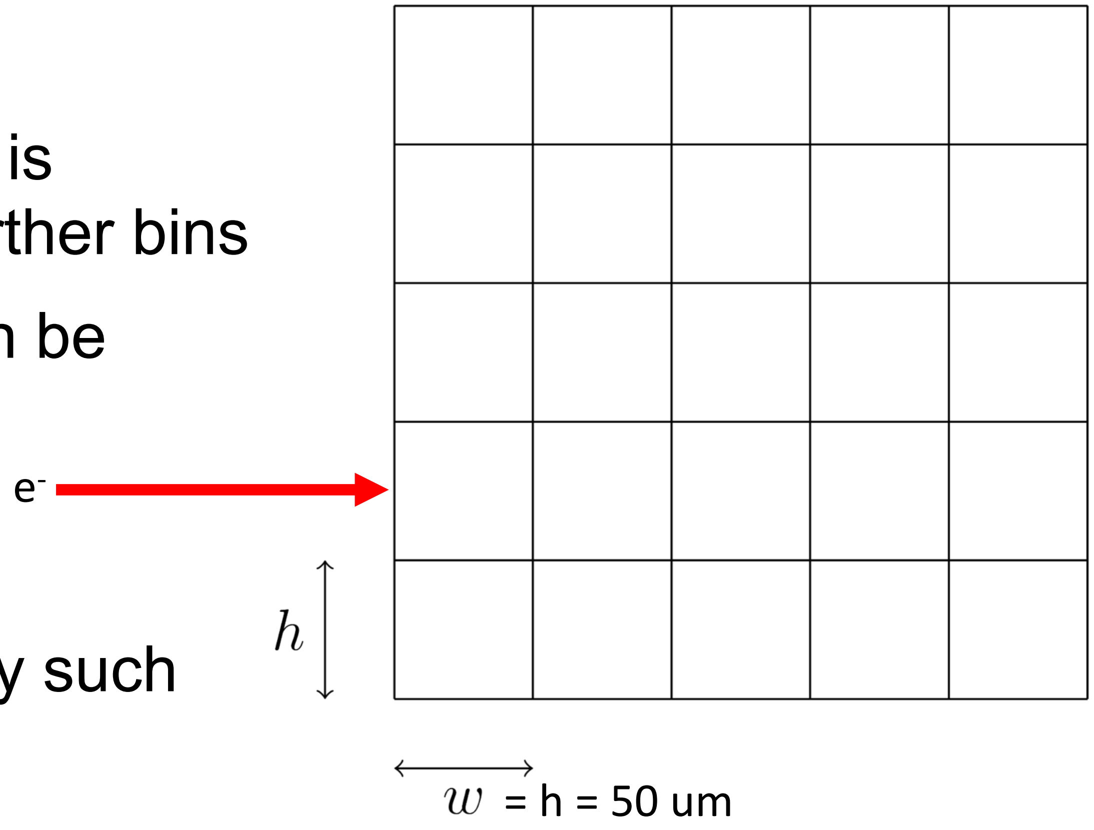
- For heavy ions: scaled from 4-HELIUM with mass ratio

Example: 10-MeV e^- in water

- Suppose a Cartesian USRBIN where each bin has height=width=depth of 50 µm
- Let 10 MeV electrons impinge from the left (on, say, water):
- What are meaningful threshold values?

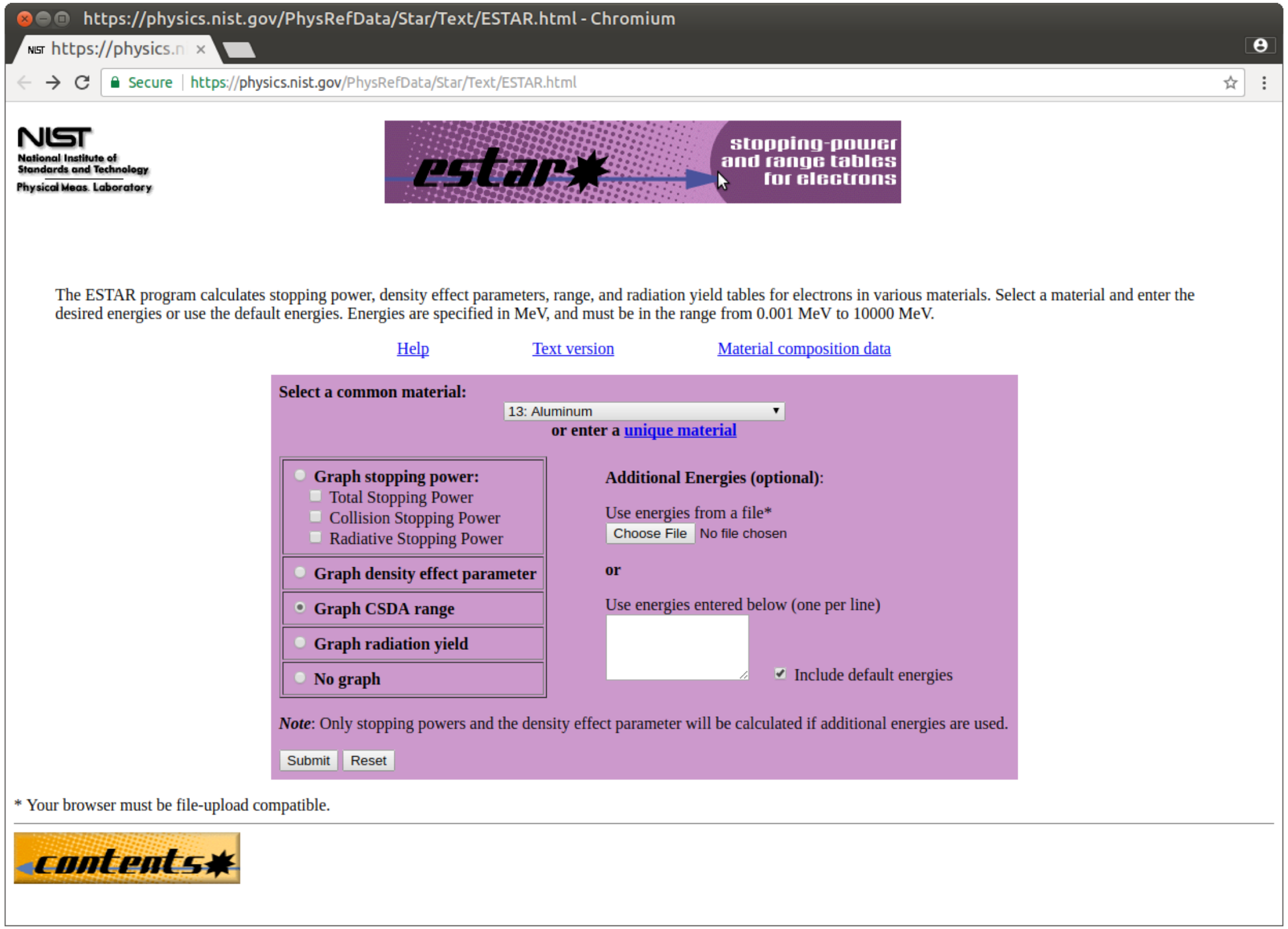
- If we kill electrons at too high energies, this is premature: they could have traveled into farther bins
- If we kill electrons at too low energies: it can be an overkill: anyway the energy would be deposited in the same bin

- Basic idea: put transport threshold at energy such that the range is smaller than the bin length



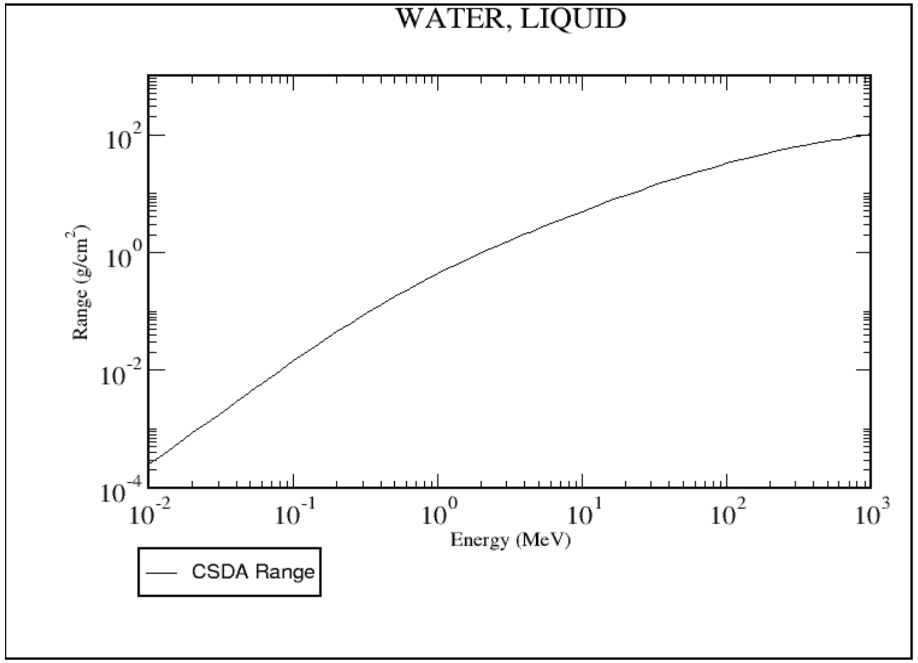
Quick way to examine particle ranges

e.g. https://physics.nist.gov/PhysRefData/Star/Text/ESTAR.html



Electron range in water

- ESTAR/PSTAR give ranges in mass units. Have to divide by the density.
- Note the jump of 2 decades in the ordinates…



- What if we kill electrons below 1 MeV?
  - Range is O(1 mm) = 1000 um
  - The geometry has L = 50 um
  - We would kill them prematurely and get distorted energy deposition maps
- Let's kill electrons below 10 keV:
  - Range is O(10^{-4} cm) = 1 um
  - Depositing them on the spot in a 50 um is fine

- If your geometries/scoring grids are coarser, higher thresholds can be perfectly fine!

A few guidelines

- Threshold values depend on the “granularity” of the scoring grid / geometry.
- Range tables are useful guidelines.

- Warnings:
  - To correctly reproduce electronic equilibrium, neighboring regions should have the same electron energy (not range!) threshold.
  - Photons travel farther than electrons: their thresholds should be lower than for electrons
  - Alas, low thresholds for e-/e+/photons are ruthless CPU-time consumers.

- Delta-ray-production threshold:
  - $T_\delta <$ e- transport threshold: CPU wasted in producing and dumping delta-rays on the spot.
  - $T_\delta >$ e- transport threshold: the latter is increased.

Check e⁻⁺/photon transport thresholds in *.out

```
1 Correspondence of regions and EMF-FLUKA material numbers and names:
       Region          EMF                        FLUKA

          1          0   VACUUM                   1   BLCKHOLE
     Ecut =  0.0000E+00 MeV,    Pcut =  0.0000E+00 MeV,    BIAS = F,   Ray. = F,   S(q,Z) = F,  Pz(q,Z) = F
          2          0   VACUUM                   2   VACUUM
     Ecut =  0.0000E+00 MeV,    Pcut =  0.0000E+00 MeV,    BIAS = F,   Ray. = F,   S(q,Z) = F,  Pz(q,Z) = F
          3          1   WATER                   26   WATER
     Ecut =  6.1100E-01 MeV,    Pcut =  5.0000E-03 MeV,    BIAS = F,   Ray. = T,   S(q,Z) = T,  Pz(q,Z) = T
          4          2   LEAD                    17   LEAD
     Ecut =  6.1100E-01 MeV,    Pcut =  5.0000E-03 MeV,    BIAS = F,   Ray. = T,   S(q,Z) = T,  Pz(q,Z) = T
          5          3   ALUMINUM                10   ALUMINUM
     Ecut =  6.1100E-01 MeV,    Pcut =  5.0000E-03 MeV,    BIAS = F,   Ray. = T,   S(q,Z) = T,  Pz(q,Z) = T
```

- Ecut: electron transport threshold given as total energy (!) in MeV
- Pcut: photon transport threshold in MeV

Other particle transport thresholds in *.out

```
 === Particle transport thresholds:

Global cut-off kinetic energy for particle transport:  1.000E-04 GeV
The cut-off kinetic energy is superseded by individual particle thresholds if set


  Cut-off kinetic energy for 4-HELIUM transport:  1.000E-04 GeV

  Cut-off kinetic energy for 3-HELIUM transport:  1.000E-04 GeV

  Cut-off kinetic energy for TRITON   transport:  1.000E-04 GeV

  Cut-off kinetic energy for DEUTERON transport:  1.000E-04 GeV

  Cut-off kinetic energy for PROTON   transport:  1.000E-04 GeV

  Cut-off kinetic energy for APROTON  transport:  1.000E-04 GeV

  Cut-off kinetic energy for ELECTRON transport defined in the Emfcut card

  Cut-off kinetic energy for POSITRON transport defined in the Emfcut card

  Cut-off kinetic energy for NEUTRIE  transport:  0.000E+00 GeV

  Cut-off kinetic energy for ANEUTRIE transport:  0.000E+00 GeV

  Cut-off kinetic energy for PHOTON   transport defined in the Emfcut card

  Cut-off kinetic energy for NEUTRON  transport:  1.000E-14 GeV
```

Electron and photon production thresholds in the .out file

```
1 Quantities/Biasing associated with each media:



 WATER
      Rho =    1.00000     g/cm**3     Rlc=    36.0830     cm
      Ae =   0.610999      MeV     Ue =    11521.6      MeV
      Ap =   5.000000E-03 MeV     Up =    11521.1      MeV
      dE/dx fluctuations activated for this medium, level  1
      below the threshold for explicit secondary electron production
     (up to  2I discrete levels, up to   2 K-edges)

 LEAD
      Rho =    11.3500     g/cm**3     Rlc=   0.561207     cm
      Ae =   0.610999      MeV     Ue =    11521.6      MeV
      Ap =   5.000000E-03 MeV     Up =    11521.1      MeV
      dE/dx fluctuations activated for this medium, level  1
      below the threshold for explicit secondary electron production
     (up to  2I discrete levels, up to   2 K-edges)

 ALUMINUM
      Rho =    2.69900     g/cm**3     Rlc=    8.89633     cm
      Ae =   0.610999      MeV     Ue =    11521.6      MeV
      Ap =   5.000000E-03 MeV     Up =    11521.1      MeV
      dE/dx fluctuations activated for this medium, level  1
      below the threshold for explicit secondary electron production
     (up to  2I discrete levels, up to   2 K-edges)
```

- Ae: delta-ray production threshold, given as **total energy** (!) in MeV
- Ap: photon production threshold in MeV

FLUKA card summary

EMFCUT : transport thresholds for electrons, positrons, and photons

PART-THR : transport thresholds for hadrons, muons, and ions

Summary

- General overview of EM interactions
- Transport of charged particles in FLUKA (ionization and multiple scattering)
- Introduction to particle thresholds
- How to set them by way of example
- Resolving spikes/steps when scoring quantities in thin geometries

FLUKA

Stopping power of charged particles

- Spin-0 particles:

~ln $\beta^4\gamma^4$
relativistic rise

$$\left(\frac{dE}{dx}\right)_0 = \frac{2\pi n_e r_e^2 m_e c^2 z^2}{\beta^2}\left[\ln\left(\frac{2m_e c^2\beta^2 T_{max}}{I^2(1-\beta^2)}\right) - 2\beta^2 + 2zL_1(\beta) + 2z^2 L_2(\beta) - 2\frac{C}{Z} - \delta + G\right], \qquad T_{t,max} = \frac{2m_t\beta_p^2\gamma_p^2}{1 + 2\left(\frac{m_t}{m_p}\right)\gamma_p + \left(\frac{m_t}{m_p}\right)^2}$$

- z : projectile charge
  n_e : material electron density (~Z/A)
  I : mean excitation energy

- Bethe formula: 1st-order perturbation theory with plane waves, assuming $v_p \gg v_t$:

  - δ: density correction, important at high energies
  - C: is the shell correction, important at low energies
  - L_1: Barkas correction (z^3)
  - L_2: Bloch (z^4) correction
  - G: Mott corrections