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!)

Outline

- **Coulomb scattering**

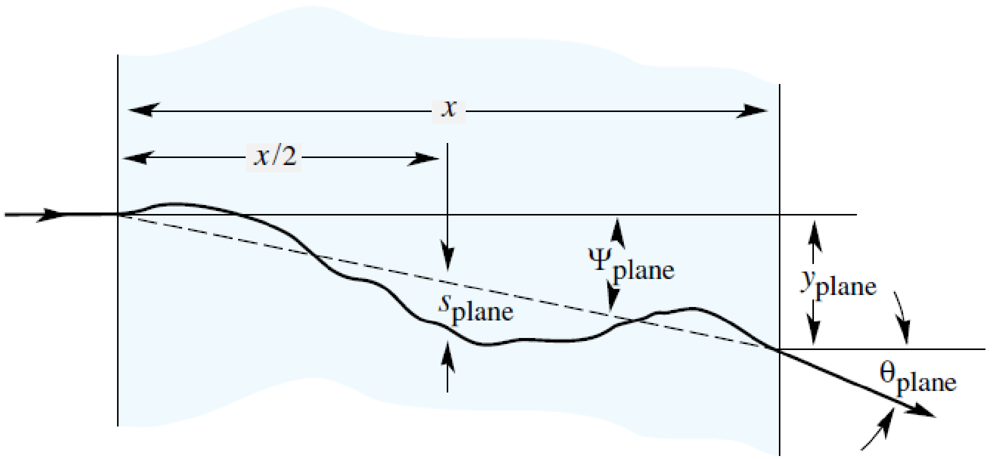
  Elastic scattering of charged particles on screened electrostatic potential of target atoms

  - Condensed multiple Coulomb scattering
  - Single scattering
- **Stopping power for ionizing particles**
  - Continuous energy loss along a particle step: stopping power (dE/dx) description + fluctuations
  - Discrete energy losses (delta ray production)
- **Photon and electron interactions in matter**
  - Radiation length
  - **$e^{\pm}$** : Radiative losses (Bremsstrahlung)
  - **γ** : photo-electric, Compton, pair production
  - **γ** : a note on photonuclear
- **Ions**
  - Corrections in the stopping power: effective charge, Mott correction, etc.
  - Additional EM processes: direct e-/e+ pair production, electromagnetic dissociation

Coulomb scattering

The problem

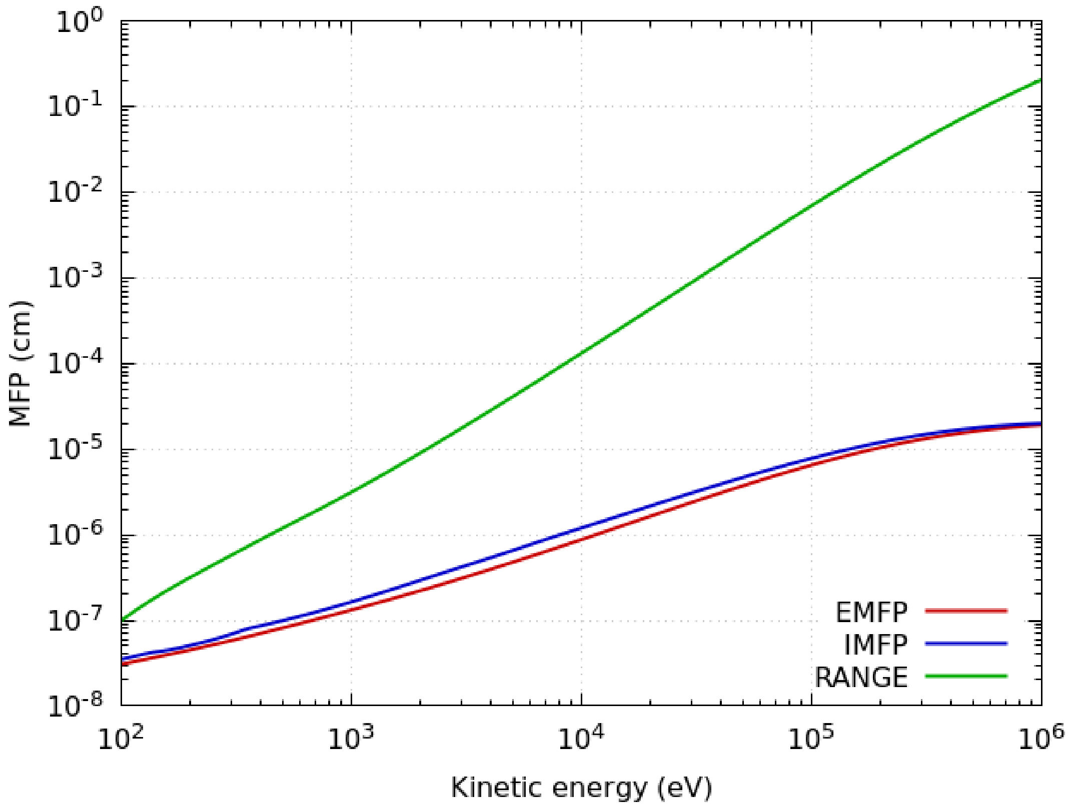
- Charged particles are elastically scattered from (screened) electrostatic potential of atoms
- Elastic collisions are very frequent



How frequent ??

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

Electrons in Al

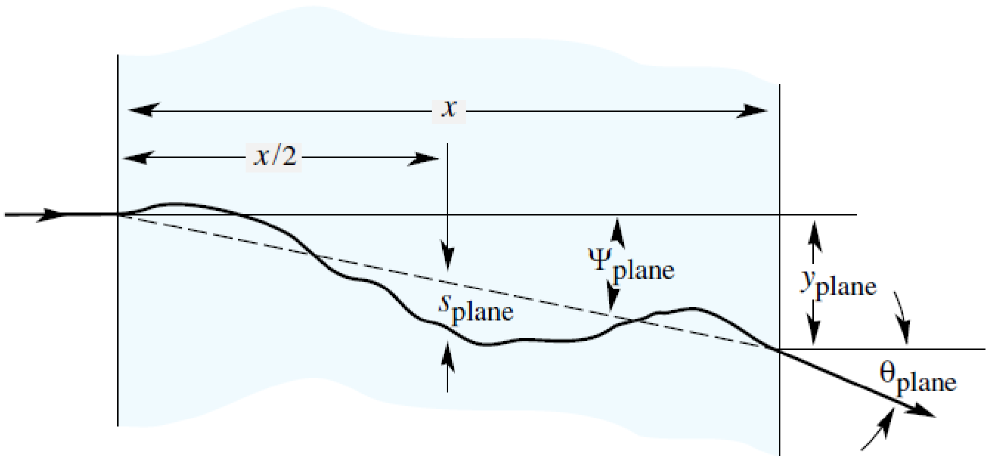


- Estimate number of ionization losses:
  - N=RANGE/IMFP
  - e.g. for a 1-MeV electron, **N~10^4**
- Estimate number of Coulomb losses:
  - N=RANGE/EMFP
  - e.g. for a 1-MeV electron, **N~10^4**
- **Too many to simulate explicitly!**
- A more practical approach is necessary to keep CPU time within acceptable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

The problem

- Charged particles are elastically scattered from (screened) electrostatic potential of atoms
- Elastic collisions are very frequent

  → Impractical to sample individually



- **Multiple** scattering theory: effective scheme to describe effect of many deflections along a particle step

After a given 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

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

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

- Distribution of angles after step t:

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

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

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

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

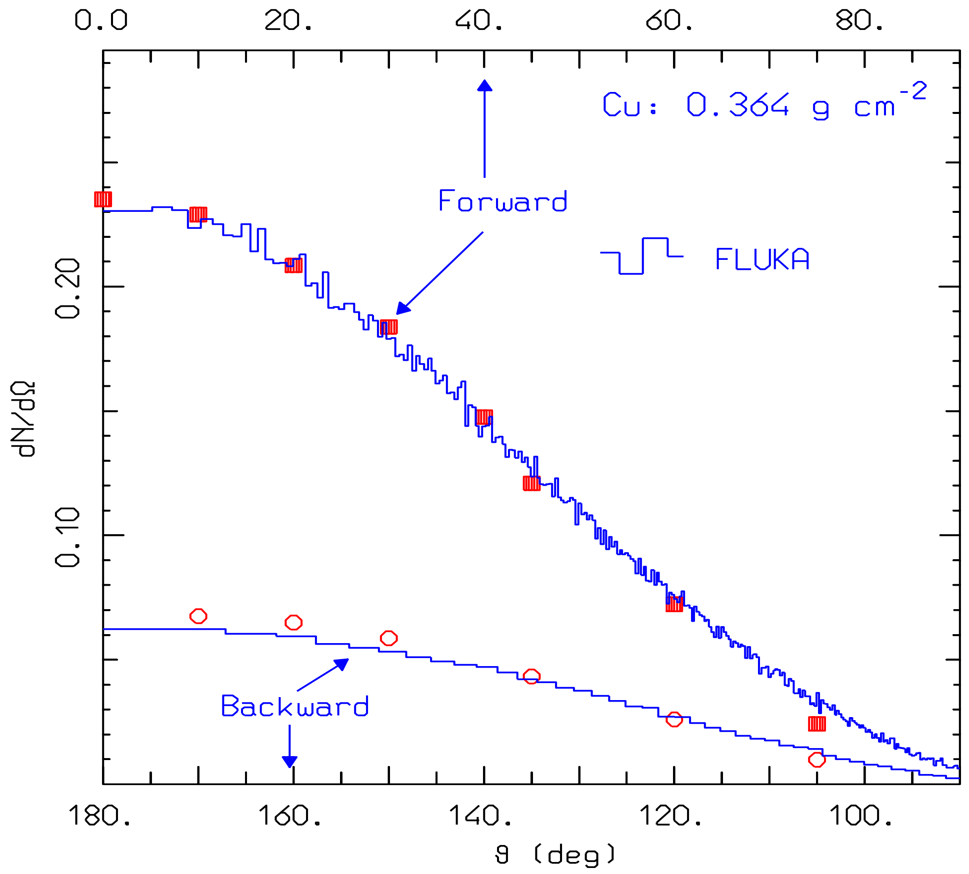
Model performance in demanding circumstances

- 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



Electronic energy loss of heavy charged particles

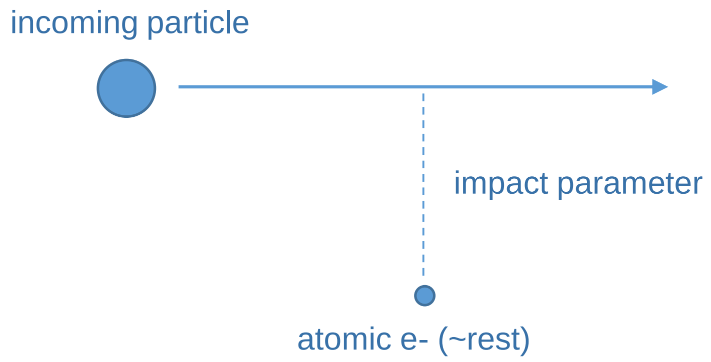
The problem

- Fast charged particles interact with matter electrons, and lose part of their energy
  - Ionization
  - Excitation

  } of atoms along their passage
- In most cases, the energy transfer is small !
- Very large number of such interactions taking place

→ Impractical to sample individually (again...)

(see slide 5)

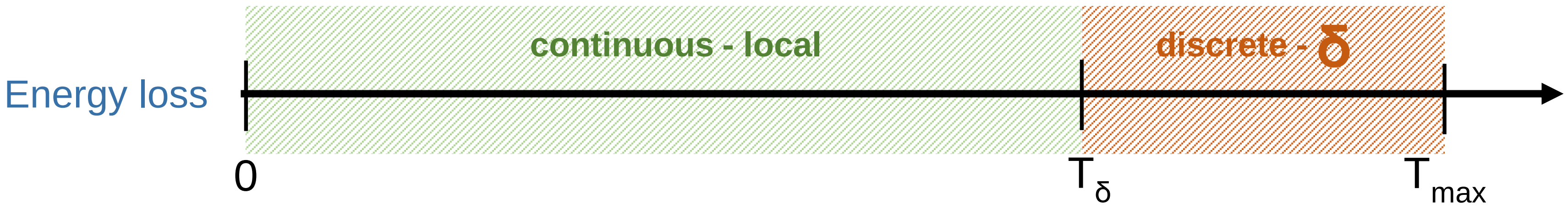


After a given step length, what does the energy distribution look like?

...and what of the energy lost ?

Ionization energy losses

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



- Ionization loss cross sections $\propto 1/T^2$
  → Small losses are dominant
  Expensive CPU-wise to simulate them all

- Need for aggregation along particle step:
  - Determine average energy loss per unit path length up to T_δ (restricted stopping power)
  - Random fluctuations applied on top

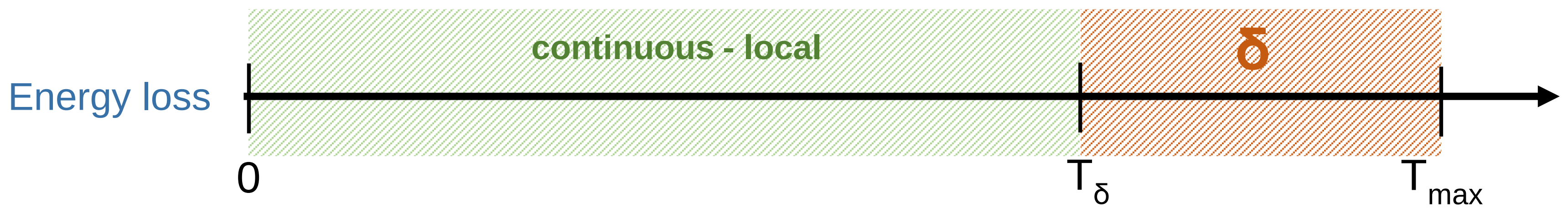
Energy is deposited **locally along the step**

- Transferred energy sets target electron in motion
  → δ ray

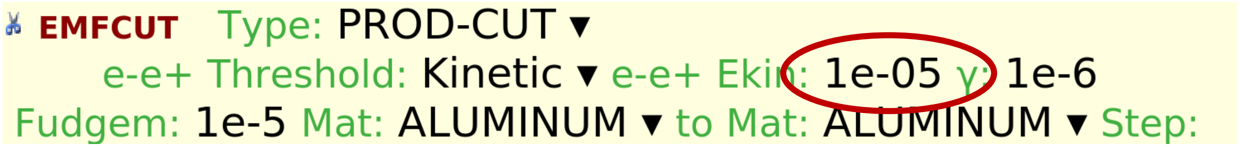
- δ rays
  - are energetic
  - can transport energy away from origin
  → are explicitly produced/transported in FLUKA

- Cross sections depends on projectile
  - Moller (e-)
  - Bhabha (e+)
  - generic spin-0, spin-1/2…

Delta-ray production threshold



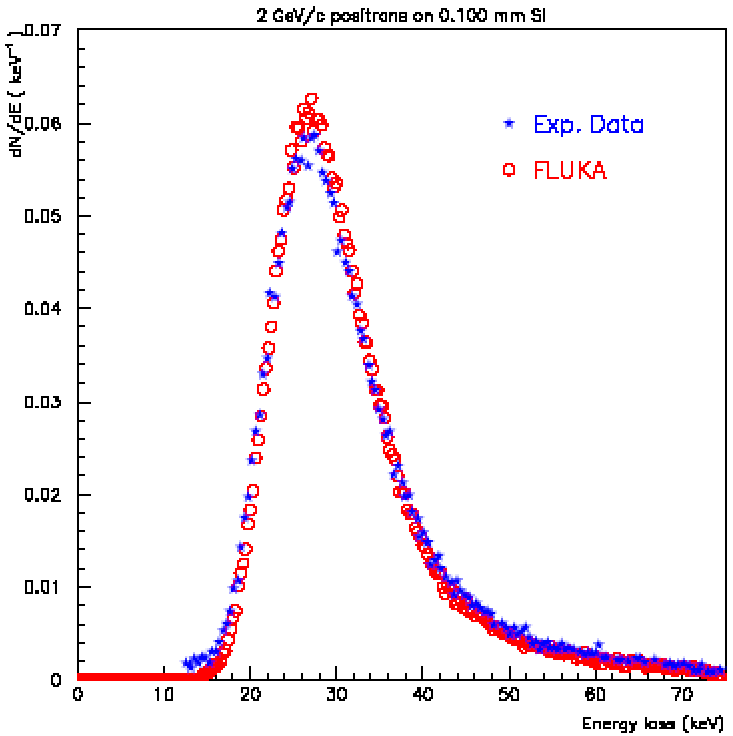
- **T_δ = delta-ray production threshold**
- FLUKA sets default values, not necessarily appropriate for your problem!
- Cards to override (rule of thumb below):
  - Electrons and positrons: **EMFCUT** card with SDUM=PROD-CUT

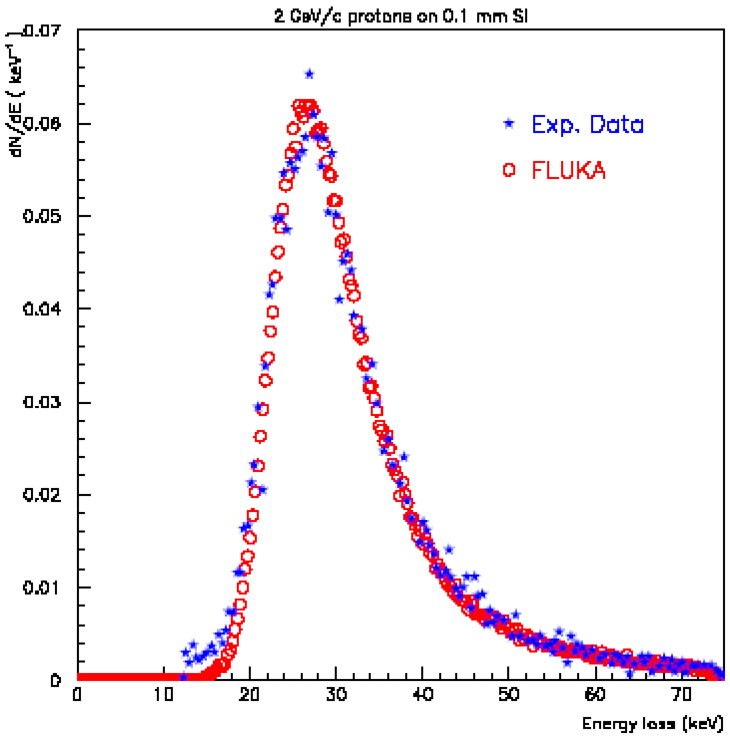


  - Charged hadrons, muons, and ions: **DELTARAY** card

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.





- Skewed Landau-Vavilov distribution (+ corrections depending on projectile)
- J. Bak et al, NPB 288, 681 (1987)

Printing the electronic stopping power

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

```
EMFFIX   Mat1: ALUMINUM ▾ Max Frac.1:  Print: PRINT ▾
         Mat2:  ▾ Max Frac.2:
         Mat3:  ▾ Max Frac.3:
```

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

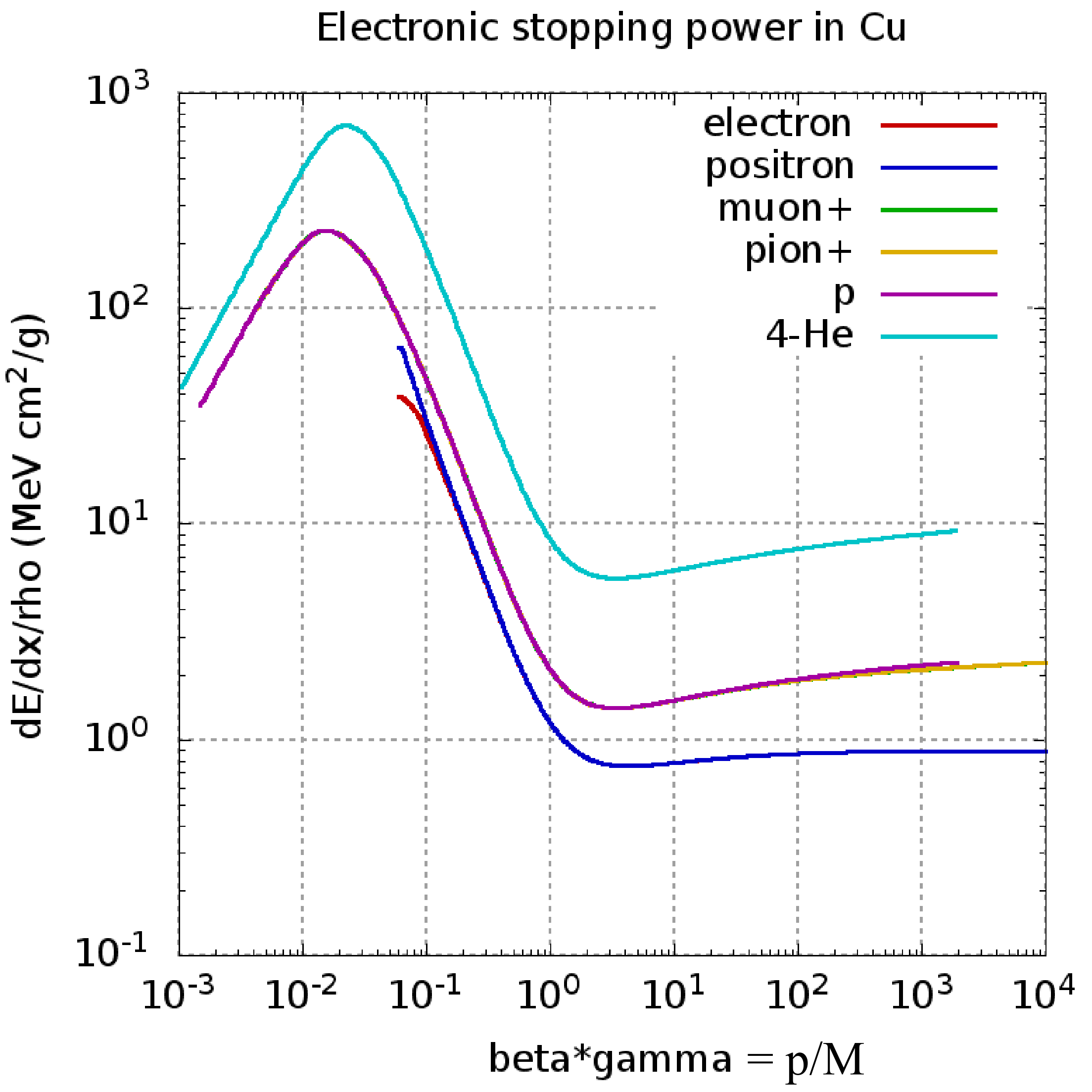
```
DELTARAY   E thres: 1e-5 # Log dp/dx:  Log width dp/dx:
Print: PRINT ▾ Mat: ALUMINUM ▾ to Mat: ALUMINUM ▾ Step:
```

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

Electronic energy loss overview

Example of printing from FLUKA

Check easily that all energy loss curves are consistent with each other (dependence on Z)



Z_{alpha}=2

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

|Z|=1

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

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

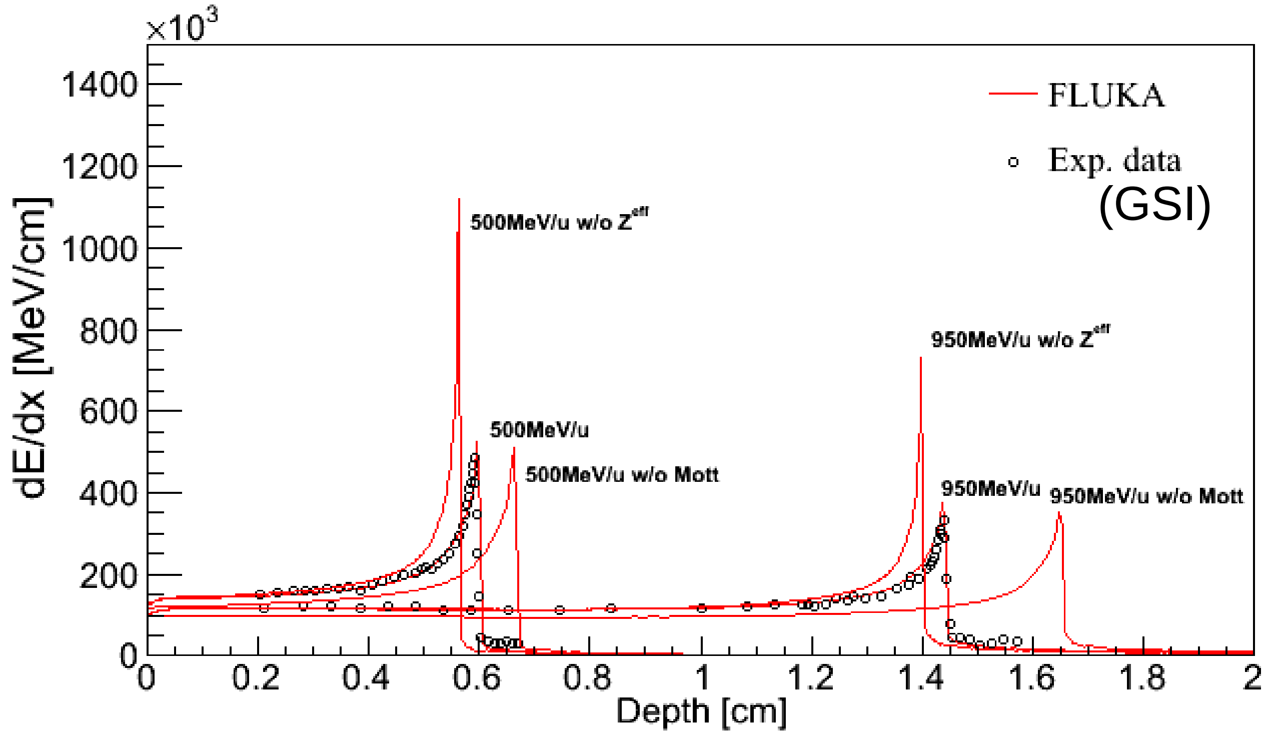
- Heavy ions require the following refinements:

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 : electronic energy loss for heavy particles

- 2 treatments for ionization energy losses in FLUKA
  - large energy losses : δ ray emission (transported explicitly)
  - small energy losses : aggregated and described along particle step
  - Importance of the δ-ray threshold !

- Reality (as always) more complex:
  - Low energy : non-relativistic Ziegler, LSS,...
  - High energy : radiative losses become predominant
- Dedicated effort for ions leads to good agreement with experiments

FLUKA card summary

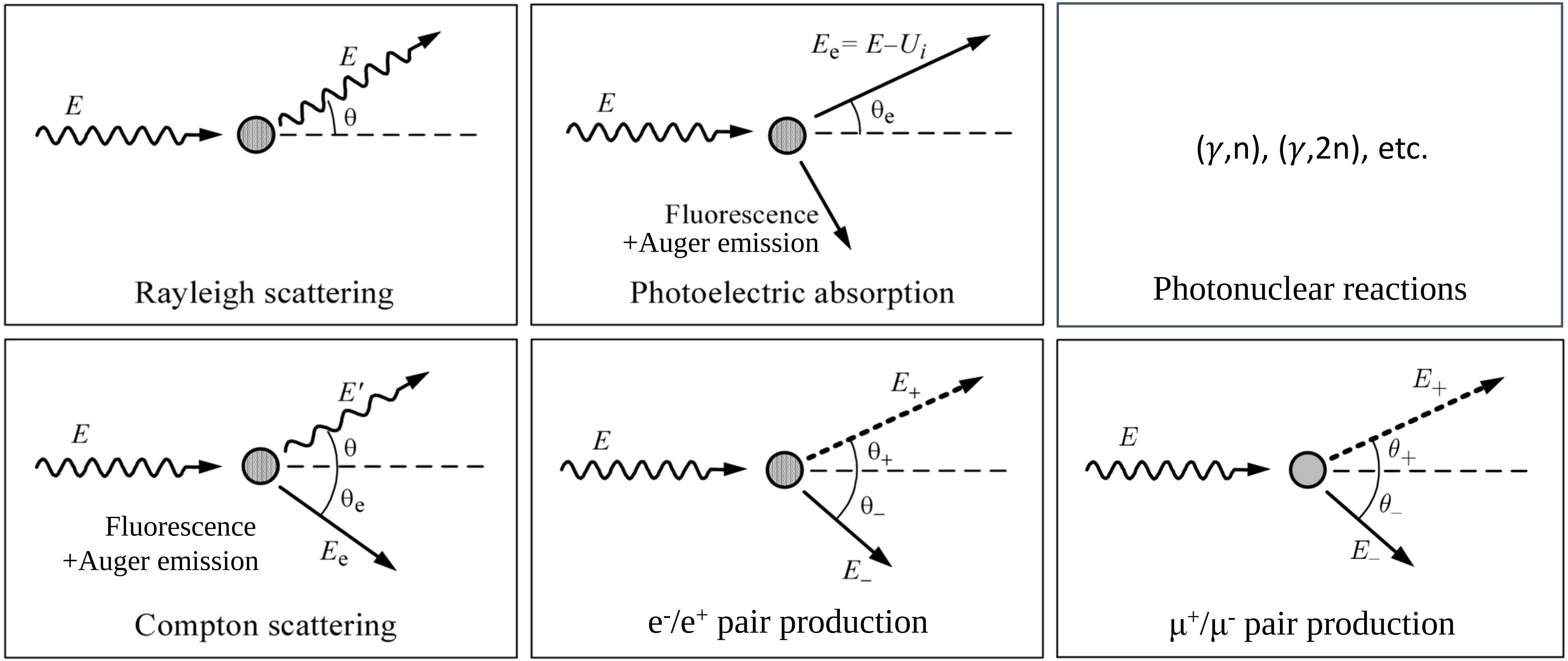
EMFCUT : set delta ray production threshold for electrons and positrons

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

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

Photon interactions



(Figures kindly shared by the PENELOPE authors)

Photon interaction cross sections

Low energy

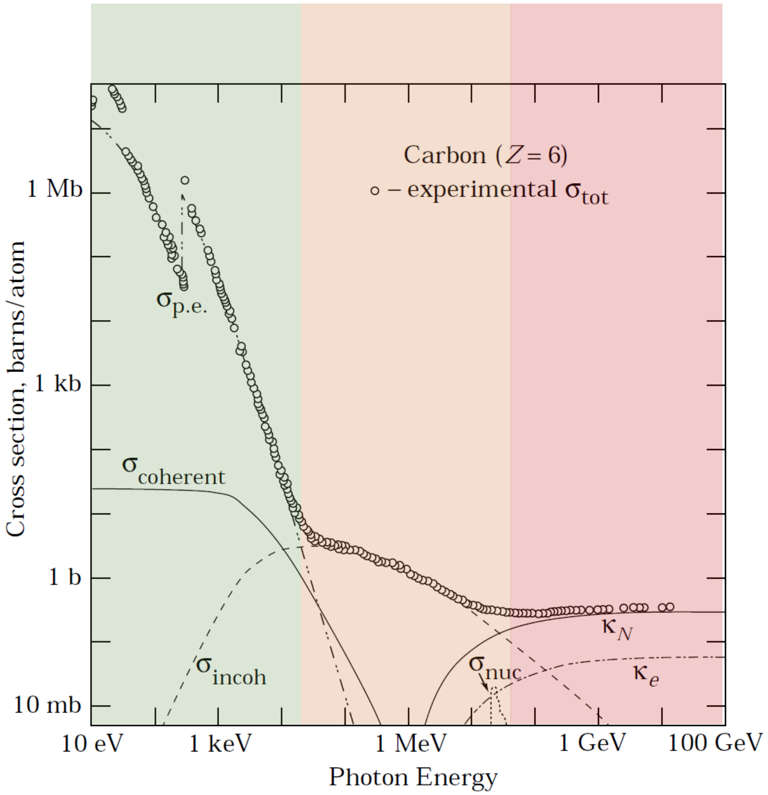
- photoelectric effect $\sigma \propto Z^5$
- atomic shell structure signature

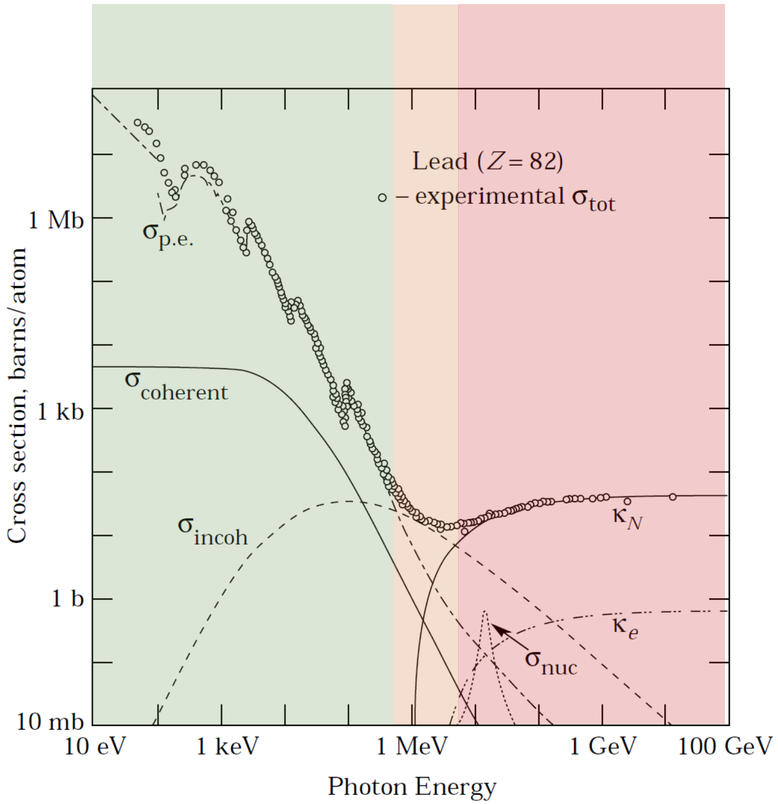
Intermediate energy

- Compton scattering $\sigma \propto Z$

High energy

- At 1.022 MeV, e-/e+ pair production opens $\sigma \propto Z^2$
- Minor contribution from photonuclear





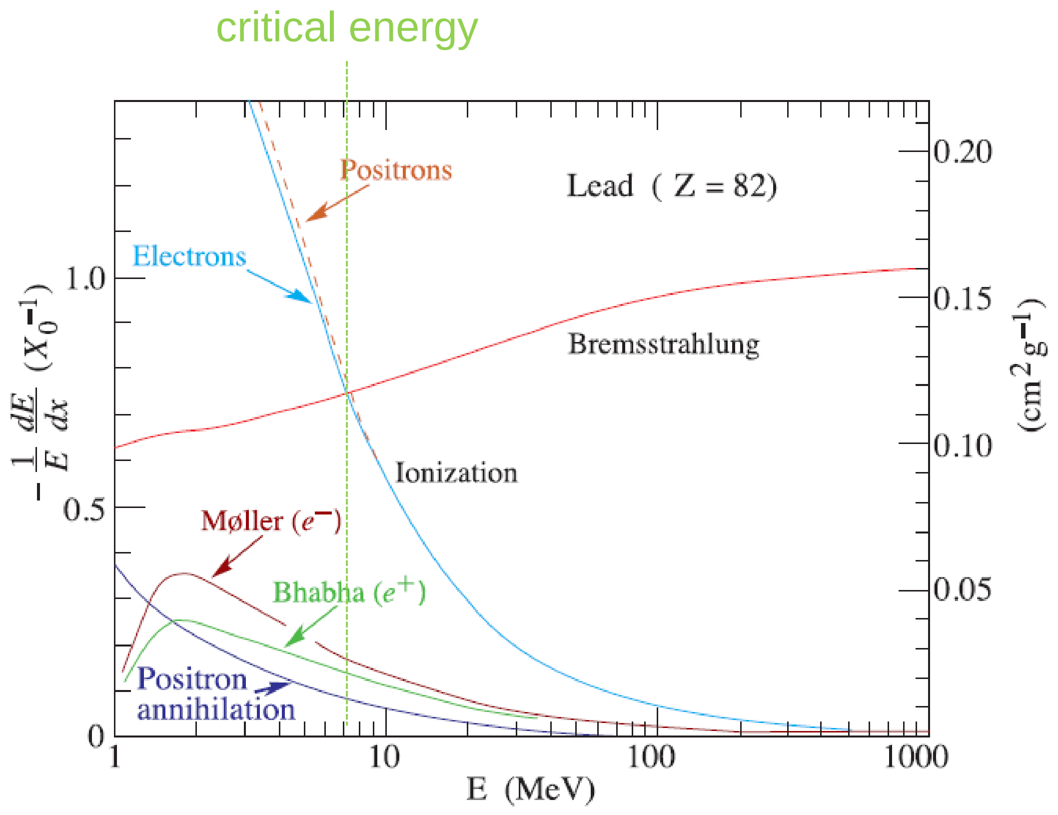
Electron/positron interactions

Below critical energy

- **Ionization** (cf. before) with a twist, due to projectile and target symmetry
- **Møller** (e-) or **Bhabha** (e+) scattering (→ δ-rays)

Above the critical energy

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



Positron annihilation

- Both at rest and in flight
- For annihilation at rest, account for mutual polarization of the two emitted photons

+ electro-nuclear... (see hadronic physics)

Photon and e± physics package in FLUKA

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

  EMF : OFF ▼

  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

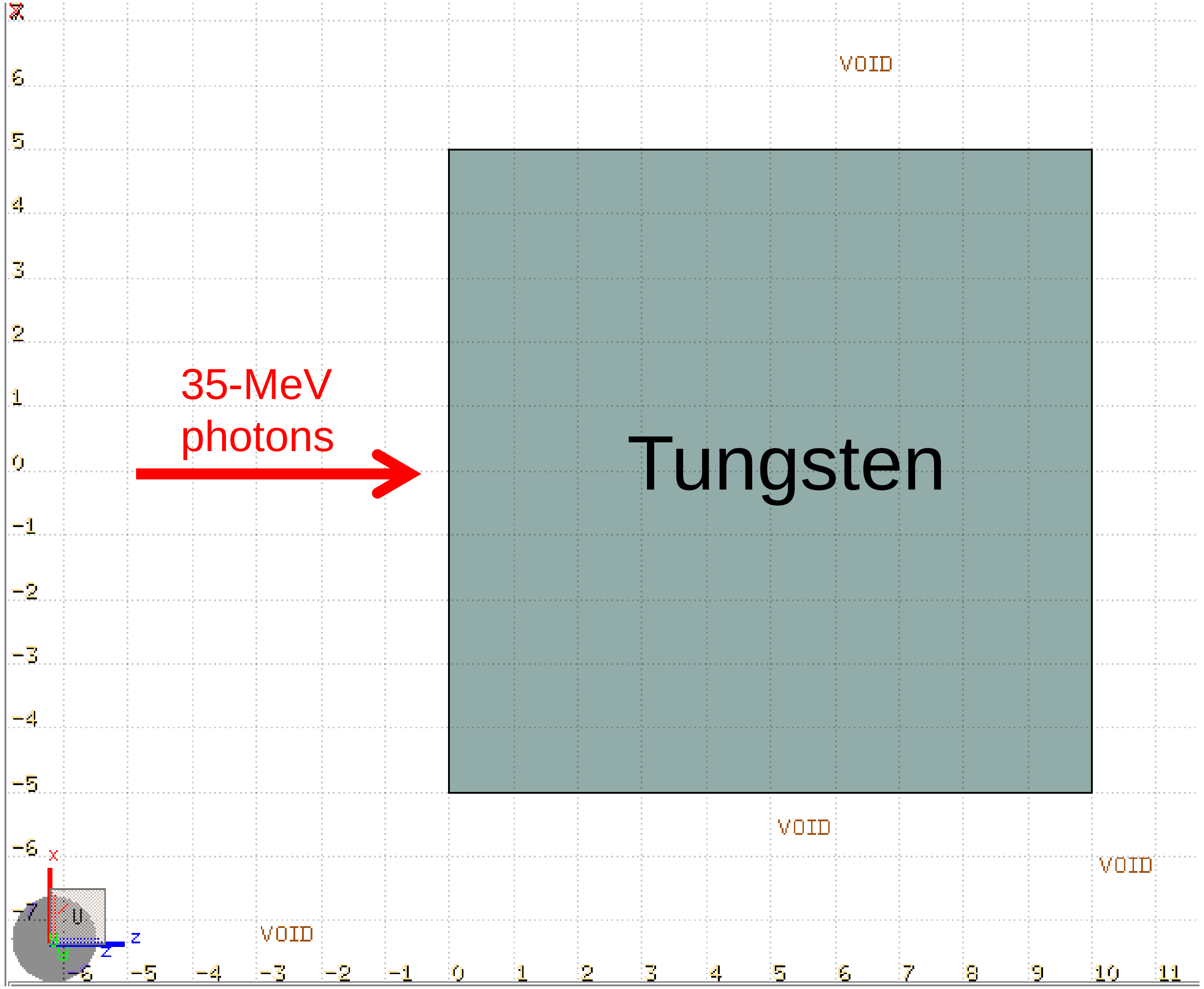
- Up-to-date γ cross sections from the EPDL database

- Energy conservation is ensured within computer precision

Full coupling between EM and hadronic shower

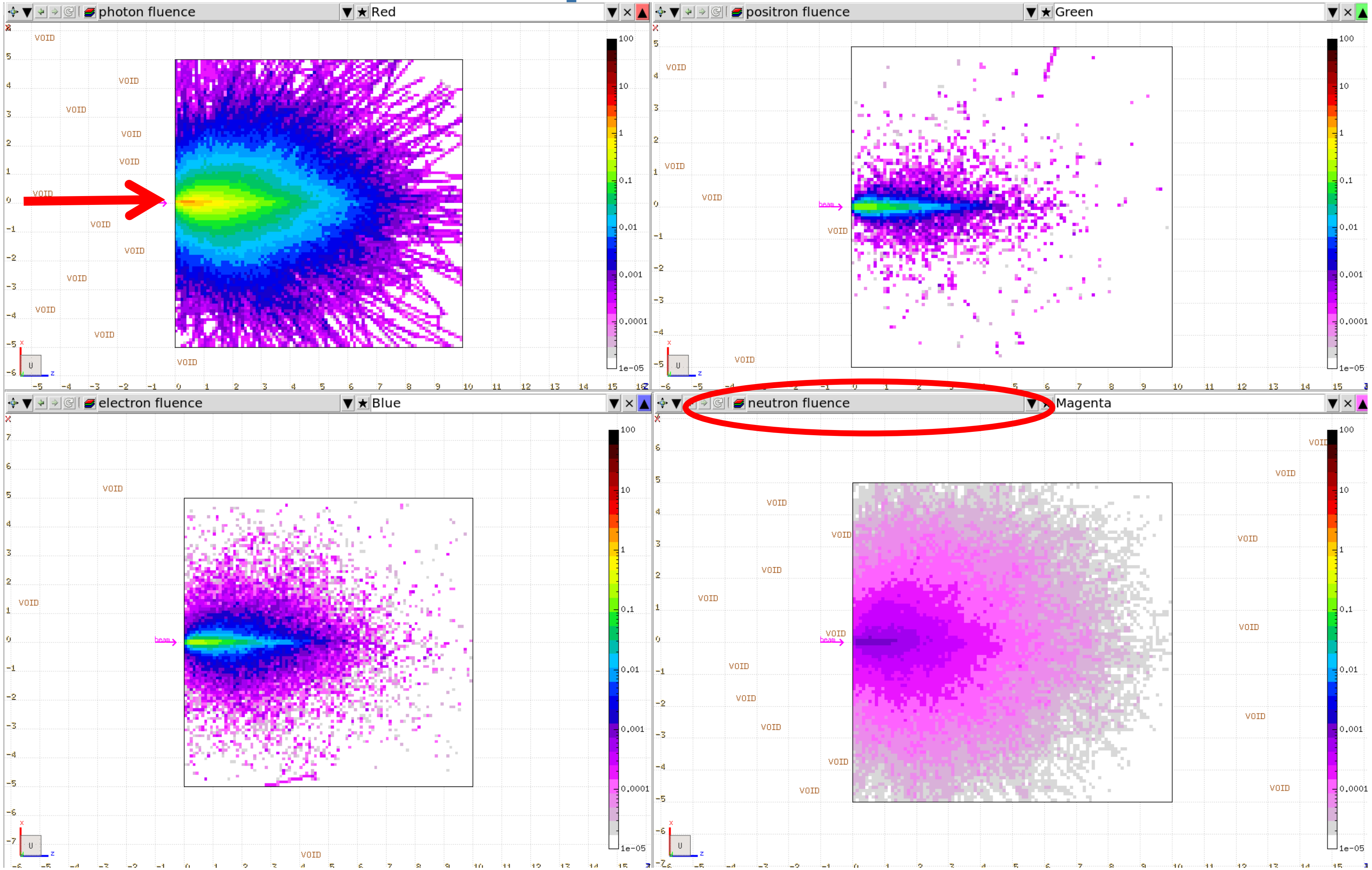
- E.g. 35-MeV photons on W target
- Start with a purely EM shower
- Photons may undergo photonuclear reactions
- E.g. neutrons can be produced (!)

- Let's examine various particle fluences….



Particle fluences from 35-MeV photons on W

35-MeV photons



All fluences in 1/cm^2/primary photon

Note of caution for photonuclear interactions

- Are discussed in more detail during the Hadronic physics lecture
- 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

- 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. 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:

FLUKA card summary

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

EM thresholds

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:

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

Let 10 MeV electrons impinge on water from the left

Cartesian USRBIN with bin height=width=depth of 50 μm

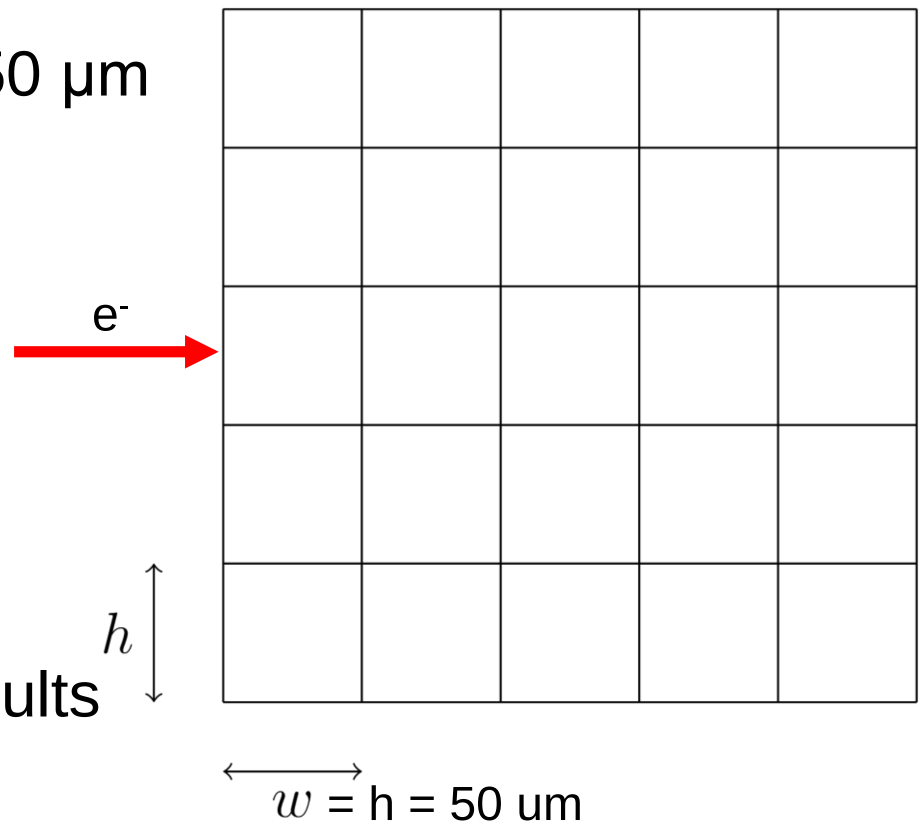
What are meaningful threshold values?

Threshold too high

→ premature: electrons could have traveled further

Threshold too low

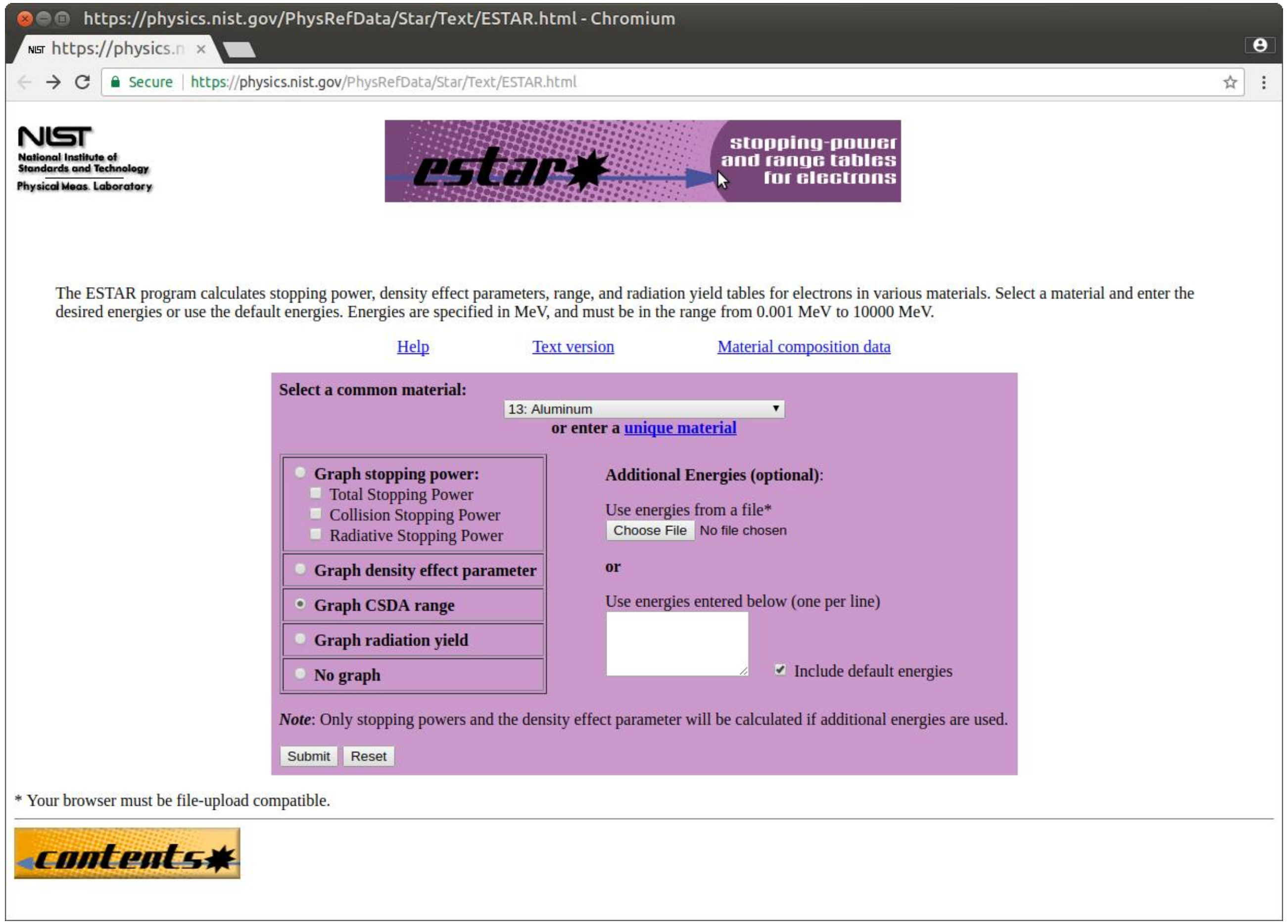
→ waste of time without gaining anything on the results



Put transport threshold at energy such that the range is smaller than the bin length

Quick way to examine particle ranges

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



Electron range in water

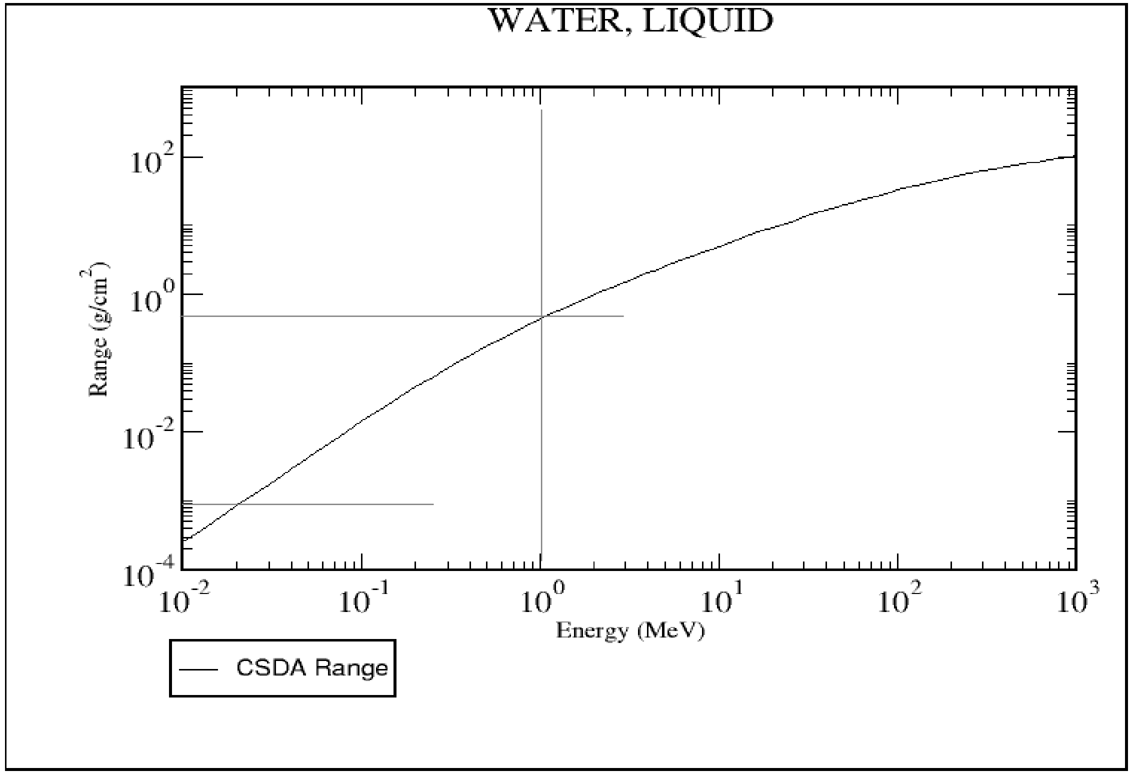
Consider our example scoring with dimensions of 50 μm.

What if we kill electrons below 1 MeV?

- Range at 1 MeV is ~5 mm = 5000 um
- The geometry has L = 50 um
- We would end the transport prematurely and get distorted energy deposition maps

Let's consider a range of 10 μm

- Depositing them on the spot in a 50μm bin is reasonable
- Corresponding energy is **~20 keV**



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

Summary: how to set your thresholds ?

e+/e- and γ transport thresholds

- Values depend on the geometry granularity
- Refer to range tables

e+/e- and γ production thresholds

- At least equal to transport threshold

δ-ray production thresholds

- At least equal to e- transport threshold, otherwise wasting cpu-time producing and dumping electrons on the spot
- If transport threshold is lower than δ-ray production threshold, it is increased automatically

WARNING

- Photons travel farther than electrons: their thresholds should be lower than for electrons
- Low thresholds for e-/e+/γ are ruthless CPU-time consumers

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

The FUDGEM parameter (avoid a FLUKA stop!)

When setting the delta-ray-production threshold,

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

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:

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:

- 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 +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

EMFCUT : careful with FUDGEM

MULSOPT : request single scattering, fine-tune MCS parameters

Summary

General overview of EM interactions

- Charged particles
  - Coulomb scattering → deflection
  - Ionization → energy loss
  - Radiative effects
- Photons
  - Photo-electric
  - Compton
  - Pair production
- Interdependence of e+/e- and photon cascades (and hadronic)
- Importance of the thresholds !

And now

Practical application of thresholds and their effect on your simulation

- Accuracy
- CPU time

FLUKA

Beyond the "simple" picture of energy loss

Electrons

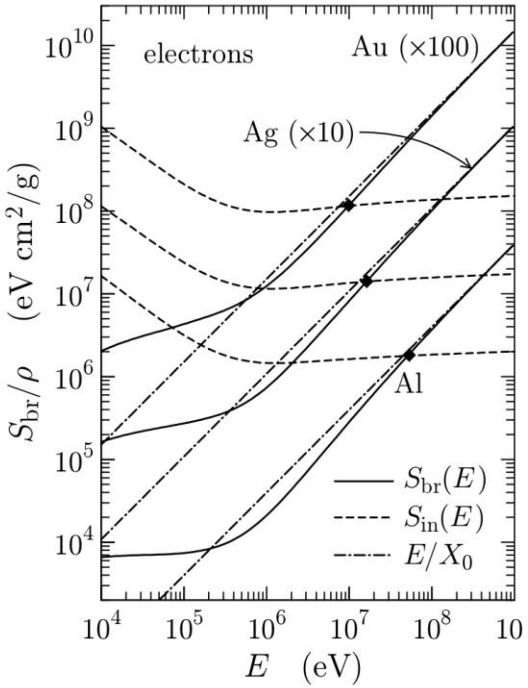
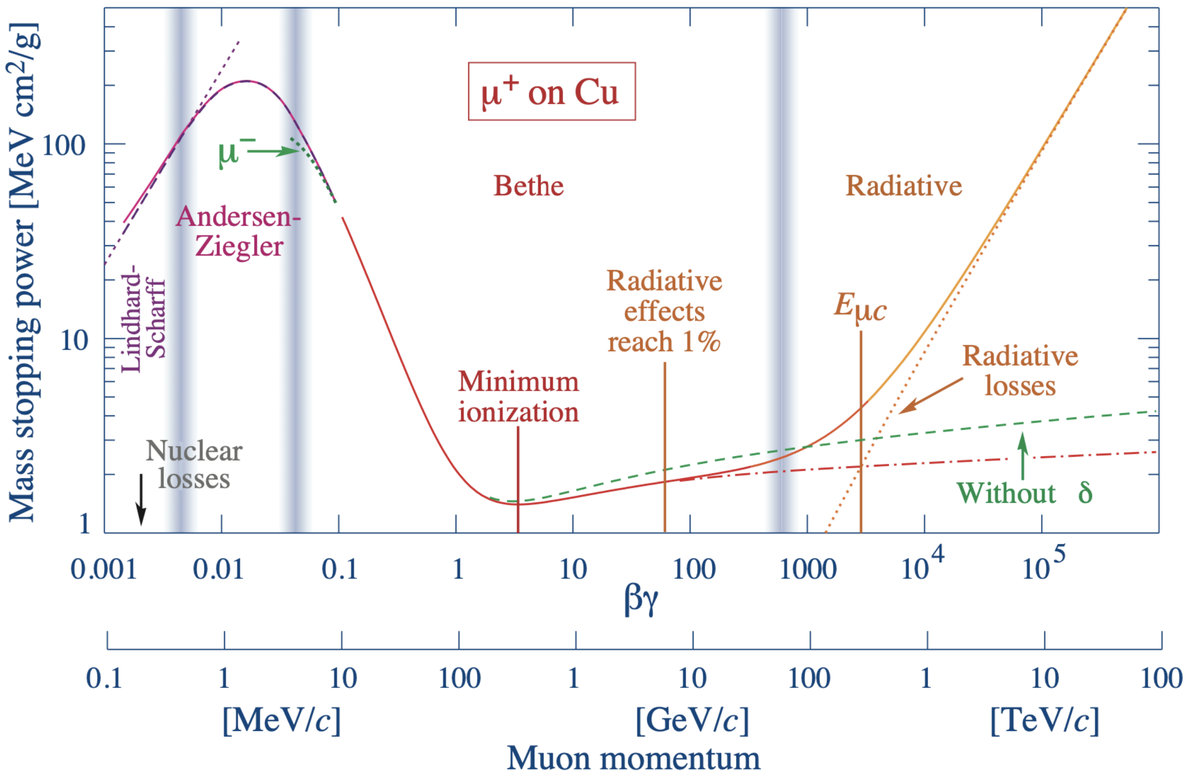


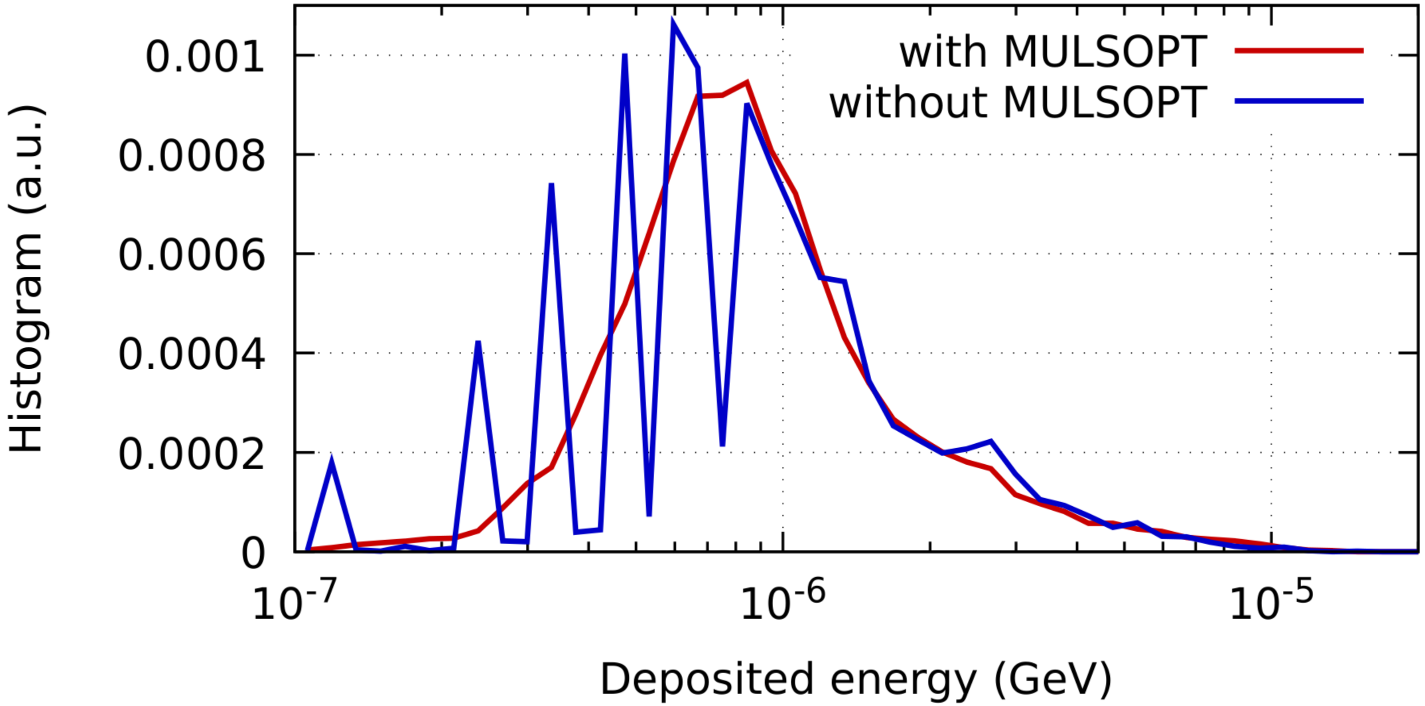
Figure 3.15: Radiative and collision stopping powers for electrons in aluminium, silver (×10) and gold (×100) as functions of the kinetic energy (solid and dashed curves, respectively). Dot-dashed lines represent the high-energy approximation given by Eq. (3.160). Diamonds indicate the critical energy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

muons in Cu



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`**)



Stopping power of charged particles

- Spin-0 particles:

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

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

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

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