

CURSO INTRODUTÓRIO



23 DE JANEIRO
A 8 DE MARÇO
DE 2023

FLUKA

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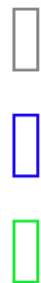
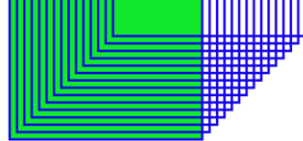
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AULA 09

Cartões de transporte e física

Iniciaremos em breve



Código Monte Carlo de interação e transporte de partículas

01

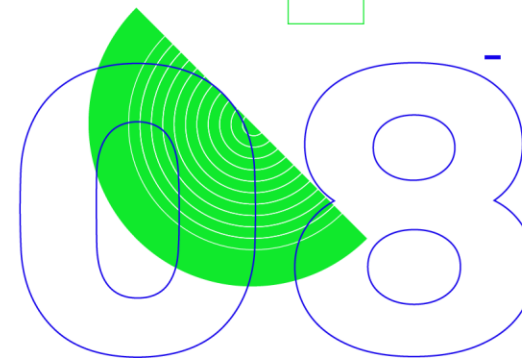
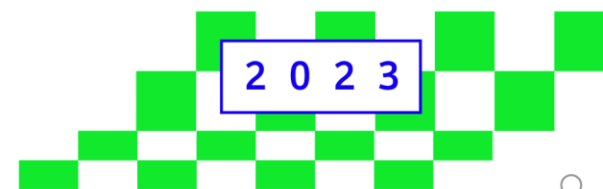
02

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01

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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

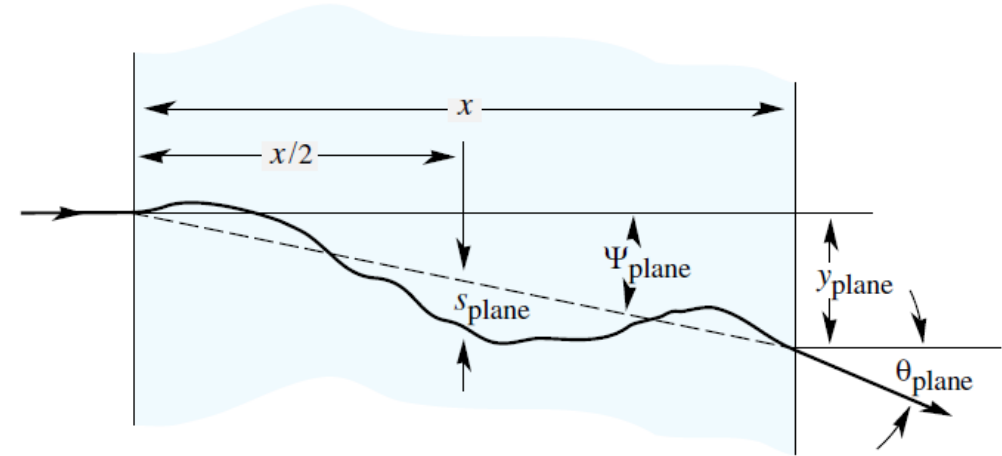
- **Ions**

- 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
→ 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

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

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

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

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

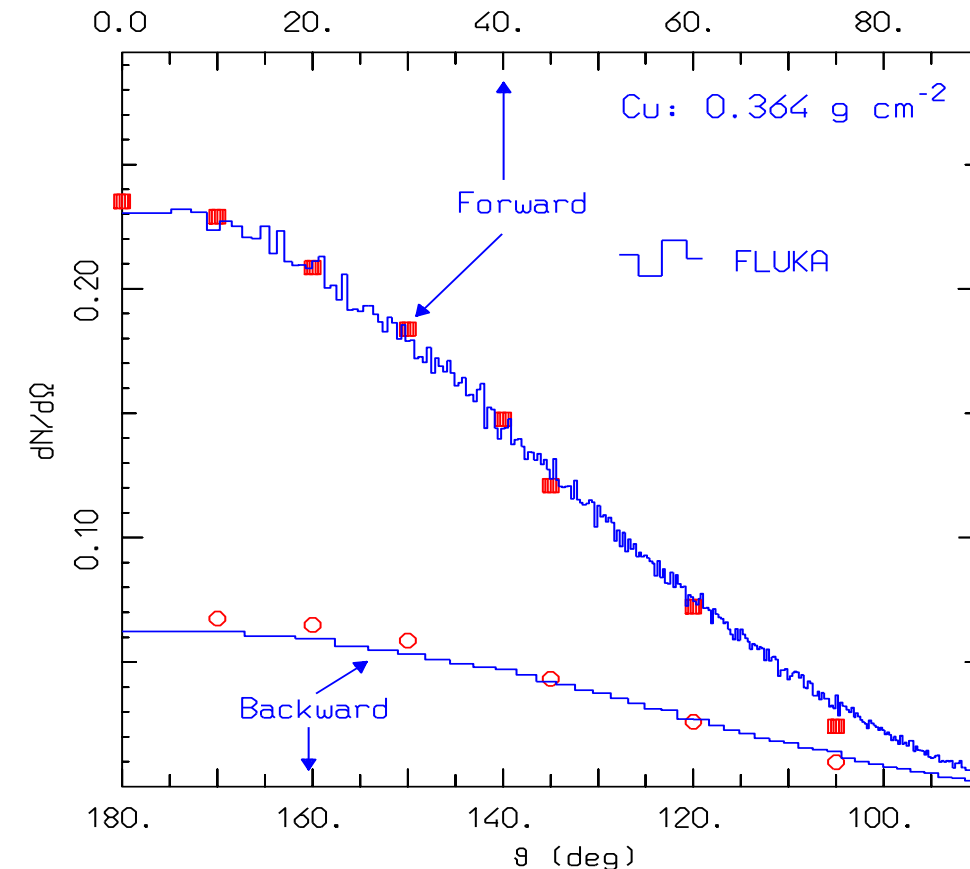
- At every step t, we sample aggregate deflection from F_{Mol}

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

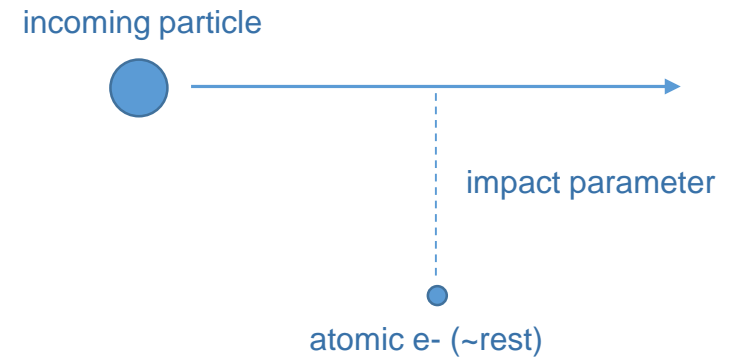
- As a result of the modelling effort, even demanding situations like electron backscattering can be modelled, in most cases without resorting to single scattering (not bad for an algorithm based on the Moliere theory!)
- E.g.: 1.75 MeV electrons on 0.364 g/cm² Cu foil
- Transmitted (forward scattered) 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)

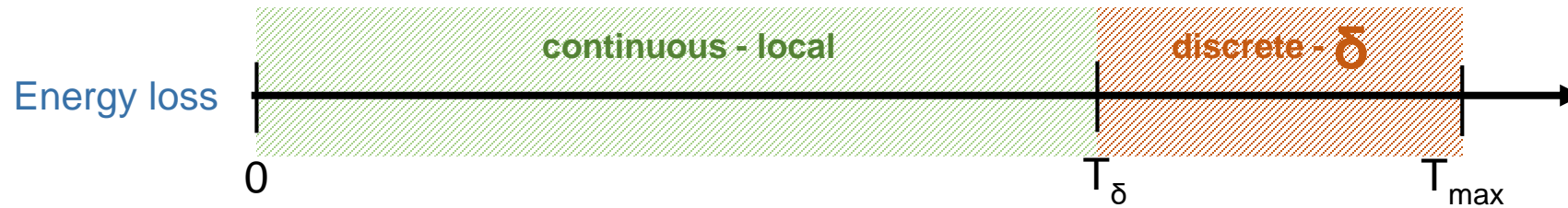


After a given step length, what does the energy distribution look like?

...and what of the energy lost ?

Ionization energy losses

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

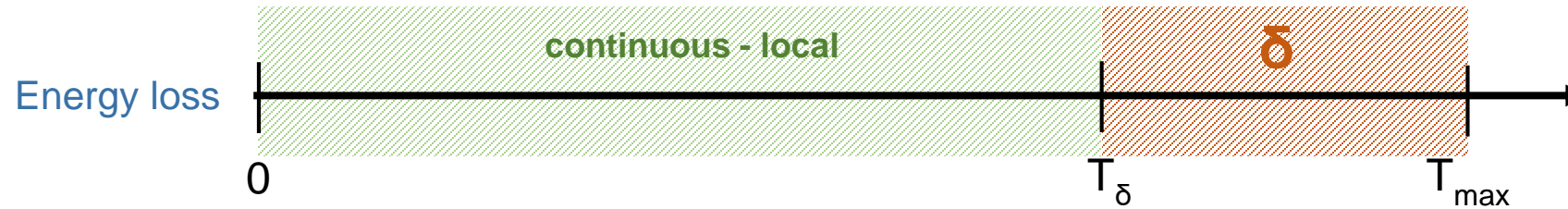


- Ionization loss cross sections $\propto 1/T^2$
→ Small losses are dominant
Expensive CPU-wise to simulate them all
- Need for aggregation along particle step:
 - Determine average energy loss per unit path length up to T_δ (restricted stopping power)
 - Random fluctuations applied on top

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

```
⌘ 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

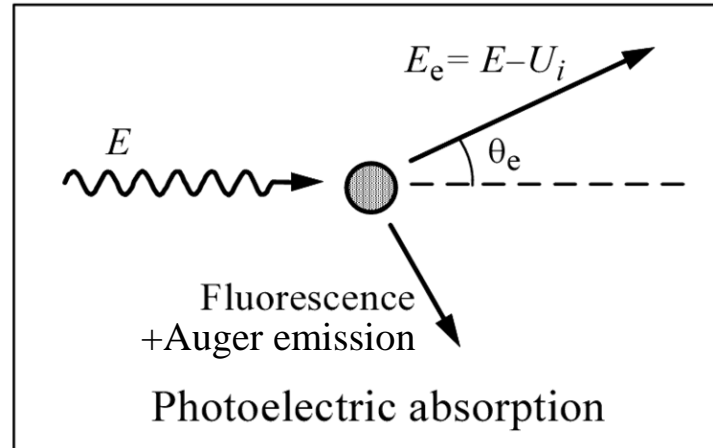
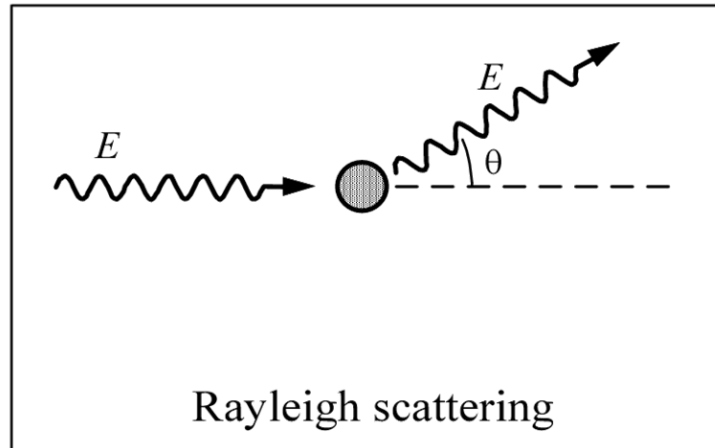
```
⌘ DELTARAY E thres: 1e-5 # Log dp/dx: Log width dp/dx:  
Print: NOPRINT ▼ Mat: ALUMINUM ▼ to Mat: ALUMINUM ▼ Step:
```

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

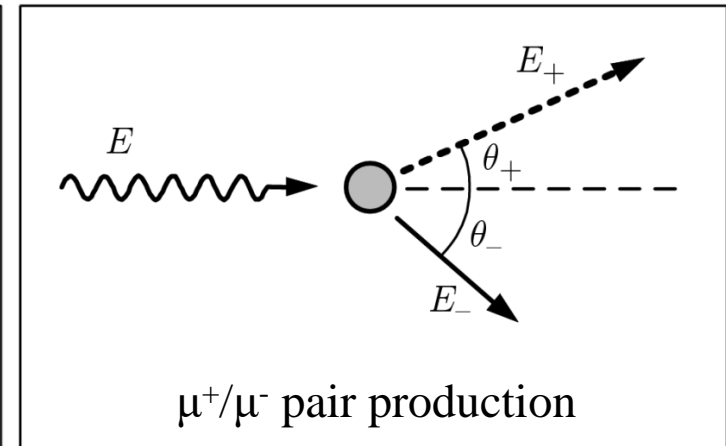
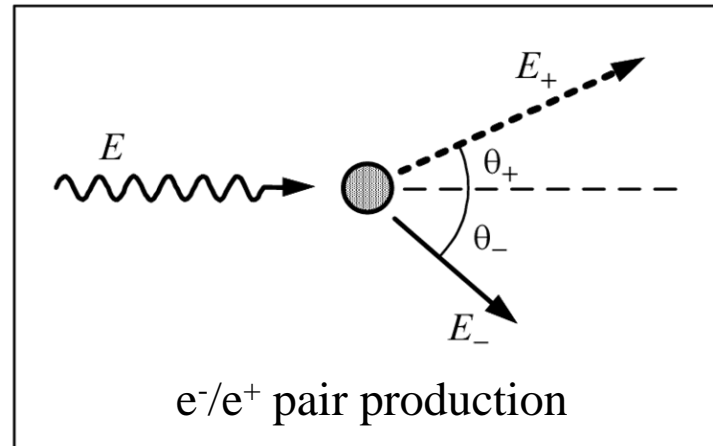
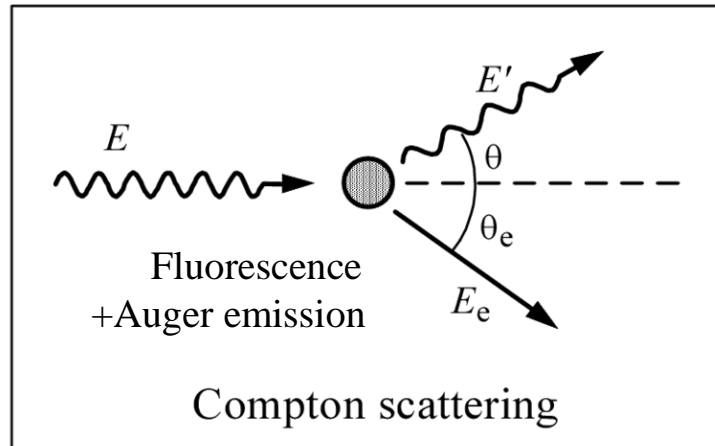
Photon and e^\pm interactions in matter

Photon interactions



(γ, n) , $(\gamma, 2n)$, etc.

Photonuclear reactions



(Figures kindly shared by the PENELOPE authors)

Photon interaction cross sections

Low energy

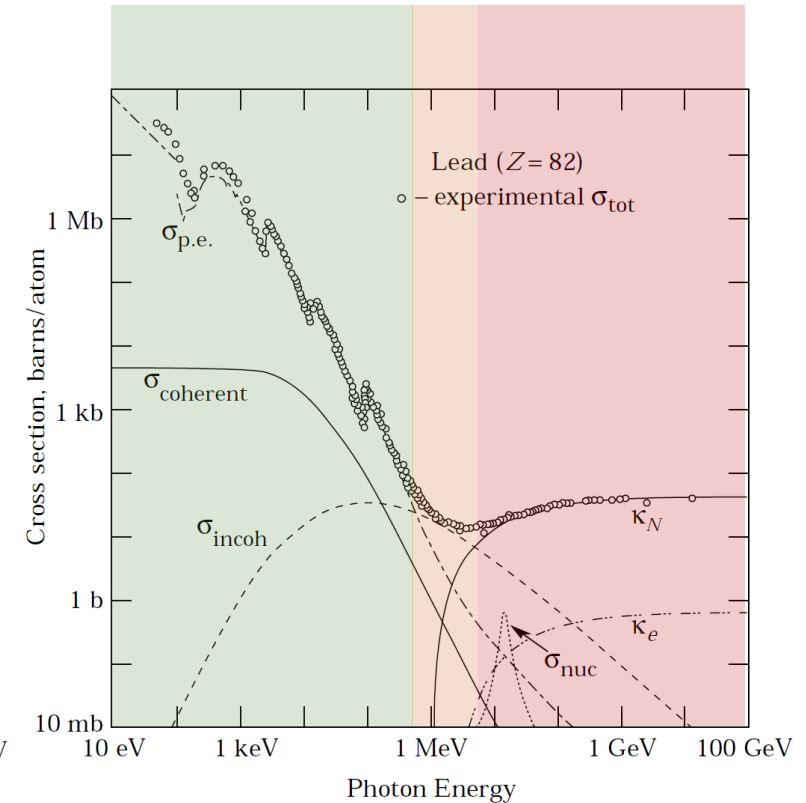
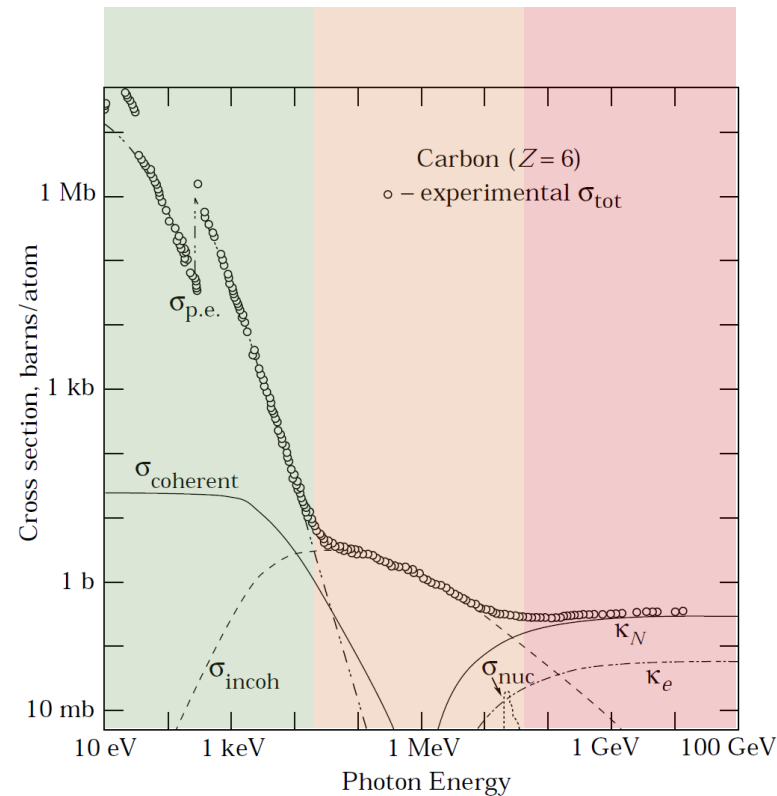
- photoelectric effect $\sigma \propto Z^5$
- atomic shell structure signature

Intermediate energy

- Compton scattering $\sigma \propto Z$

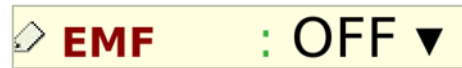
High energy

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



Photon and e^\pm physics package in FLUKA

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

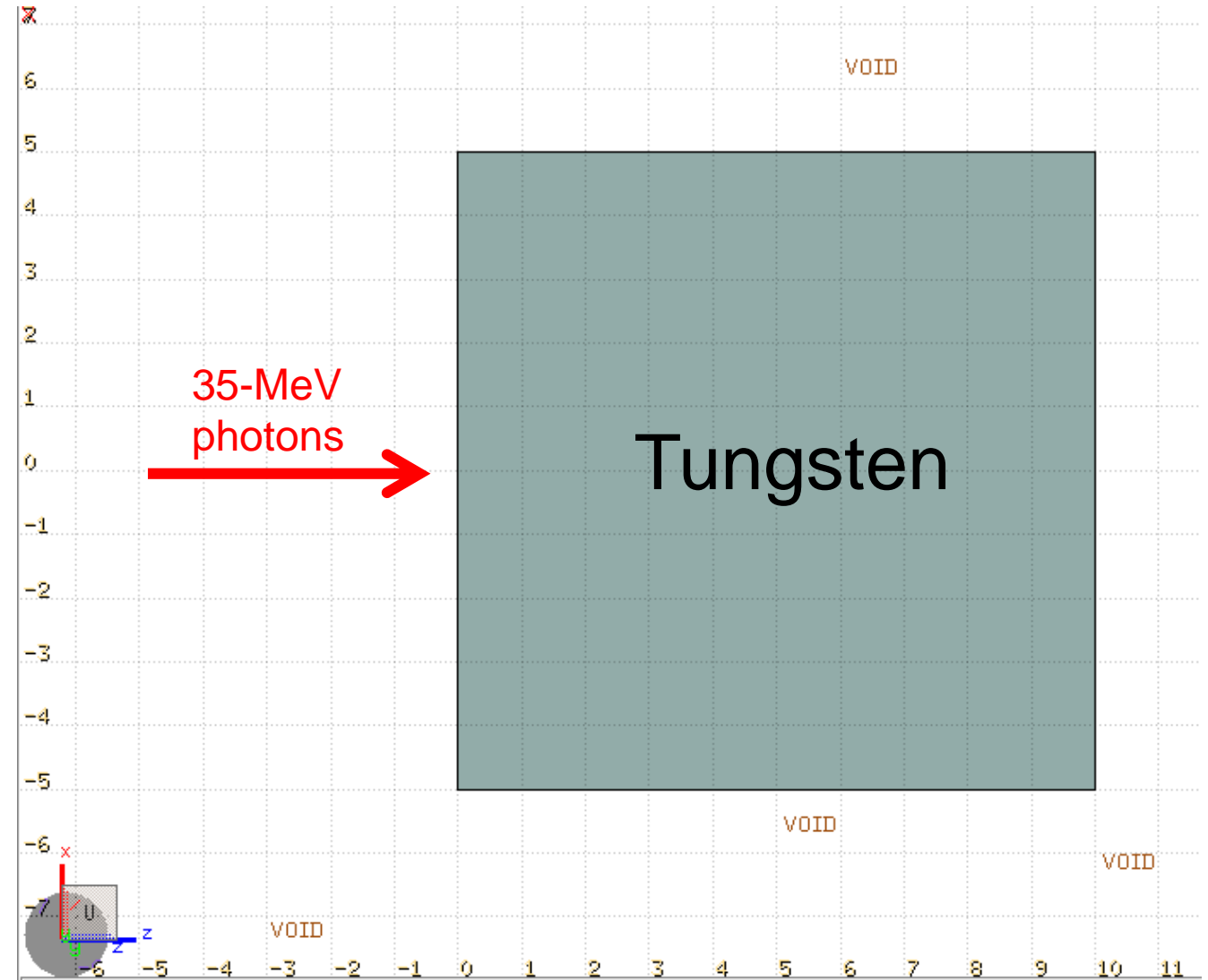
 EMF : OFF ▼

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

- Energy range: e^\pm : 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

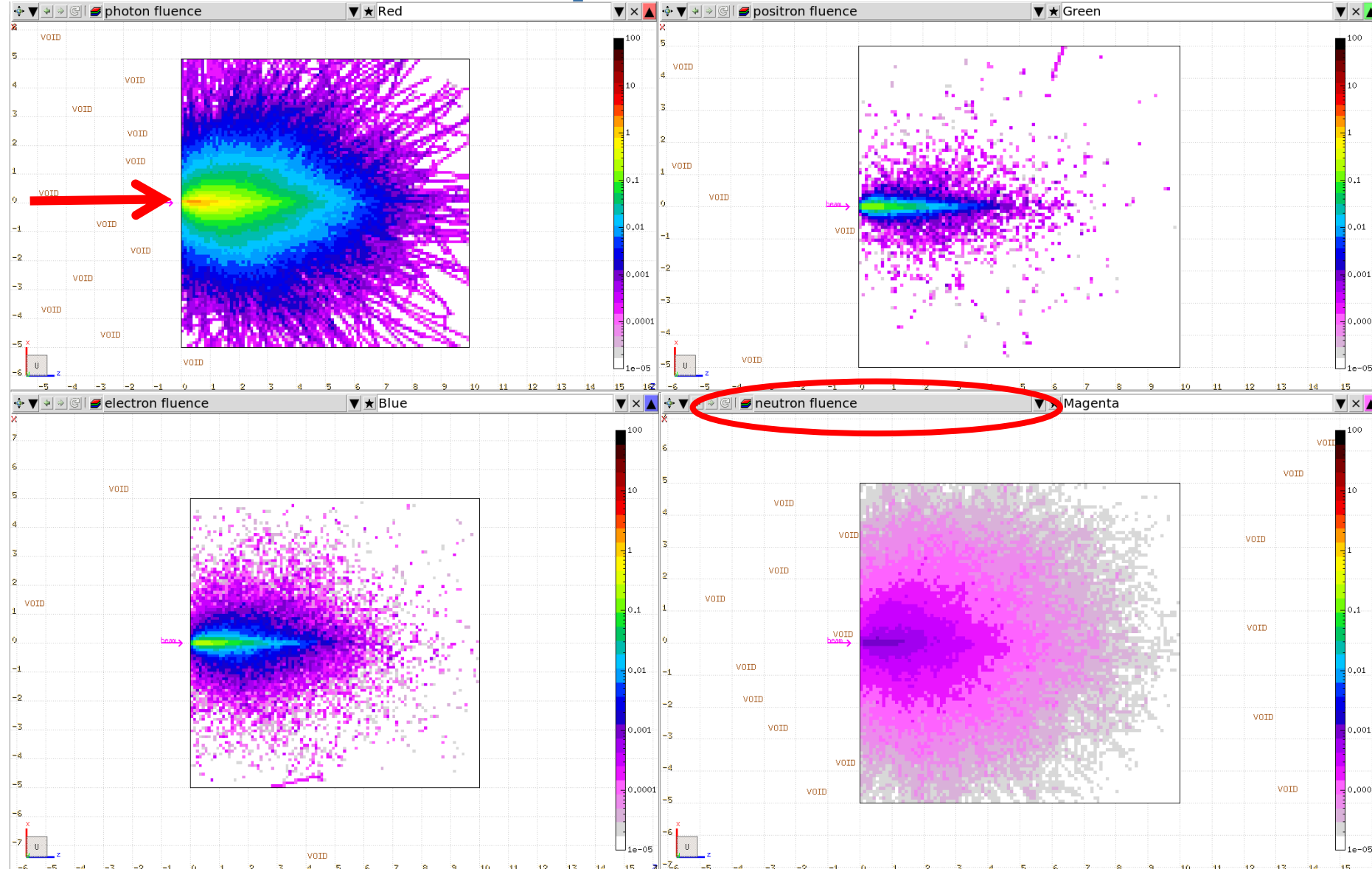
Full coupling between EM and hadronic shower

- 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 $1/\text{cm}^2/\text{primary photon}$

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 ▼  $\Delta$  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: ▼  $\times$  mean life: 0  $\times$   $\lambda$  inelastic: 0.01  
Mat: LEAD ▼ Part: PHOTON ▼ to Part: ▼ Step:
```

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

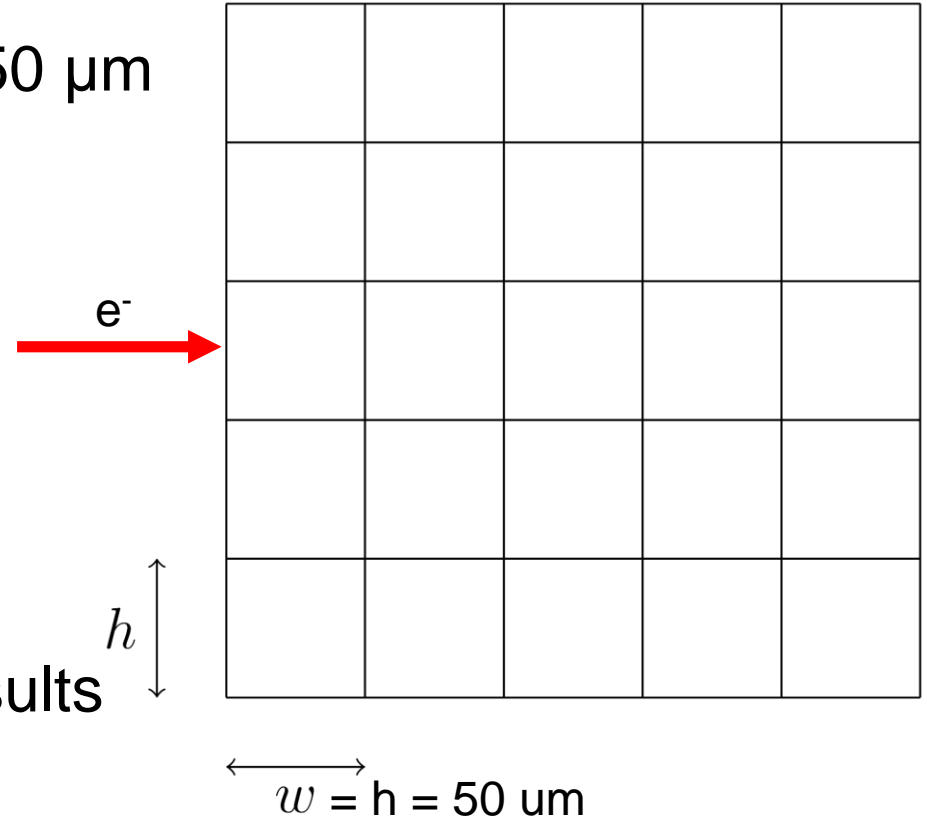
What are meaningful threshold values?

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>

NIST
National Institute of
Standards and Technology
Physical Meas. Laboratory

estars stopping-power and range tables for electrons

The ESTAR program calculates stopping power, density effect parameters, range, and radiation yield tables for electrons in various materials. Select a material and enter the desired energies or use the default energies. Energies are specified in MeV, and must be in the range from 0.001 MeV to 10000 MeV.

[Help](#) [Text version](#) [Material composition data](#)

Select a common material:
13: Aluminum
or enter a [unique material](#)

Graph stopping power:
 Total Stopping Power
 Collision Stopping Power
 Radiative Stopping Power

Graph density effect parameter

Graph CSDA range

Graph radiation yield

No graph

Additional Energies (optional):
Use energies from a file*
Choose File No file chosen

or
Use energies entered below (one per line)

 Include default energies

Note: Only stopping powers and the density effect parameter will be calculated if additional energies are used.

Submit Reset

* Your browser must be file-upload compatible.

[contents](#)

Electron range in water

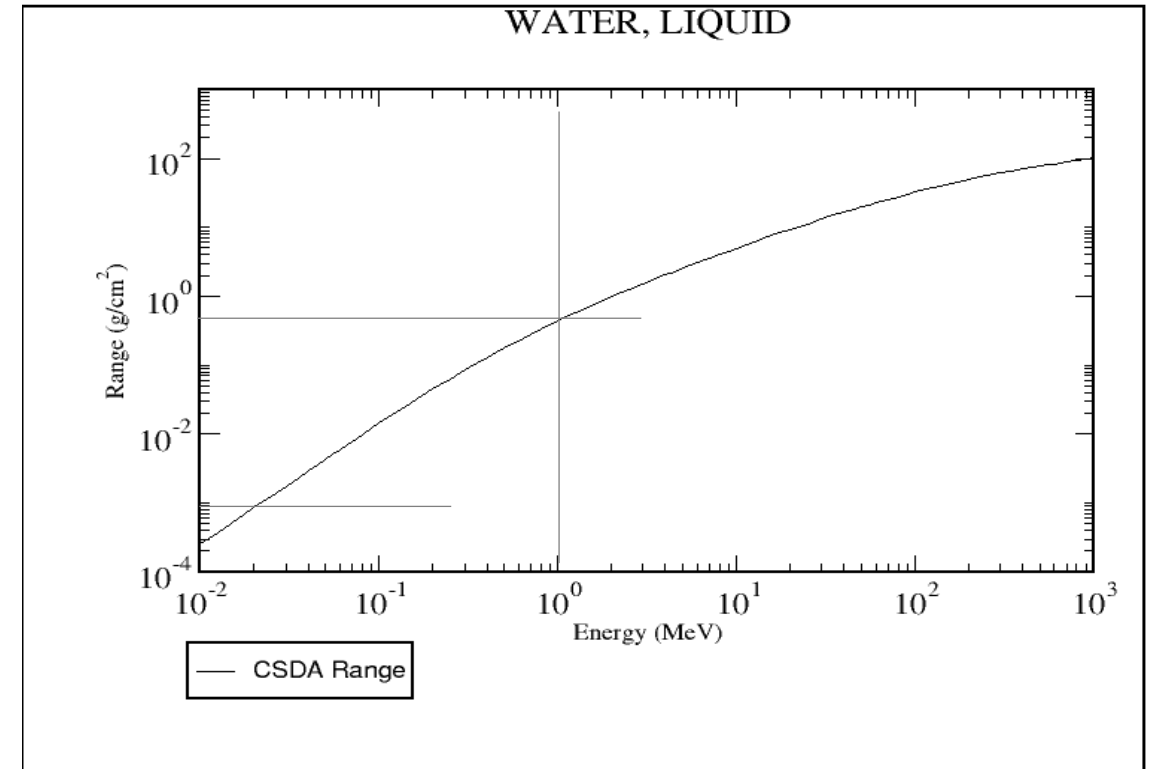
Consider our example scoring with dimensions of 50 μm .

What if we kill electrons below 1 MeV?

- Range at 1 MeV is $\sim 5 \text{ mm} = 5000 \mu\text{m}$
- The geometry has $L = 50 \mu\text{m}$
- 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 50 μm bin is reasonable
- Corresponding energy is **$\sim 20 \text{ keV}$**



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

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

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  $\gamma$ : 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 $T_\delta \sim 1$ keV, $FUDGEM=1e-5$ (zero)



Hadronic & photonuclear interactions

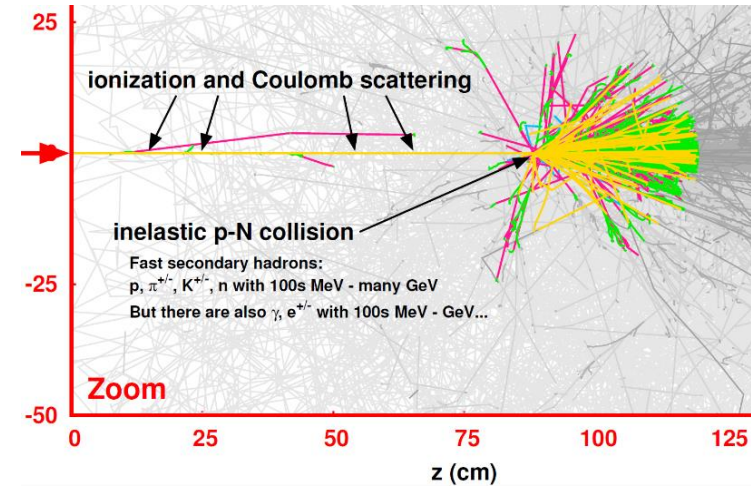
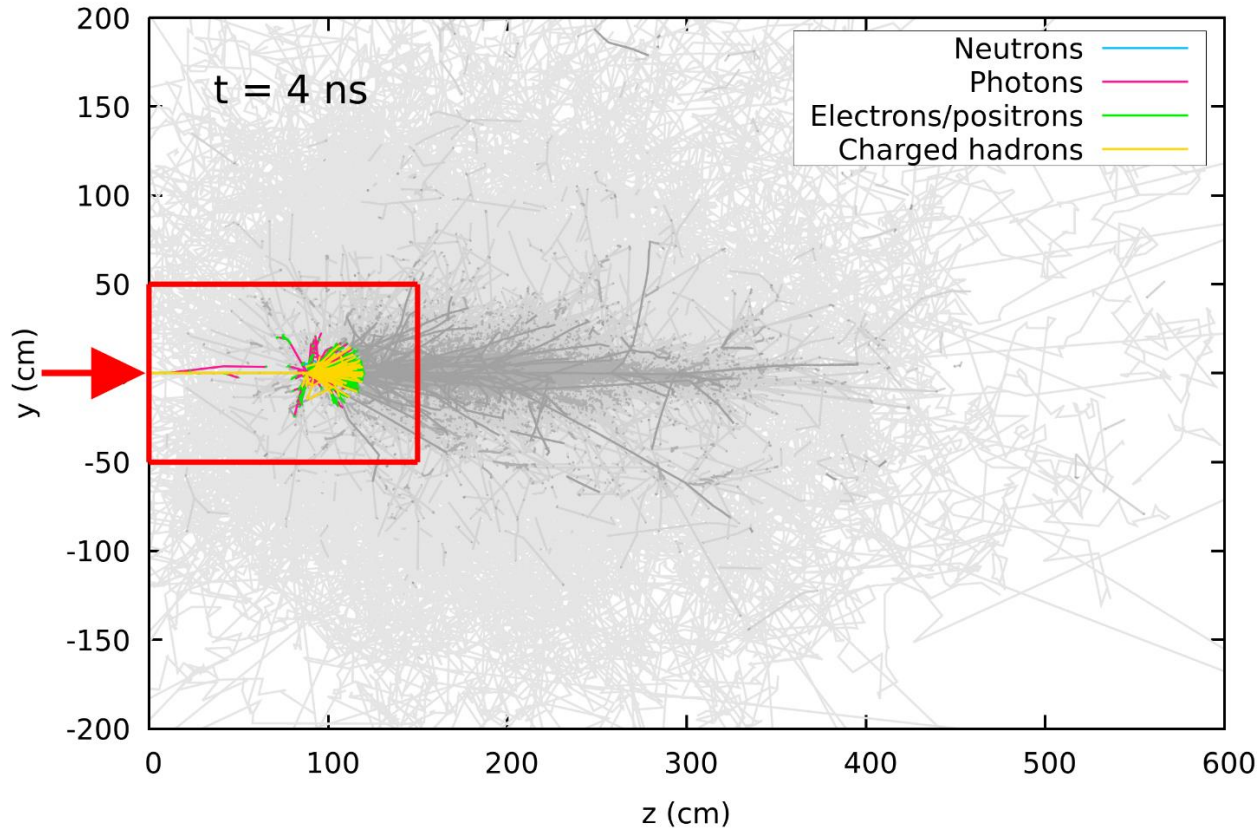
Hadron-nucleus, nucleus-nucleus and photon-nucleus reactions

Hadronic interactions [I]

Hadron-nucleus reactions

The microscopic view [I]

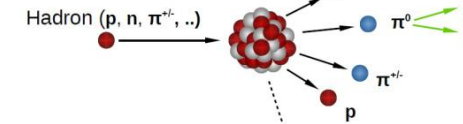
one 450 GeV proton on aluminum



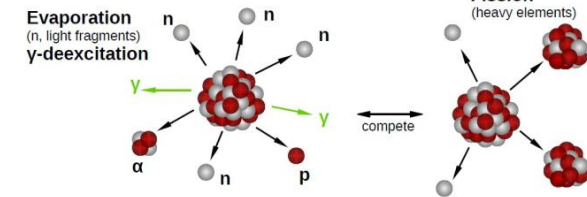
high energy nuclear reaction

$$\lambda \rho = \frac{A}{\sigma_R N_A} \quad \sigma_R \simeq \pi r_0^2 A^{2/3}$$

Fast stage (10^{-22} s)



Slow stage (10^{-16} s)

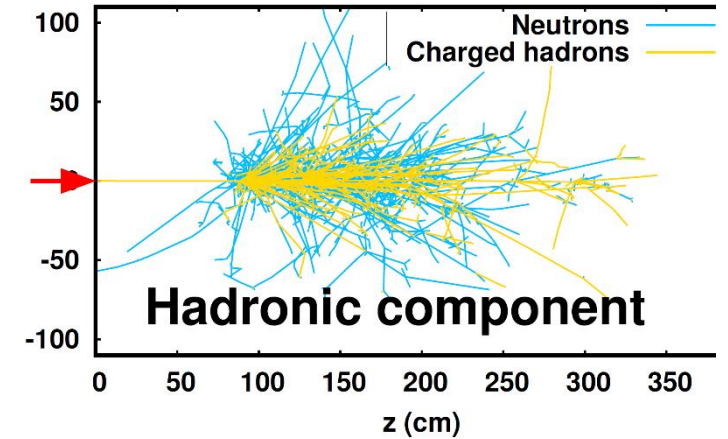
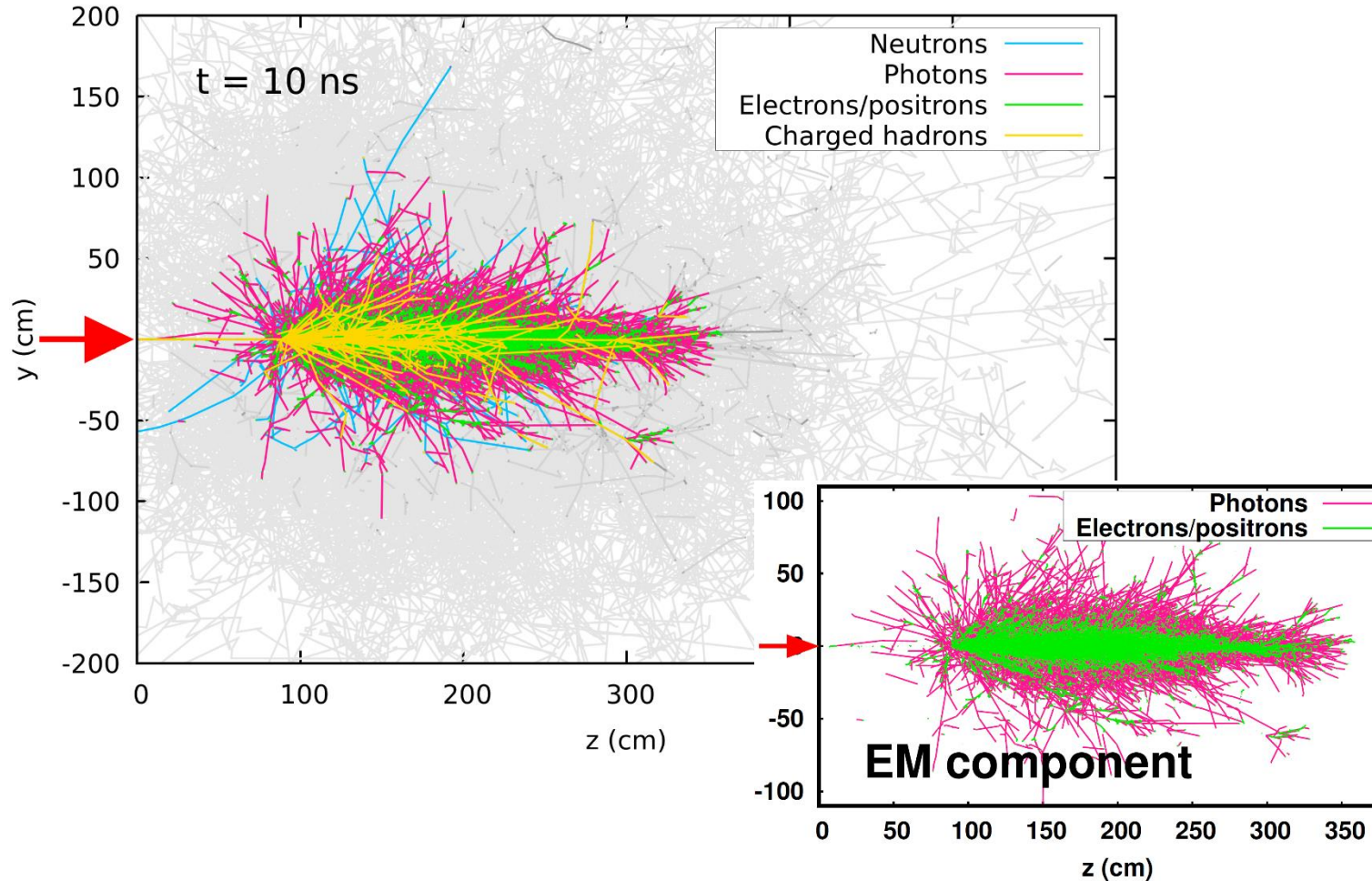


Residual nuclei can be unstable (radioactive)

Fission products can also undergo evaporation

The microscopic view [II]

one 450 GeV proton on aluminum

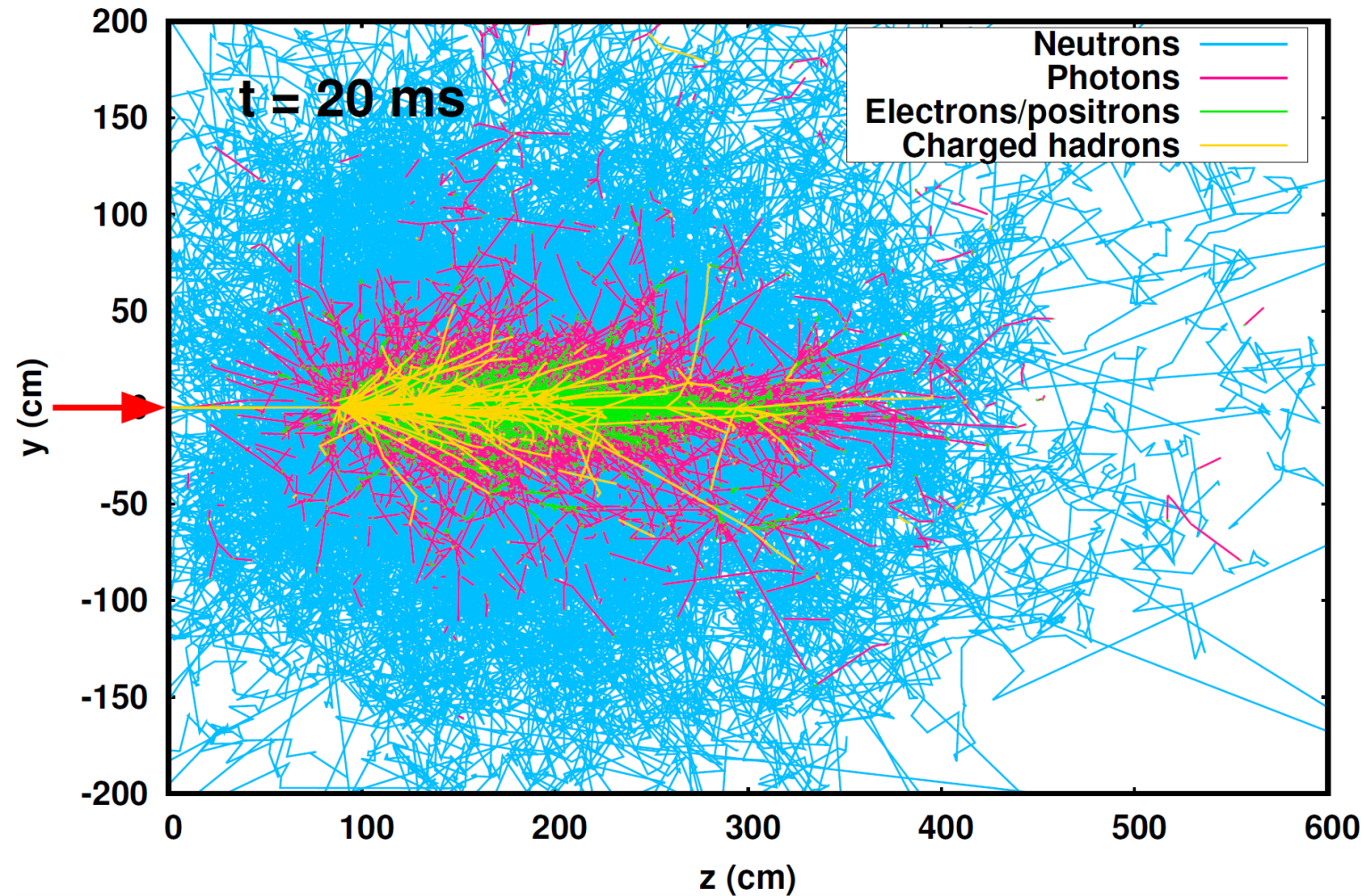


hadronic shower continues until particle energy falls below pion production threshold

non-negligible fraction of initial energy goes to mass by nuclear binding breaking

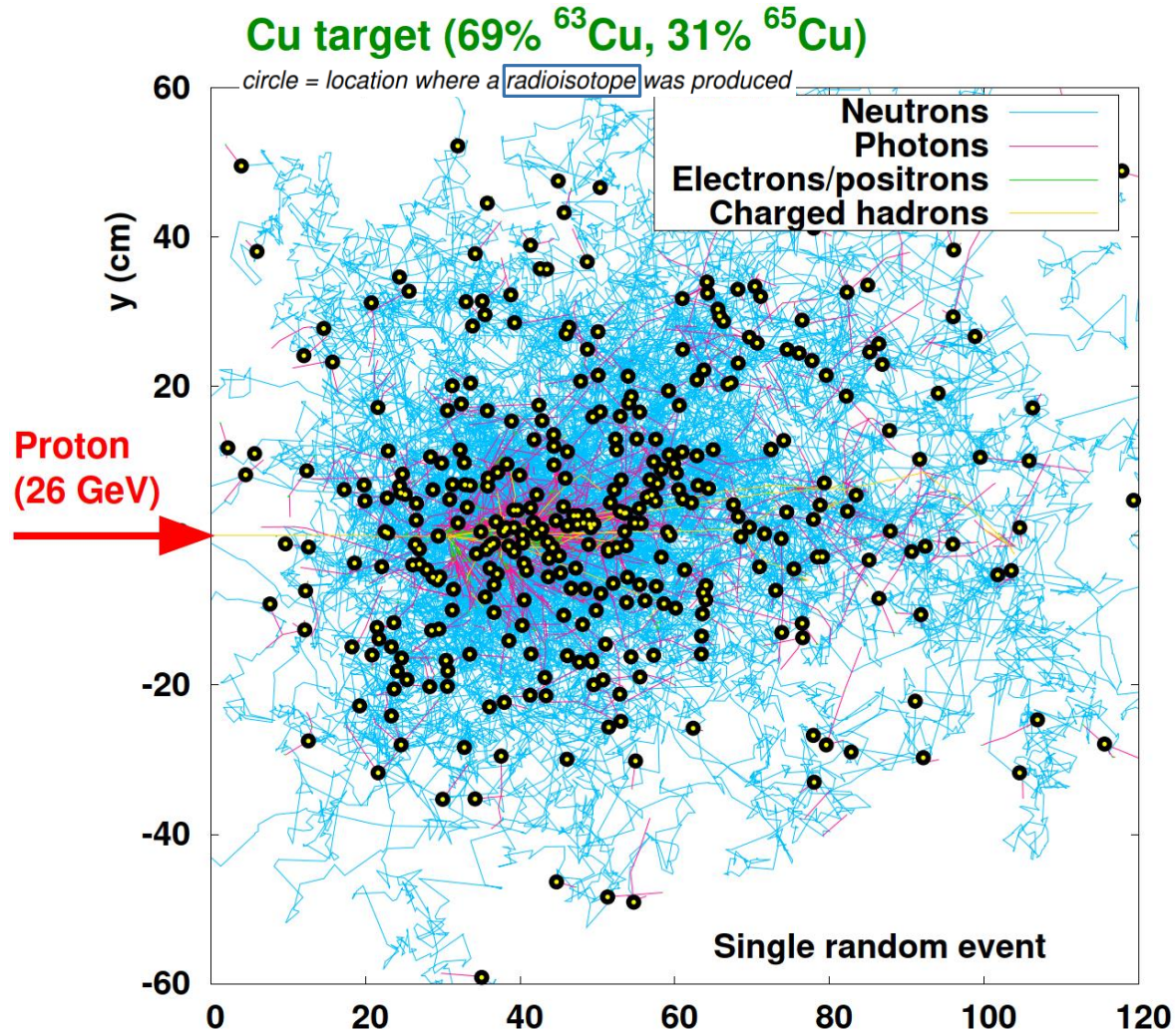
The microscopic view [III]

one 450 GeV proton on aluminum



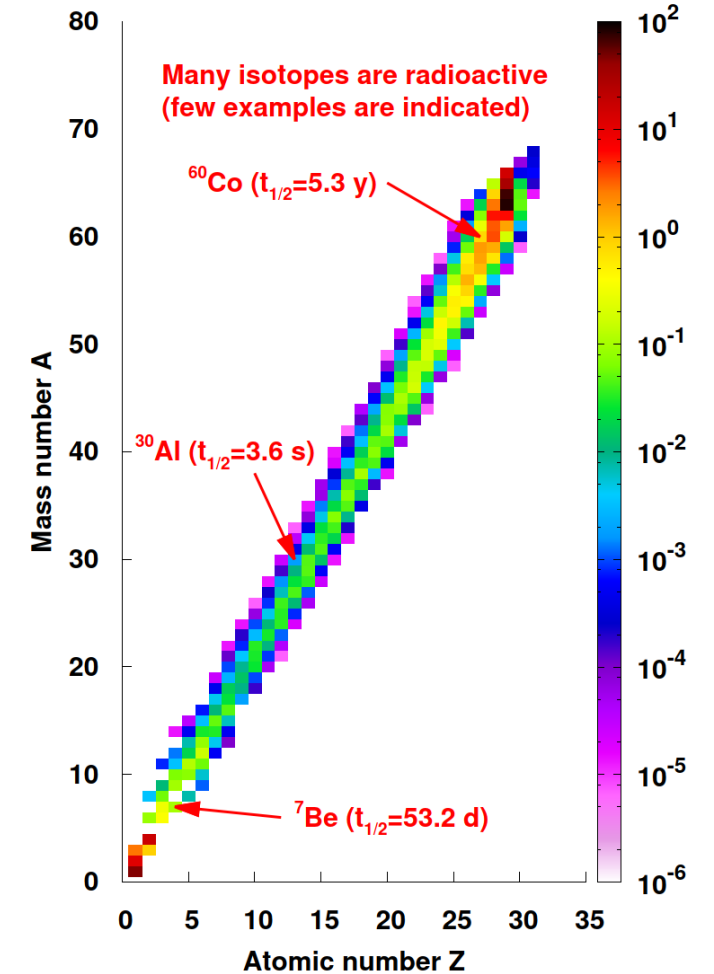
The microscopic view [IV]

one 26 GeV proton on copper



THE MACROSCOPIC VIEW: ACTIVATION

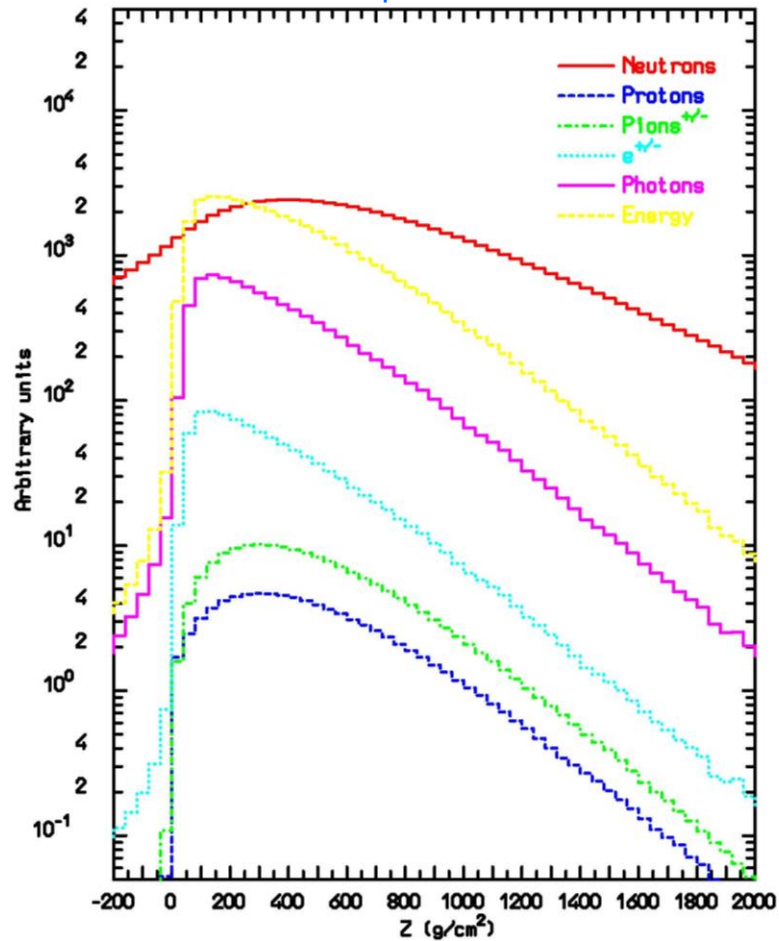
Average # of isotopes produced per impacting proton



The macroscopic view of high energy showers

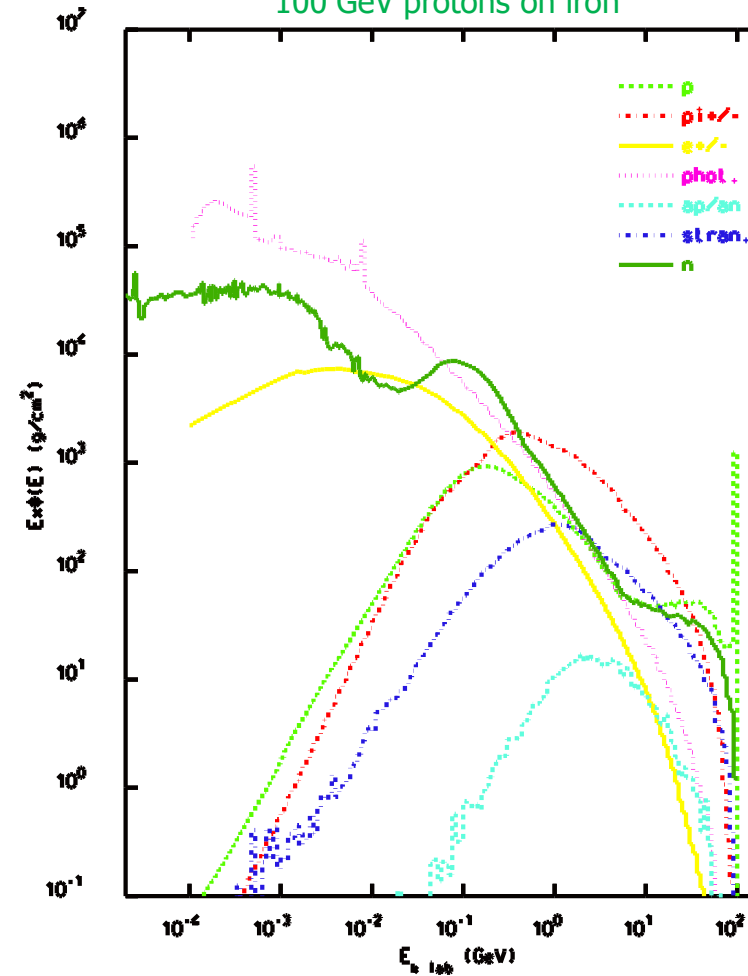
particle fluence and energy deposition profile

100 GeV protons on lead



volume-averaged particle spectra

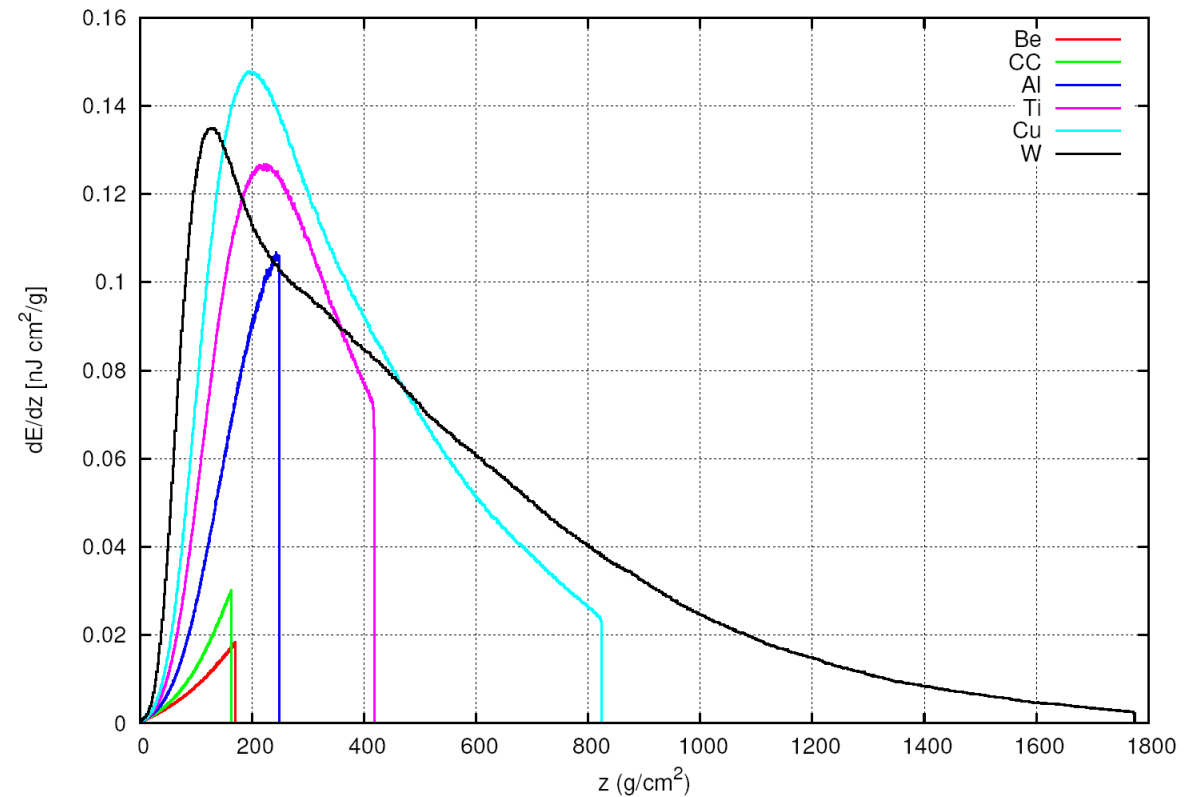
100 GeV protons on iron



Material dependence

	ρ [g/cm ³]	Z	χ_0 [cm]	λ [cm] for 7 TeV p
Be	1.85	4	35.28	37.06
CC	1.77	6	24.12	42.09
Al	2.70	13	8.90	35.35
Ti	4.54	22	3.56	25.04
Fe	7.9	26	1.76	15.1
Cu	8.96	29	1.44	13.86
W	19.3	74	0.35	8.90

energy deposition transversally integrated
 [different from *peak density* profile, which depends on beam size]
 for a 7 TeV proton impacting on a 92 cm long jaw



Nuclear reactions

In general there are two kinds of nuclear reactions:

- **Elastic interactions** are those that **do not change the internal structure** of the projectile/target and **do not produce new particles**. Their effect is to transfer part of the projectile energy to the target (lab system), or equivalently to deflect in opposite directions target and projectile in the Centre-of-Mass system with no change in their energy.

There is no threshold for elastic interactions.

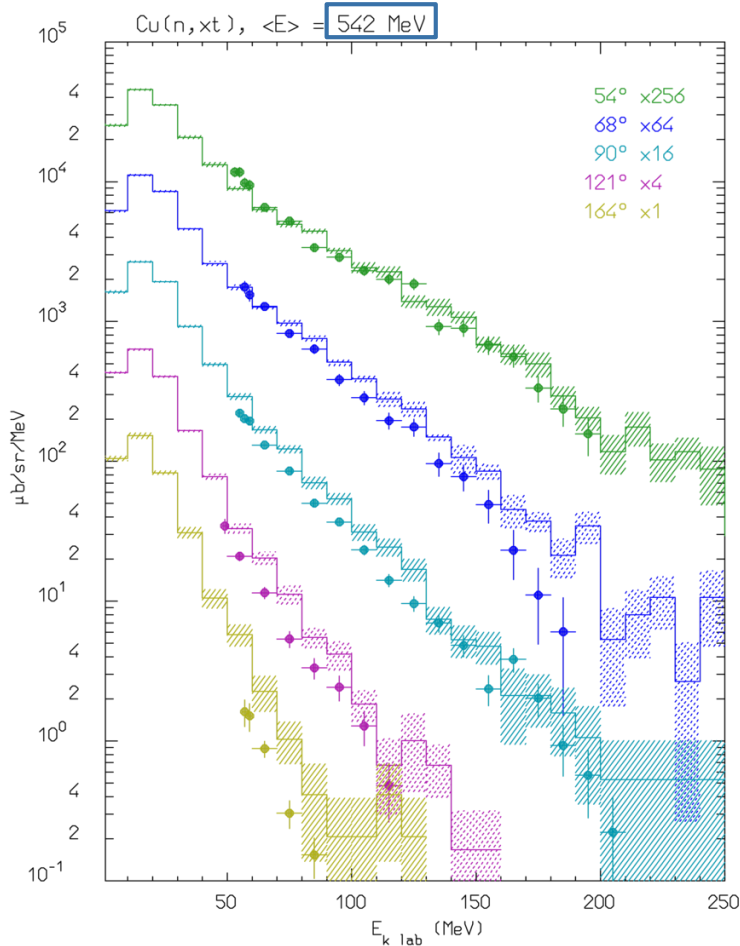
- **Non-elastic reactions** are those where **new particles are produced** and/or the **internal structure** of the projectile/target **is changed** (e.g. the nucleus is excited).

A specific non-elastic reaction has usually an energy threshold below which it cannot occur (the exception being neutron capture).

Coalescence

High energy light fragments can be produced by a mechanism joining together nucleons that are near in the phase space.

NEUTRON – Cu



double-differential triton spectra

To be activated when light fragment spectra or residual nuclei are of interest:

```

PHYSICS Type: COALESCE Activate: On
*...+...1...+...2...+...3...+...4...+...5...+...6...+...7...+...
PHYSICS 1. COALESCE
  
```

N.B. Remove the card previously required to invoke low energy *deuteron splitting at interaction*:

```


PHYSICS Type: IONSPLIT Ion Split: On Splitting: Nonelastic
Emin: 0.005 Emax: 0.15 Amin: 2 Amax: 2
*...+...1...+...2...+...3...+...4...+...5...+...6...+...7...+...
PHYSICS 1. 0.005 0.15 2. 2. 5. IONSPLIT

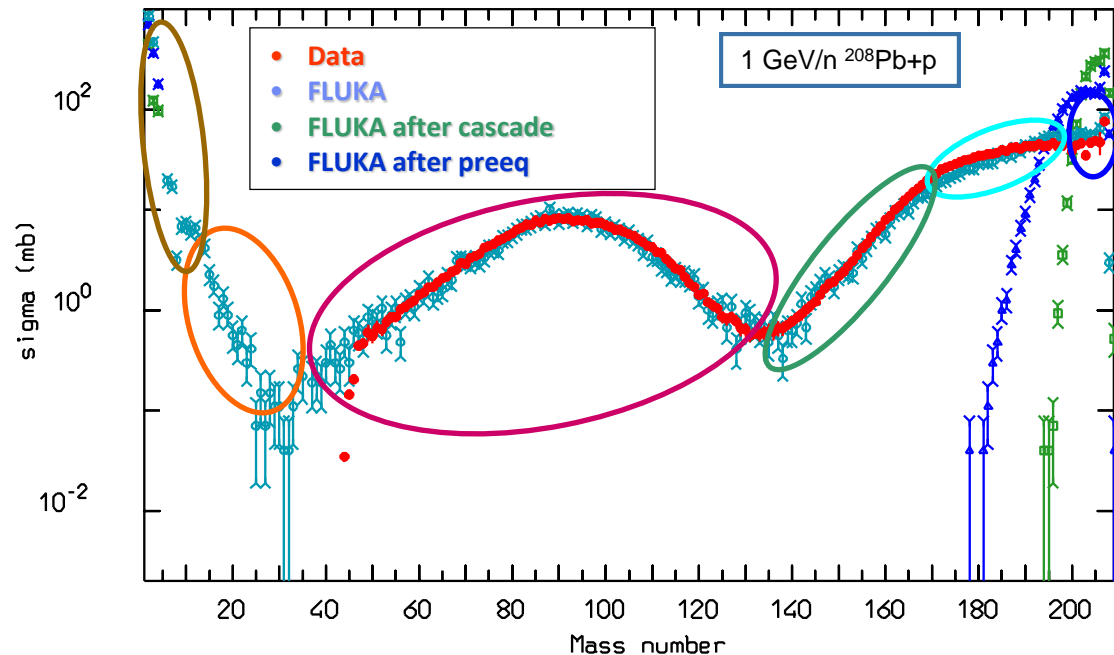
  
```

A dedicated **deuteron interaction** model is now available since FLUKA-4.2.0 and invoked by default (unless splitting is requested) !

Evaporation

In the final stage of the nuclear reaction, a nucleus of given charge (Z), mass (A) and excitation energy undergoes **evaporation** (Weisskopf-Ewing) or **fission** (Myers and Swiatecki), or **fragmentation** (Fermi break-up for $A < 18$), and γ de-excitation.

Pb – PROTON



Inclusive fragment production

Points: exp. data (T. Enqvist, Nucl. Phys. A 686 (2001) 481)

The evaporation of heavy fragments (up to $A=24$) has to be activated when residual nuclei are of interest:

```

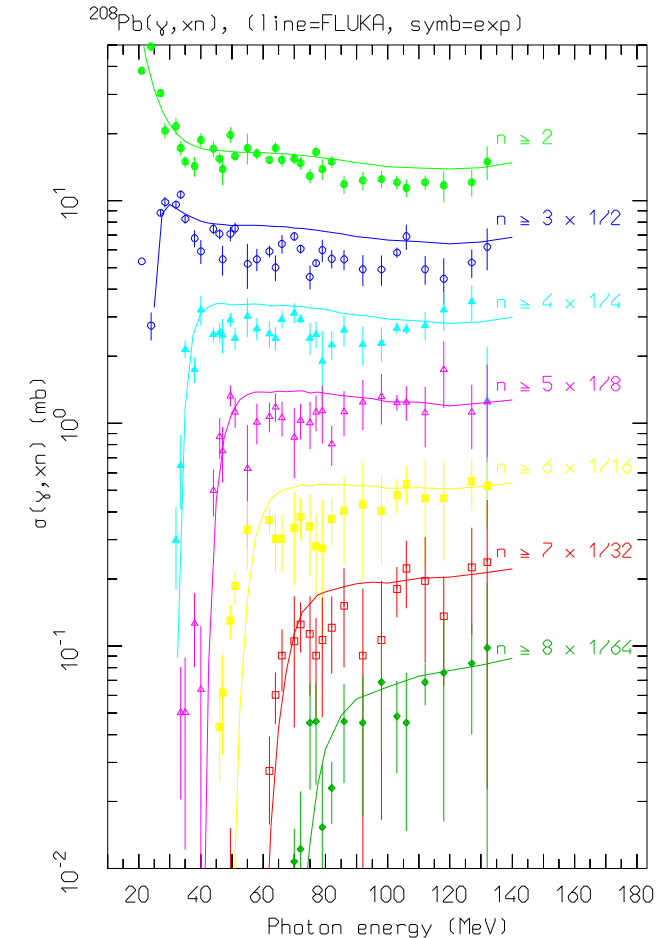
PHYSICS      Type: EVAPORAT  Model: New Evap with heavy frag
              Zmax: 0        Amax: 0
*...+...1...+...2...+...3...+...4...+...5...+...6...+...7...+...
PHYSICS      3              EVAPORAT
    
```

To be activated when relevant:

PHOTONUC	Type: ▾	All E: On ▾	
E>0.7GeV: off ▾	Δ resonance: off ▾	Quasi D: off ▾	Giant Dipole: off ▾
	Mat: COPPER ▾	to Mat: ▾	Step:
*...+...1...+...2...+...3...+...4...+...5...+...6...+...7... ▾ +...			
PHOTONUC	1	COPPER	

- The **reaction cross section** features four energy ranges:
 - Giant Dipole Resonance (6-60 MeV, stored in a special database)
 - Quasi-deuteron
 - Delta resonance
 - Vector Meson Dominance (high energy > 0.7 GeV)
- The **reaction outcome** is calculated through the IntraNuclear Cascade, pre-equilibrium and evaporation stages
- Photonuclear reactions need to be biased by the **LAM-BIAS** card (see the Biasing lecture)

$\gamma - \text{Pb}$



cross section for multiple neutron emission
data: NPA367, 237 (1981) and NPA390, 221 (1982)

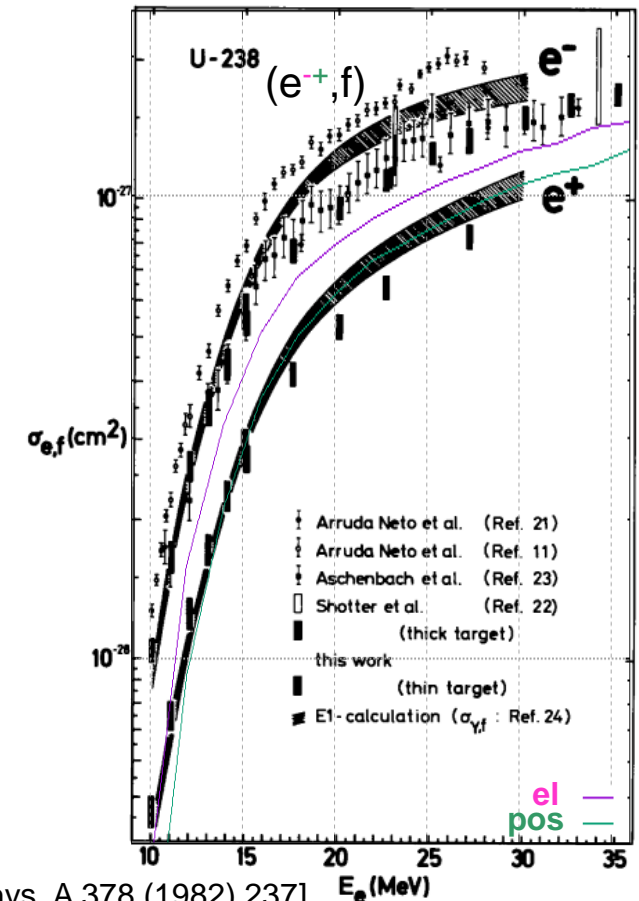
μ -A, e^- -A, e^+ -A

Virtual photon reactions are also implemented:

- muon photonuclear interactions (normally on by default, no need for the **MUPHOTON** card)
- electronuclear interactions, to be activated:

PHOTNUC	Typ: ELECTNUC	All On
E>0.7GeV: off	Δ resonance: off	Quasi D: off
	Mat: LEAD	Giant Dipole: off
	to Mat:	Step:
...+...1...+...2...+...3...+...4...+...5...+...6...+...7...+...		
PHOTNUC	LEAD	ELECTNUC

- For *electron/positron beams*, they play a role in case of thin target. As the material thickness exceeds the respective radiation length, reactions by real bremsstrahlung photons dominate.
- The card above activates automatically real photon reactions too (*no need for an additional card as in the previous slide*)

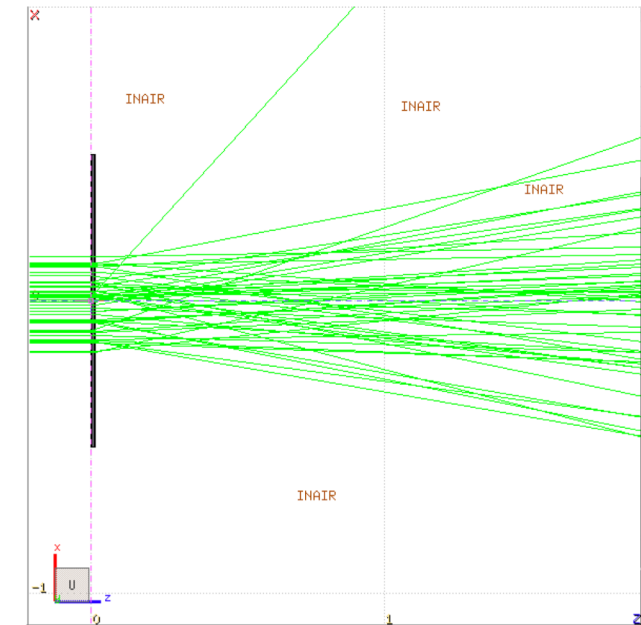


[H. Ströher et al, Nucl. Phys. A 378 (1982) 237]

Exercise : Thresholds

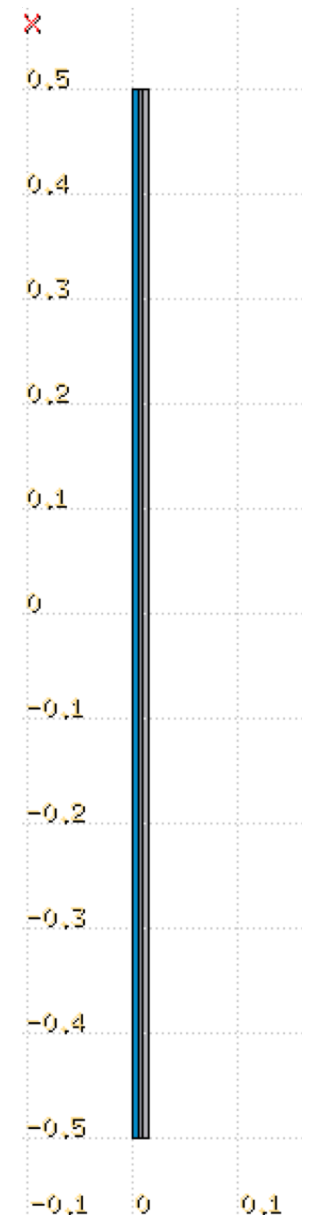
Aim of the exercise:

- Examine the effect of setting different threshold values
- Further interaction with the FLUKA manual
- Practice the use of preprocessor directives
- Strengthen plotting skills



Input file

- 10 MeV electron beam
 - Circular beam with 2 mm radius
- 5-mm radius target split in three layers, each 50 μm thick
 - Set to $\text{H}_2\text{O} - \text{Pb} - \text{Al}$
- Thin layers require high tracking precision. Thus, we set
 - **DEFAULT PRECISION** (should already be there)
- Notice that three preprocessor variables are defined
 - HI-THR, LOW-THR, VLOW-THR
- **USRBIN** scoring DOSE over the entire target
 - 1 μm bins in z, 1 μm bins in R, unformatted unit 55



Add EMFCUT and DELTARAY cards

- Set both production and transport thresholds in all materials
 - Hint: when specifying the range of materials/regions, use @LASTMAT/@LASTREG as needed to refer to the last material or region, respectively

- Threshold cases:

```
#if HI-THR
```

```
    photons: 1 keV ,      electrons: 1 MeV kinetic energy,      FUDGEM=1
```

```
#elif LOW-THR
```

```
    photons: 1 keV ,      electrons: 100 keV kinetic energy,      FUDGEM=1
```

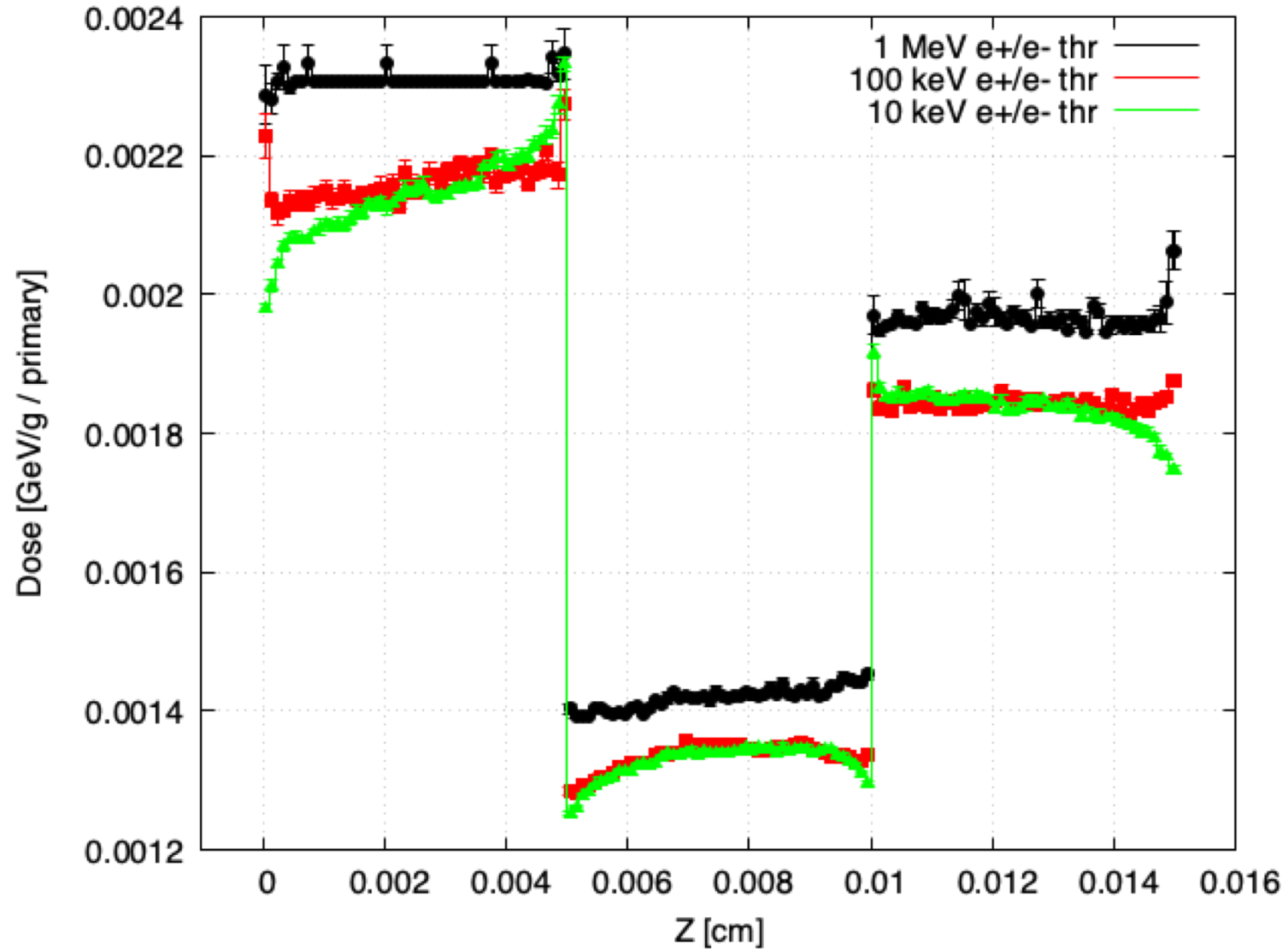
```
#elif VLOW-THR
```

```
    photons: 1 keV ,      electrons: 10 keV kinetic energy,      FUDGEM=0.5
```

```
#endif
```

- Note that the electron threshold is 100 keV in case of **PRECISION**
- Reminder: stopping powers and ranges for electrons, protons, and He ions are available on the NIST webpage: <https://physics.nist.gov/PhysRefData/Star/Text/intro.html>

Result : Compare thresholds



CURSO INTRODUTÓRIO



23 DE JANEIRO
A 8 DE MARÇO
DE 2023

FLUKA

FLUKA

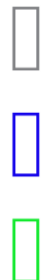
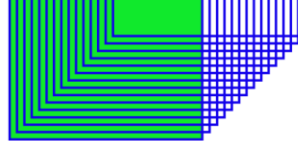
FLUKA

FLUKA

FLUKA

AULA 09 Cartões de transporte e física

Obrigado pela participação



Código Monte Carlo de interação e transporte de partículas

01

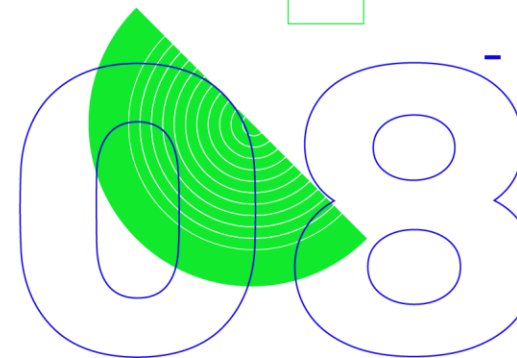
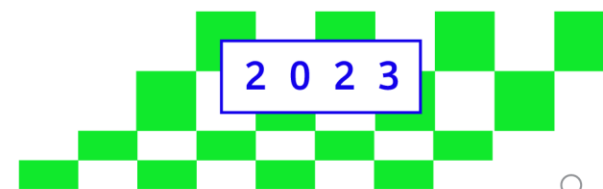
02

03

04

05

06



01

02

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