

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

Overview of lepton and photon interactions

Transport of charged particles

Particle transport and delta-ray-production thresholds (exercise!)

EM process overview

- Elastic scattering of charged particles on screened electrostatic potential of target atoms (Coulomb scattering):
 - Condensed multiple Coulomb scattering
 - Single 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)
- lons:
 - 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.

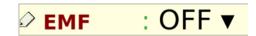


Photon and e± interactions in FLUKA



Photon and e± interactions in FLUKA

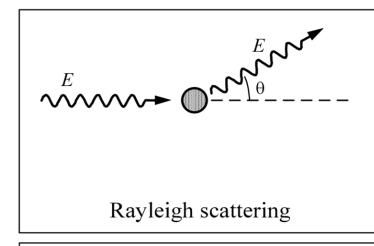
• FLUKA's e± and γ physics package (EMF) is already enabled with most **DEFAULT**s except: EET-TRAN, NEUTRONS, SHIELDING. To deactivate:

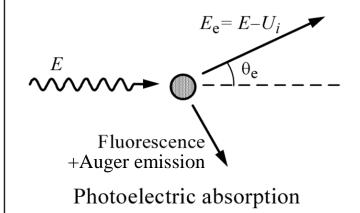


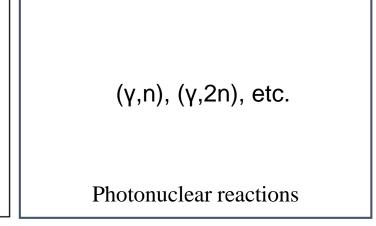
 Note: If EMF is disabled, the energy of electrons/positrons/photons is deposited on the spot!

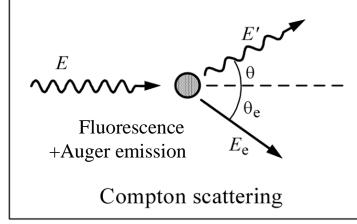
- Energy range: e[±]: 1 keV 1000 TeV, γ: 100 eV 1000 TeV
- Up-to-date γ cross sections from the EPDL database
- Energy conservation is ensured within computer precision

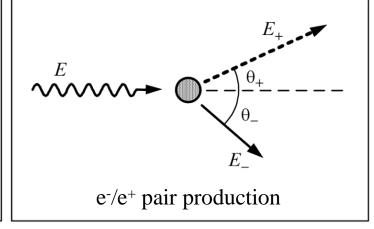
Photon interactions overview

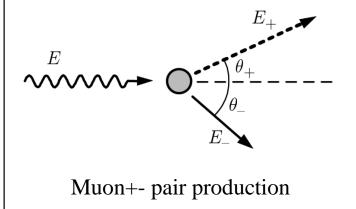










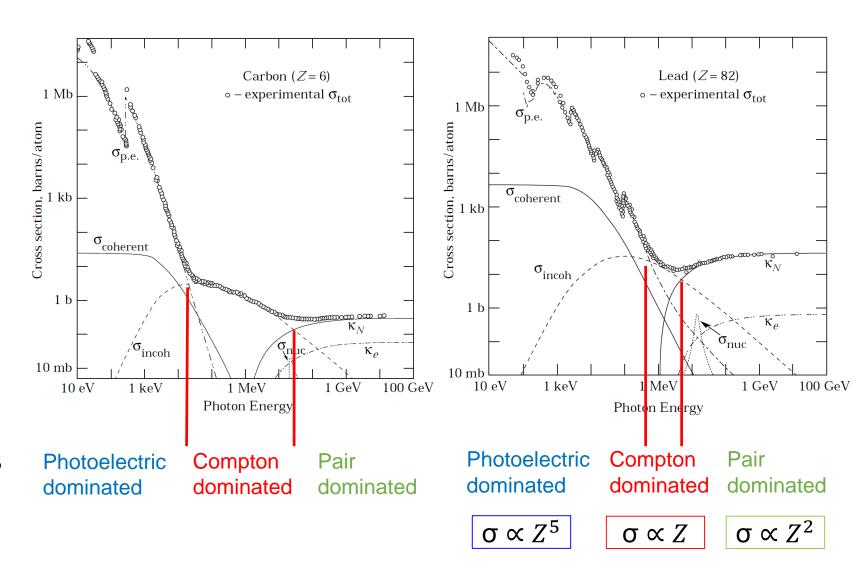


(Figures kindly shared by the PENELOPE authors)



Photon interaction cross sections overview

- At low energies, photoelectric effect dominates
- Clear signature of atomic shell structure
- Compton scattering dominates at intermediate energies
- At 1.022 MeV, e⁻/e⁺
 pair production opens
- Photonuclear reactions are not dominating

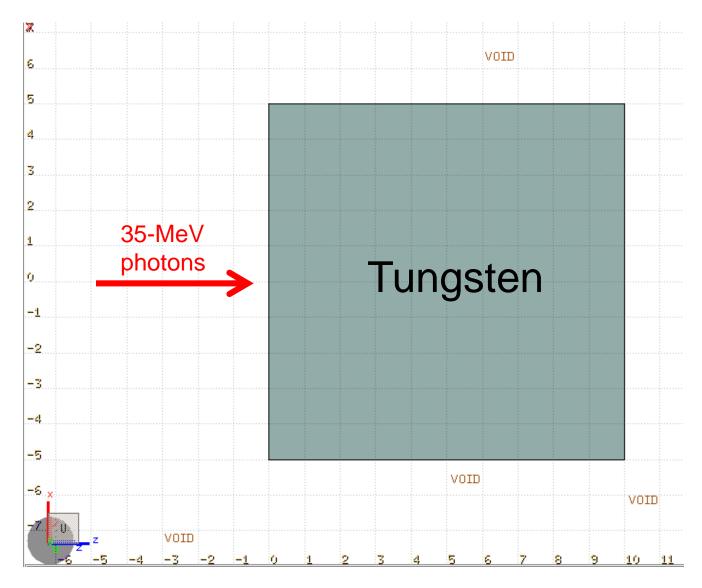




Full coupling between EM and hadronic shower

 Note: we almost never have a pure EM shower, except for low energies

- E.g. 35 MeV photons on W target
 - Start with a purely EM shower
 - Photons may undergo photonuclear reactions
 - E.g. neutrons can be produced (!)
- Let's examine various particle fluences....



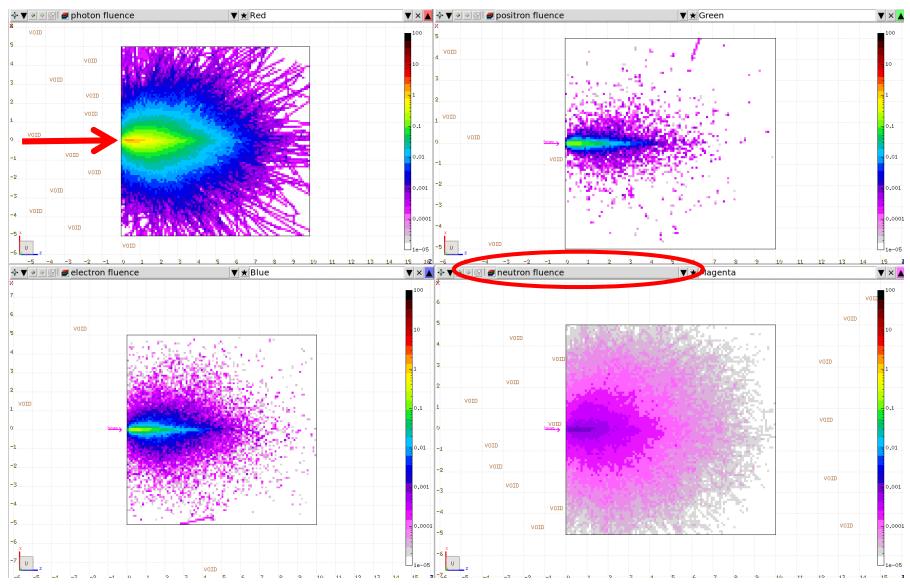


Particle fluences from 35-MeV photons on W

35 MeV photons

All fluences in 1/cm²/primary photon

(See slide 8 for a relevant note on photonuclear reactions)





Note of caution for photonuclear interactions

- Photonuclear interactions are discussed in more detail in the hadronic interactions lecture
- They are **not on by default** (!). You request them via the **PHOTONUC** card:

```
▶ PHOTONUC Type: ▼ All E: On ▼
E>0.7GeV: off ▼ Δ resonance: off ▼ Quasi D: off ▼ Giant Dipole: off ▼ Mat: BLCKHOLE ▼ to Mat: @LASTMAT ▼ Step: 1
```

• They are **suppressed compared to other processes**. In a next lecture, we will introduce biasing techniques, which allow to effectively sample these rare (but important) events. For completeness, one can request to shorten the mean free path for this process (e.g. by a factor 50-100) with the **LAM-BIAS** card:

```
    ∠ LAM-BIAS Type: ▼ × mean life: 0 × λ inelastic: 0.01
    Mat: LEAD ▼ Part: PHOTON ▼ to Part: ▼ Step:
```



e⁻⁺ interaction overview

- Ionization losses (see block on ionization and transport below):
 - Delta-ray production respectively modelled via the Møller and Bhabha cross sections
 - Delta-ray-production threshold

- Bremsstrahlung production
 - Differential cross sections from the Berger and Seltzer (NIST) database
 - Consideration of Landau-Pomeranchuk-Migdal effect *

* reduction of the bremsstrahlung and pair production cross sections at high energies or high densities

- Positron annihilation
 - Both at rest and in flight
 - For annihilation at rest, account for mutual polarization of the two emitted photons.
- Electro-nuclear interactions (treated in the Hadronic physics lecture)



FLUKA card summary (so far)

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

- ...and for photonuclear reactions:
 - **PHOTONUC**: activate photonuclear reactions
 - LAM-BIAS: transport of electrons, positrons, and photons on/off



Ionization and transport



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)

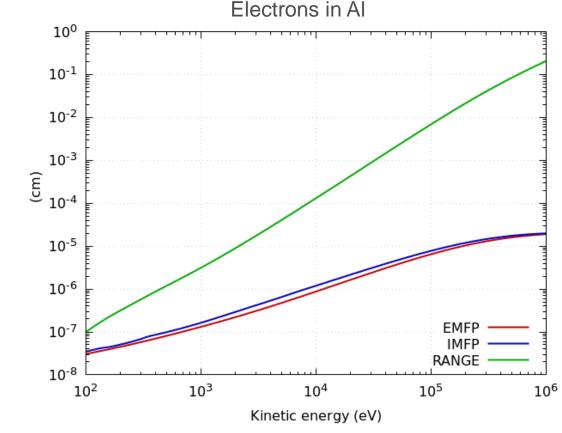
- We will already introduce:
 - Transport threshold
 - Delta-ray-production threshold



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

- Estimated number of ionization losses:
 - N = RANGE / IMFP
 - e.g. for a 1-MeV electron, N~10⁴
- Estimated number of Coulomb losses:
 - N = RANGE / EMFP
 - e.g. for a 1-MeV electron, N~10⁴
- Too many to simulate explicitly!
- A more practical approach is necessary to keep CPU time within acceptable bounds.



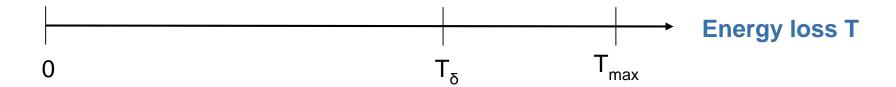
Condensed simulation of ionization losses

- 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)



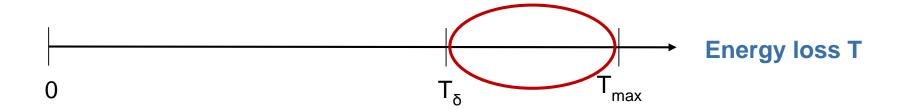
Ionization energy losses in FLUKA

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





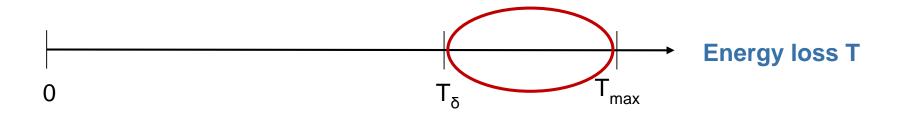
Large ionization energy losses (detailed sampling)



- Large energy loss $T>T_{\delta}$ transferred to a target electron
- Invested in setting in motion this target electron (δ ray)
- δ rays are typically energetic and can transport energy away from their point of origin, so they are explicitly produced and transported in FLUKA

• Differential cross sections: Moller (e⁻), Bhabha (e⁺), generic spin-0, spin-1/2...

Delta-ray production threshold



- T_δ is called the delta-ray production threshold
- FLUKA sets default values, not necessarily appropriate for your problem!

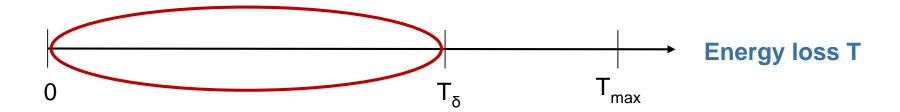
- Cards to override (rule of thumb below):
 - Electrons and positrons: EMFCUT card with SDUM=PROD-CUT

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:
```



Small energy losses (condensed description)

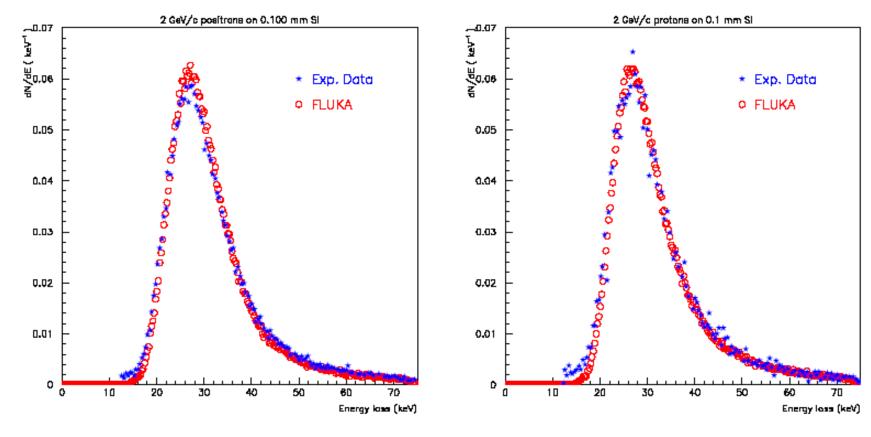


- Ionization loss cross sections go like 1/T², so
 - Small losses are dominant
 - Expensive CPU-wise to simulate them all
- We account for the aggregate effect of small losses $(T < T_{\delta})$ along particle step:
 - Determine average energy loss per unit path length up to T_{δ} (restricted stopping 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

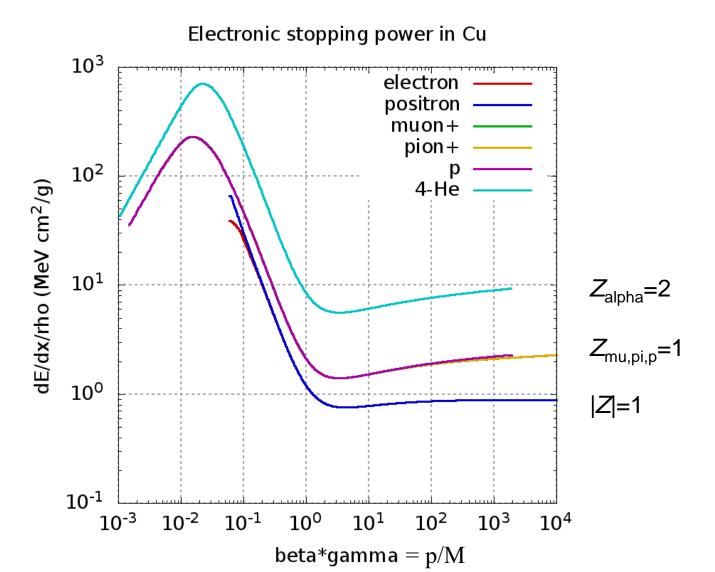
Electrons and positrons: EMFFIX and SDUM=PRINT

Charged particles: DELTARAY and SDUM=PRINT

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

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

Electronic stopping power overview



A bit more detail in the extra slides



Radiative stopping power (dominant above E_{crit})

Electrons

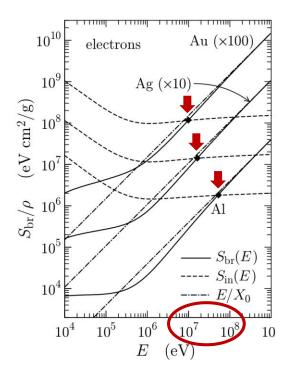
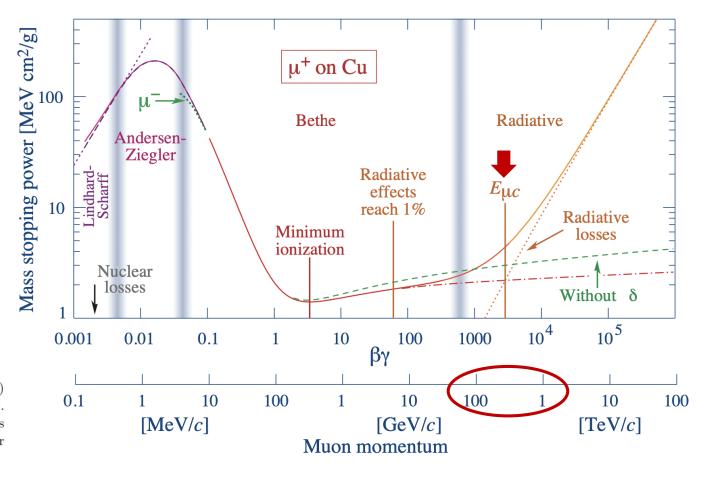


Figure 3.15: Radiative and collision stopping powers for electrons in aluminium, silver ($\times 10$) and gold ($\times 100$) as functions of the kinetic energy (solid and dashed curves, respectively). Dot-dashed lines represent the high-energy approximation given by Eq. (3.160). Diamonds indicate the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

Muons in Cu



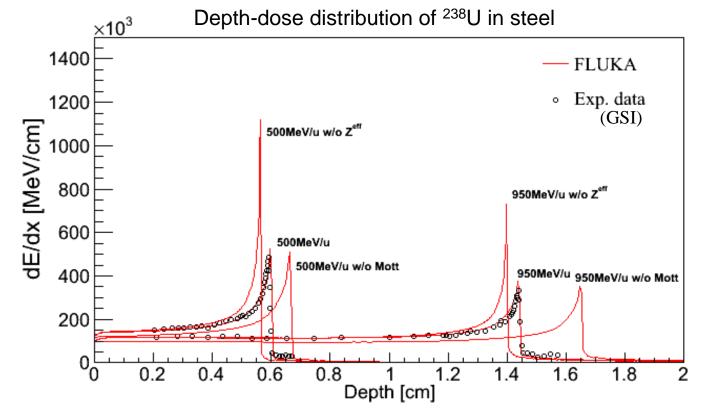
[PENELOPE manual]

[PDG]



Heavy ions

- 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 (so far)

We have discussed two separate treatments for ionization energy losses in FLUKA:
 large energy losses vs small energy losses

- Large losses (above delta ray production threshold) sampled explicitly
- Effect of many small losses is described effectively along particle step
- Dedicated effort for ions leads to good agreement with experiments

FLUKA card summary (so far)

• 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



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 **DEFAULT** 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:

For charged hadrons, muons, and ions:

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

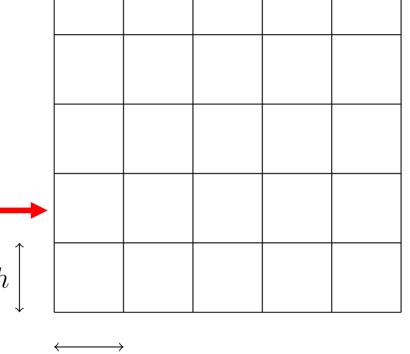
N.B.: if you set "from particle to particle", you may inadvertently kill low-energy neutrons (they can be transported down to 10⁻¹⁴ GeV); add a second **PART-THR** card resetting the neutron transport threshold

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



Example: 10-MeV e- in water

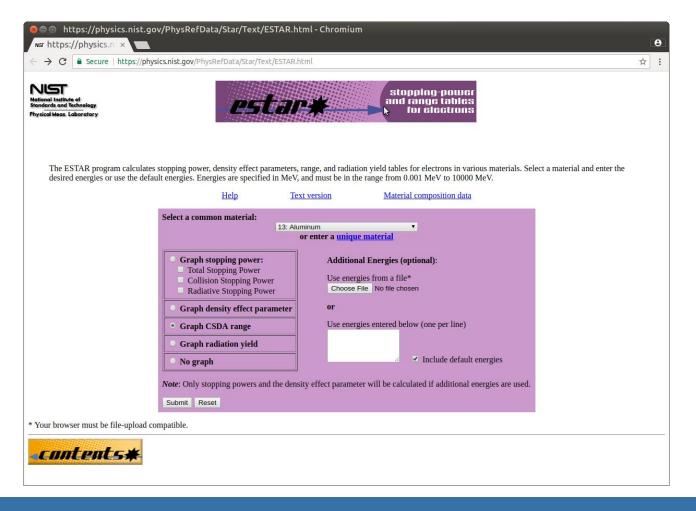
- Let 10 MeV electrons impinge from the left (on, say, water):
- Suppose a Cartesian USRBIN where each bin has height=width=depth of 50 μm
- What are meaningful threshold values?
 - If we kill electrons at too high energies, this is premature: they could have traveled into farther bins
 - If we kill electrons at too low energies: it can be an overkill; the energy would anyway be deposited in the same bin
- Basic idea: put transport threshold at energy such that the range is smaller than the bin length



$$\overrightarrow{w}$$
 = h = 50 um

Quick way to examine particle ranges

Electrons. https://physics.nist.gov/PhysRefData/Star/Text/ESTAR.html
https://physics.nist.gov/PhysRefData/Star/Text/PSTAR.html

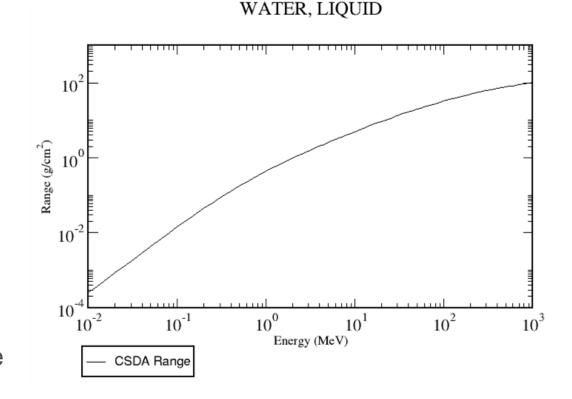




Electron range in water

Consider our example scoring with dimensions of 50 um.

- What if we kill electrons below 1 MeV?
 - Range is O(1 mm) = 1000 μm
 - The geometry has L = 50 μm
 - We would kill them prematurely and get distorted energy deposition maps
- Let's kill electrons below 10 keV:
 - Range is $O(10^{-4} \text{ cm}) = 1 \mu \text{m}$
 - Depositing them on the spot in a 50 µm layer 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, neighbouring 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 for electron projectiles:
 - T_{δ} < e⁻ transport threshold: CPU wasted in producing and dumping delta-rays on the spot.
 - T_{δ} > e⁻ transport threshold: the latter is increased



Check e⁻⁺/photon transport thresholds in the .out file

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

Region EMF FLUKA

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

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



Other particle transport thresholds in the .out file

=== 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
                         q/cm**3
                                     Rlc=
                                              36.0830
                                                         CM
           0.610999
                                       11521.6
                                                    MeV
           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
                         g/cm**3
                                     Rlc= 0.561207
     Rho =
             11.3500
                                                         cm
           0.610999
                                       11521.6
                                                    MeV
                               Up =
                                       11521.1
           5.000000E-03 MeV
                                                   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
                         q/cm**3
     Rho =
             2.69900
                                      Rlc=
                                             8.89633
                                                         CM
           0.610999
                                       11521.6
                                                    MeV
         5.000000E-03 MeV
                                       11521.1
                               Up =
                                                   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 (so far)

• **EMFCUT**: transport thresholds for electrons, positrons, and photons

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



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 given step length, what does the angular distribution look like?



The Molière distribution

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

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

- Solve the transport equation within the small-angle approximation.
- Analytical manipulations → minimum applicable step length (energy-dependent)
- Distribution of angles after step t: $F_{Mol}(\theta,t)\mathrm{d}\Omega = 2\pi\chi\mathrm{d}\chi \bigg[2\,\mathrm{e}^{-\chi^2} + \frac{1}{B}\,f_1(\chi) + \frac{1}{B^2}\,f_2(\chi) + \ldots\bigg]\bigg[\frac{\sin\theta}{\theta}\bigg]^{\frac{-2}{2}}$ $f_n(\chi) = \frac{1}{n!}\int_0^\infty u\,\mathrm{d}u\,J_0(\chi u)\mathrm{e}^{-\mathrm{u}^2/4}\bigg(\frac{u^2}{4}\ln\frac{\mathrm{u}^2}{4}\bigg)^n$
- At every step t, we sample aggregate deflection from F_{Mol}

User control of multiple-Coulomb-scattering algorithm

- There are situations where the Molière 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:

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

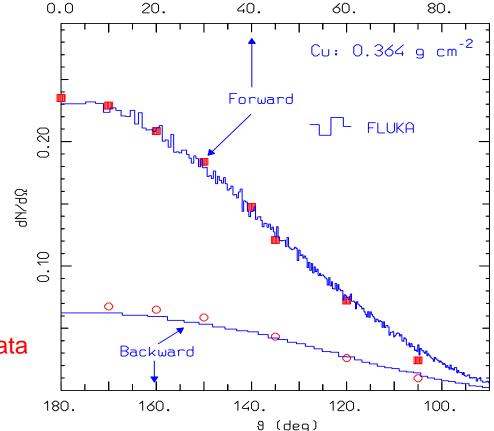


Model performance in demanding circumstances

 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 Molière theory!)

• E.g.: 1.75 MeV electrons on a 0.364 g/cm² Cu foil

 Transmitted (forward scattered) and backscattered electron angular distributions.



Dots: experimental data

Curves: FLUKA



The FUDGEM parameter (avoid a FLUKA stop!)

When setting the delta-ray-production threshold...

• ...if you forget to set the Fudgem field the code will stop with:

```
*** 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 Z² in Rutherford cross-section as Z²+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 +Z above)
- 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 (so far)

EMFCUT: careful with FUDGEM

• MULSOPT: request single scattering, fine-tune MCS parameters



Summary

- General overview of EM interactions
- Transport of charged particles in FLUKA (ionization and multiple scattering)
- Introduction to thresholds
- How to set them by way of example

Beyond: step size control (see additional slide)

- And now in the exercise you will discover the effect that thresholds have on your simulation, in terms of:
 - Accuracy
 - CPU time

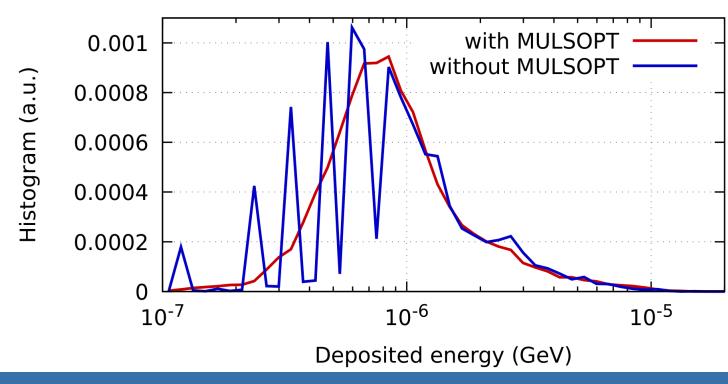




Dosimetry in micrometric volumes

- Energy deposition by a 100-MeV p beam in a 1 μm³ Si detector volume immersed in a 10 μm³ Si volume
- Spikes due to non-applicability of Molière 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)





Stopping power of charged particles

• Spin-0 particles:
$$\begin{array}{c} \sim \ln\!\beta^4\!\gamma^4 \\ \text{relativistic rise} \\ \left(\frac{dE}{dx}\right)_0 = \frac{2\pi\,n_e r_e^2 m_e c^2 z^2}{\beta^2} \left[\ln\!\left(\frac{2m_e c^2 \beta^2 T_{\text{max}}}{I^2 (1-\beta^2)}\right) - 2\beta^2 + 2z L_1(\beta) + 2z^2 L_2(\beta) - 2\frac{C}{Z} - \delta + G \right], \qquad T_{t,max} = \frac{2m_t \beta_p^2 \gamma_p^2}{1 + 2\left(\frac{m_t}{m_p}\right) \gamma_p + \left(\frac{m_t}{m_p}\right)^2} \right] \end{aligned}$$

- z : projectile charge
 - n_e : material electron density (~Z/A)
 - I : mean excitation energy
- Bethe formula: 1^{st} -order perturbation theory with plane waves, assuming $v_p >> v_t$:
 - δ : density correction, important at high energies
 - C: is the shell correction, important at low energies
 - L₁: Barkas correction (Z³)
 - L_2 : Bloch (\mathbb{Z}^4) correction
 - G: Mott corrections