Ionization and Transport

OMA School on Monte Carlo Simulations

Outline

We will give a general overview of a few topics:

- **Ionization**: energy loss of charged projectiles in collisions with electrons of medium.

- **Deflections** of charged projectiles with screened Coulomb potential of nuclei (Multiple Coulomb scattering).

- **Transport**: general picture + thresholds.

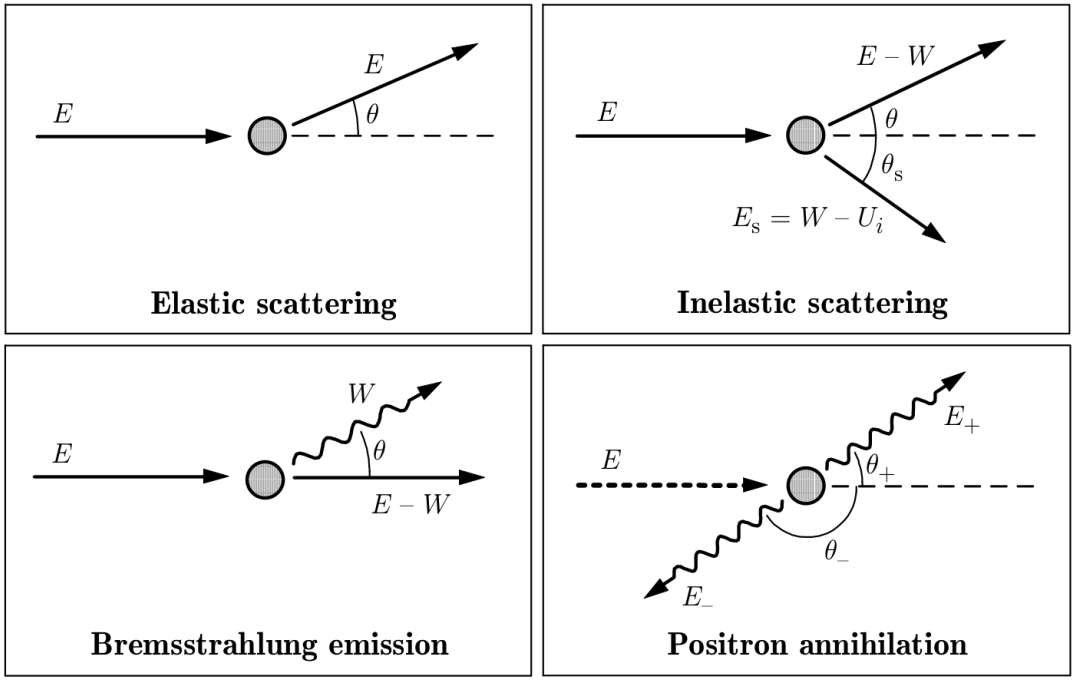
- **Biasing:** a few notions + examples.

- **Anticipated scoring example:** Compton anti-coinc shield

Disclaimer: no claim of completeness, we provide only a few general ideas.
More detail: FLUKA manual + beginner course.
Even more detail: FLUKA advanced course.

Brief reminder

From yesterday's lecture on PENELOPE, electron/positron interactions:



Additionally, in FLUKA: electronuclear reactions (next rel), high-ene corr. to Bremsstrahlung.
Not for this school, but keep in mind the tool is at your disposal.

In this lecture: FLUKA's approach to the first row, not only for e^-/e^+, but for any charged projectile (!)

Whereas PENELOPE is restricted to e^-, e^+, photons, FLUKA has to be more general.

PENELOPE is committed to energies up to 1 GeV
FLUKA up to 10 PeV

In an ideal world...

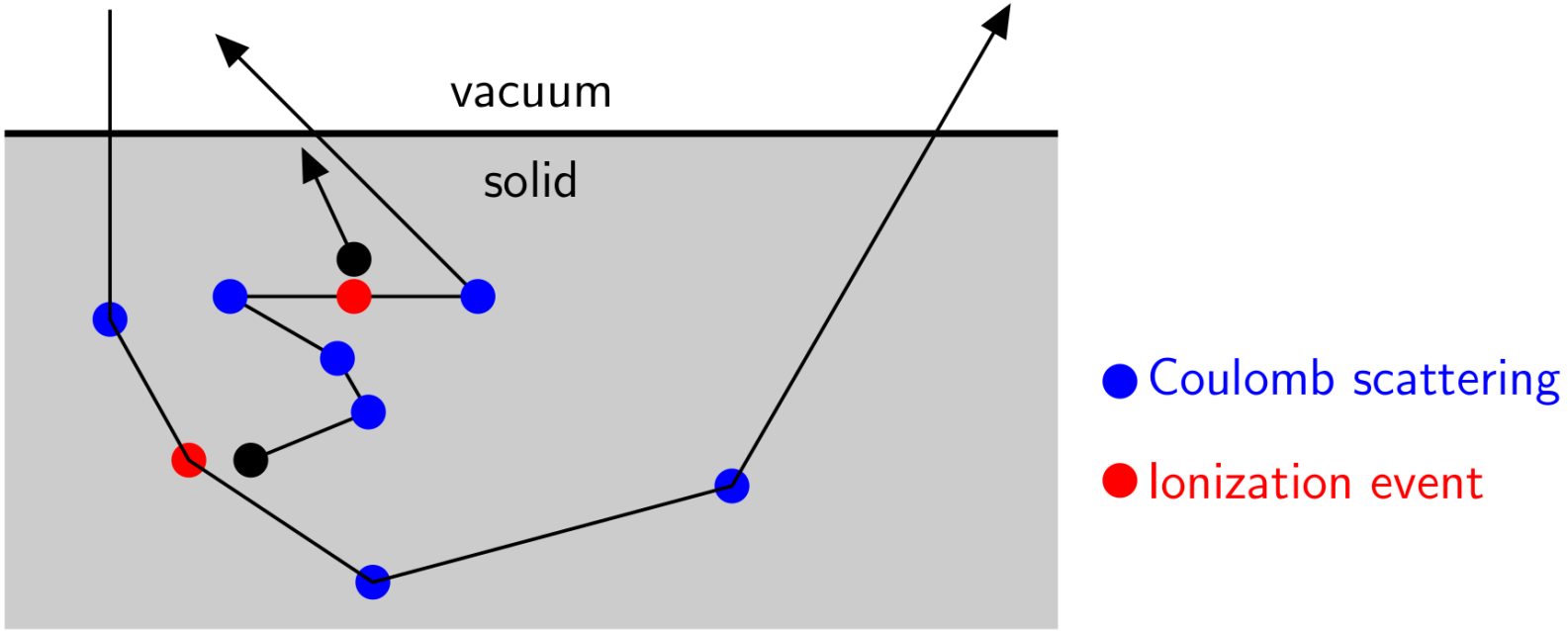
Main idea of MC: simulate ensemble of particle trajectories + statistical analysis of desired observables.

Differential cross section (dxs) for each type of event → T, angle.

E.g. only elastic (potential) scattering and ionization losses.

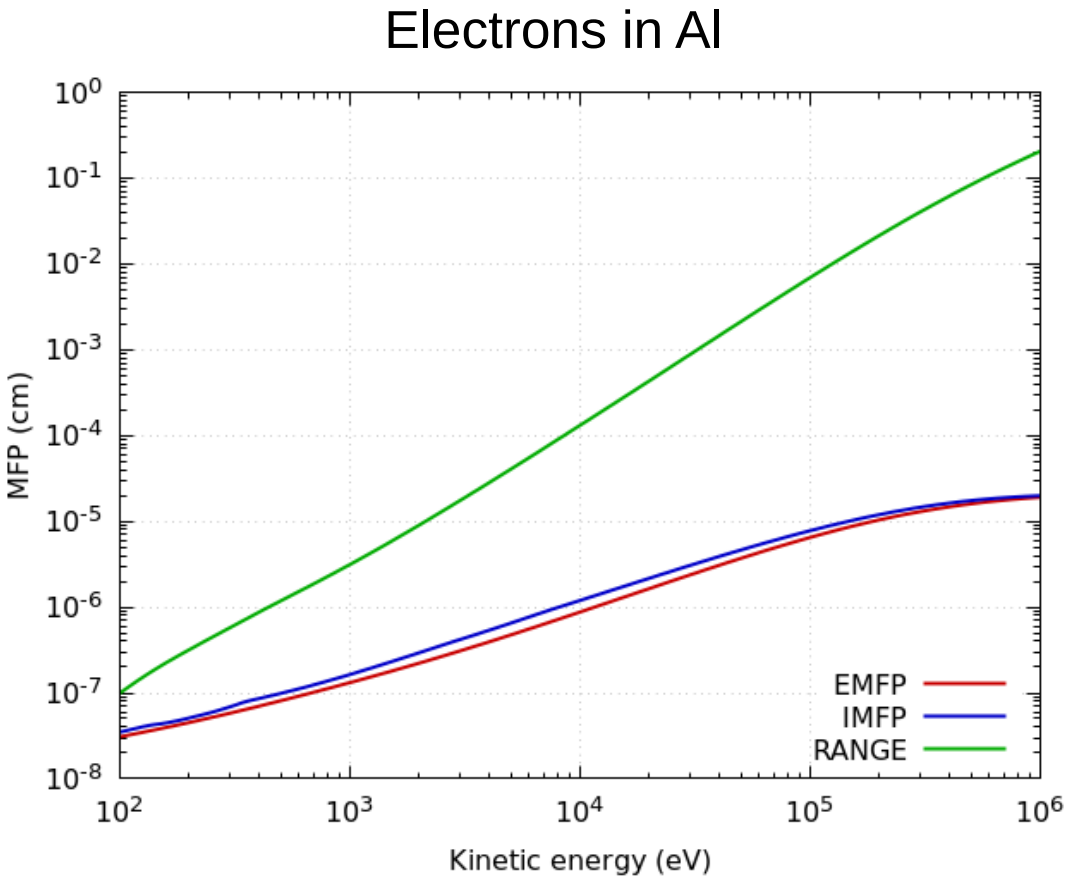
Ideally one would simulate particle trajectory event by event (detailed simulation).

Take step, decide interaction type, sample from dxs, update ene/dir. Loop.



But that is often an overkill!

How many interactions should be sampled per primary?
Rough estimate of number of collisions: Range/IMFP.



For 1-MeV electron: **~<u>10000</u>** events (!).

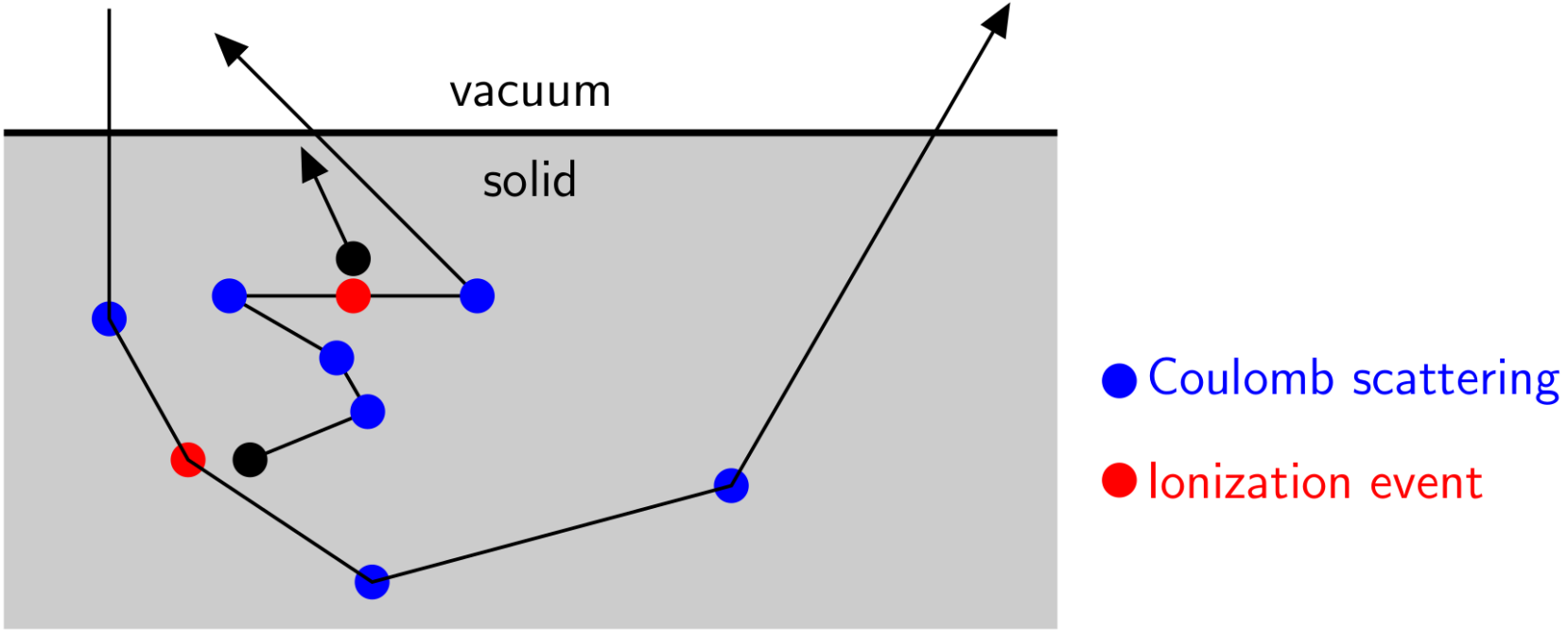
Deflections and energy losses are too frequent to simulate individually.

Sensible approach

Condensed schemes are a practical necessity to keep simulation time short.

Main idea:

- Sample individual interactions only when effect is large
- Account for global effect of small losses/deflections in an effective way (to be discussed here) at each particle step.



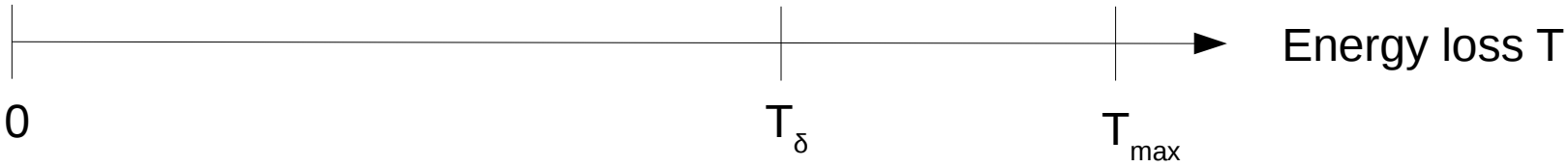
In this talk: FLUKA's approach to this condensed scheme for ionization and elastic (potential) scattering.

1/4 - Ionization energy losses

Energy losses of charged projectiles in collisions with the electrons of the medium

Ionization energy losses in FLUKA

2 different treatments: small vs large energy losses.

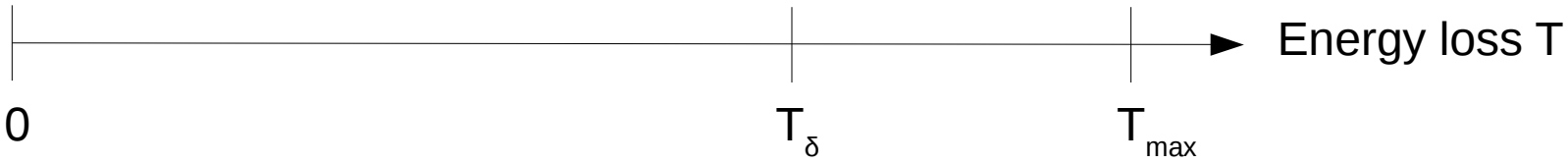


$T>T_\delta$: sampled explicitly from corresponding dxs, knock-on electron (δ ray) added to stack of particles to simulate.

$T<T_\delta$: no explicit energy loss sampling / secondary electron tracking.
Aggregate effect of many small losses described continuously during particle step.

T_δ : threshold above which it is meaningful to do detailed sampling of knock-on electrons.
δ-ray production threshold.

$T>T_{\delta}$: Discrete losses



- Large loss T transferred to a target electron.
- Invested in releasing and 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).
- … how is T sampled?

T>Tδ: detailed sampling

Depending on projectile, energy loss sampled from:

- Møller scattering (e^-)

$$\left(\frac{d\sigma}{dT_e}\right)_{Mo} = \frac{2\pi r_e^2}{\beta^2}\frac{m_e c^2}{T_e^2}\left[1+\left(\frac{T_e}{T_0 - T_e}\right)^2+\left(\frac{\gamma - 1}{\gamma}\right)^2\left(\frac{T_e}{T_0}\right)^2 - \frac{2\gamma - 1}{\gamma^2}\left(\frac{T_e}{T_0 - T_e}\right)\right]$$

- Bhabha scattering (e^+)

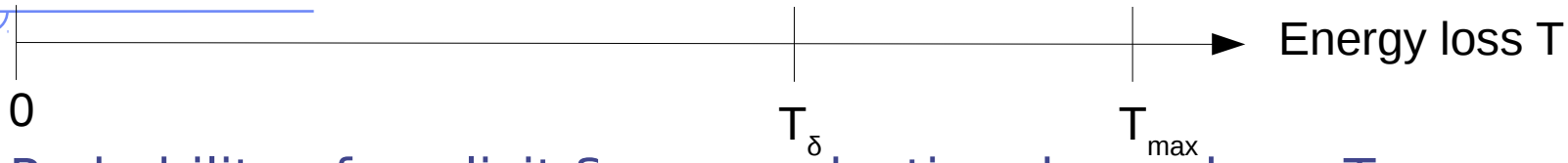
$$\left(\frac{d\sigma}{dT_e}\right)_{Bh} = \frac{2\pi r_e^2}{\beta^2}\frac{m_e c^2}{T_e^2}\left\{1 - \frac{\gamma^2 - 1}{\gamma^2}\frac{T_e}{T_0} + \frac{1}{2}\left(\frac{\gamma - 1}{\gamma}\right)^2\left(\frac{T_e}{T_0}\right)^2 - \frac{\gamma - 1}{\gamma + 1}\frac{T_e}{T_0}\left[\frac{\gamma + 2}{\gamma} - 2\frac{\gamma^2 - 1}{\gamma^2}\frac{T_e}{T_0} + \left(\frac{\gamma - 1}{\gamma}\right)^2\left(\frac{T_e}{T_0}\right)^2\right] + \left(\frac{\gamma - 1}{\gamma + 1}\right)^2\left(\frac{T_e}{T_0}\right)^2\left[\frac{1}{2} + \frac{1}{\gamma} + \frac{3}{2\gamma^2} - \left(\frac{\gamma - 1}{\gamma}\right)^2\frac{T_e}{T_0}\left(1 - \frac{T_e}{T_0}\right)\right]\right\}$$

- δ ray production by spin 0 or ½ proj (charged hadrons, muons).
- Mott for heavy ions.

T is sampled from these differential xs according to projectile type.

All moments reproduced: avg energy loss, fluctuations, etc

δ-ray production threshold



- Probability of explicit δ-ray production depends on T_δ (δ-ray production threshold).

- FLUKA sets default values, which can be overridden (rule of thumb below):

  - Electrons,positrons: EMFCUT card with PROD-CUT sdum;
  - Charged hadrons/muons: set by DELTARAY card:

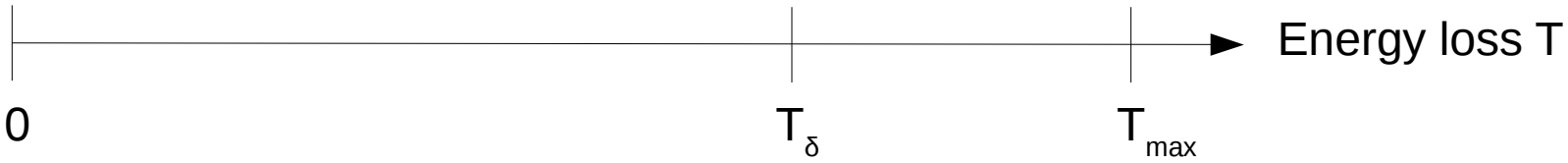
```
* ..+....1....+....2....+....3....+....4....+....5....+....6....+....7..
EMFCUT     ElePosiTh   WHAT(2)   WHAT(3)      Mat1      Mat2      StepPROD-CUT
```

```
* ..+....1....+....2....+....3....+....4....+....5....+....6....+....7..
DELTARAY     δThresh      Ntab      Wtab      Mat1      Mat2      Step PRINT
```

where:

δ_{Thresh}	production threshold, (from materials Mat1 to Mat2)
N_{tab}, W_{tab}	control the accuracy of dp/dx tabulations (advanced user)
PRINT	if set (not default), dp/dx tabulations are printed on stdout

Continuous losses ($T<T_\delta$)



- Cross sections go like T^{-2} → Small losses are frequent
  → (too much CPU effort to sample them individually).

- Idea: how to account for the aggregate effect of these small losses below the production threshold as a continuous energy loss at each particle step?

- For a given step, the continuous energy loss can be calculated by
  - determining the mean energy loss below the production threshold according to restricted stopping powers (we now briefly show how)
  - and by applying energy loss fluctuations on top to account for the stochastic nature of energy loss (we now briefly show how)

- The energy deposition due to the continuous energy loss of charged particles is local (i.e. energy not carried away by secondary particles)

Charged particle dE/dx: Bethe-Bloch

Spin 0
(spin 1/2 is similar):

~ln beta^{4}gamma^4 relativistic rise

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

- n_e : electron density of target material (~ Z/A);
- I : target mean excitation energy, material-dependent;
- T_{max}: maximum energy transfer to an electron (from kinematics)

(Bethe formula derived within 1st Born approx: 1st-order perturbation theory and plane waves, assuming v>>v_e)

To improve shortcomings, a series of corrections are used:

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

Corrections to dE/dx:

High energies: *δ* is the so called ***density correction,*** extensively discussed in the literature and connected with medium polarization

Low energies: *C* is the ***shell correction***, which takes into account the effect of atomic bounds when the projectile velocity is no longer much larger than that of atomic electrons and hence the approximations under which the Bethe-Bloch formula has been derived break down. This correction becomes important at low energies.

Higher order: L_1 is the ***Barkas (z^3)*** correction responsible for the difference stopping power for particles-antiparticles, **L_2** is the ***Bloch (z^4)*** correction (both no longer discussed in the following)

Low energies: effective charge. Partial neutralization of projectile charge due to electron capture, particularly effective at low energies.

Bethe formula gives stopping power (average energy loss per unit step length).

But what does the distribution of energy losses as a function of the step length look like?

General culture: Landau distribution

Lev Landau (1944), assuming:

- No Bremsstrahlung, only ionization events.
- Short path lengths ↔ $\Delta << E$, where Δ = total energy loss.
- Hard events via Thomson cross section:

$$\mu(W) = \mathcal{N} Z \frac{2\pi Z_0^2 e^4}{\mathrm{m_e} v^2} \frac{1}{W^2} \qquad \text{for } W > W_\mathrm{c}$$

- Distant collisions (small losses): Bethe stopping formula, no fluctuations.
- $T_\delta \rightarrow$ infinity (Laplace transform involved)

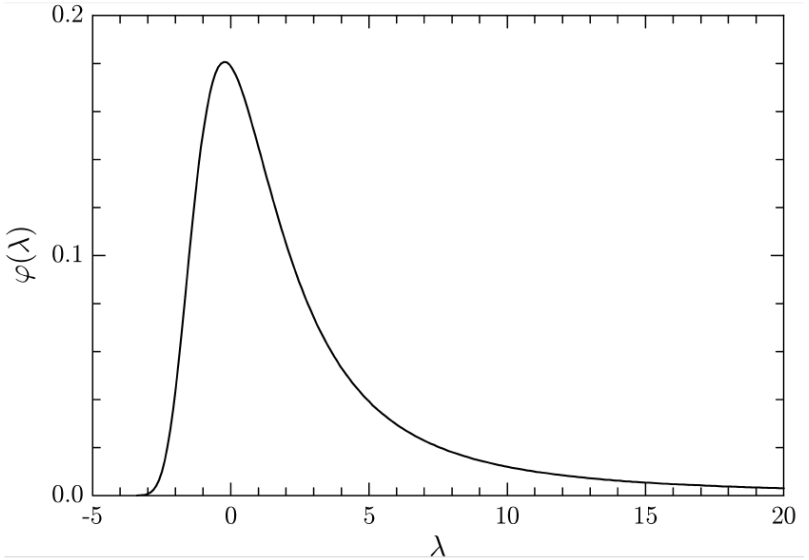
With all these approximations, he derived the distribution of energy losses after the projectile has traveled path length s

$$\Phi_\mathrm{L}(s;\Delta) = \frac{1}{\xi}\varphi(\lambda)$$

$$\varphi(\lambda) = (1/\pi)\int_0^\infty \exp(-t\ln t - \lambda t)\sin(\pi t)\,\mathrm{d}t$$

$$\lambda \equiv \frac{\Delta - \xi\left[\ln(\xi/W_1) + 1 - 0.5772\right]}{\xi}$$

$$\xi \equiv s\mathcal{N} Z \frac{2\pi Z_0^2 e^4}{\mathrm{m_e} v^2}$$



FLUKA's alternative approach

Landau distribution is somewhat impractical for FLUKA purposes:

- Differences among projectiles are not resolved (Thomson W^{-2} for all projectiles)

- For distant collisions, no fluctuations.

- Delta-ray cutoff at infinity: cannot be used for too long steps or too low ene!

FLUKA's fresh approach:

- Energy-loss in collisions with e^- described by $d\sigma/dT$ (known for given projectile type)

- In a step: N small energy losses, N~Poisson.

- Aggregate energy loss in a step is sum of T~$d\sigma/dT$ where number of terms ~ Poisson.

- Mathematical machinery: sampling aggregate energy loss from cumulants of $d\sigma/dT$

$$K_1 = m_1$$
$$K_2 = \mu_2$$
$$K_3 = \mu_3$$
$$K_4 = \mu_4 - 3\mu_2^2$$

Advantages of FLUKA approach

- As opposed to Landau distribution, no assumption on dσ/dT for ionization!
- Based on general statistical properties of the cumulants of a distribution (dσ/dT)
- Cumulants and all necessary integrals can be calculated analytically and exactly *a priori* (min. CPU time);
- Applicable to any kind of charged particle, taking into account the proper spin dependent cross section for δ ray production;
- The first 6-moments of the energy loss distribution are reproduced.

Recap: continuous energy losses

Below the δ-ray threshold, energy losses are treated as "continuous", with some **special features**:

- Fluctuations of energy loss are simulated with a FLUKA-specific algorithm
- The energy dependence of cross sections and dE/dx along the step is taken into account exactly.
- User has control on dE/dx. The latest recommended values of ionization potential and density effect parameters are implemented for each element (Sternheimer, Berger & Seltzer), but can be overridden by the user (e.g. compounds) via:

```
* ..+....1....+....2....+....3....+....4....+....5....+....6....+....7..
STERNHEI          C        X0        X1         a         m        δ0 MAT
*
MAT-PROP       Gasp      Rhosc      Ion       Mat1      Mat2      Step
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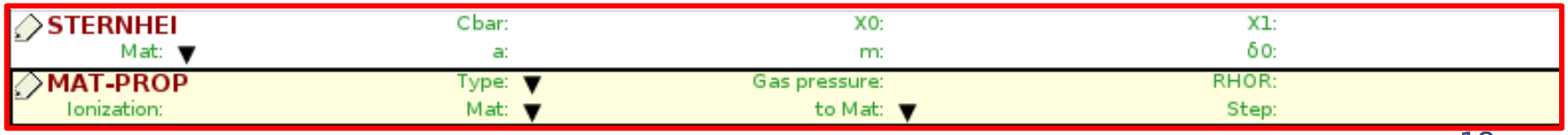
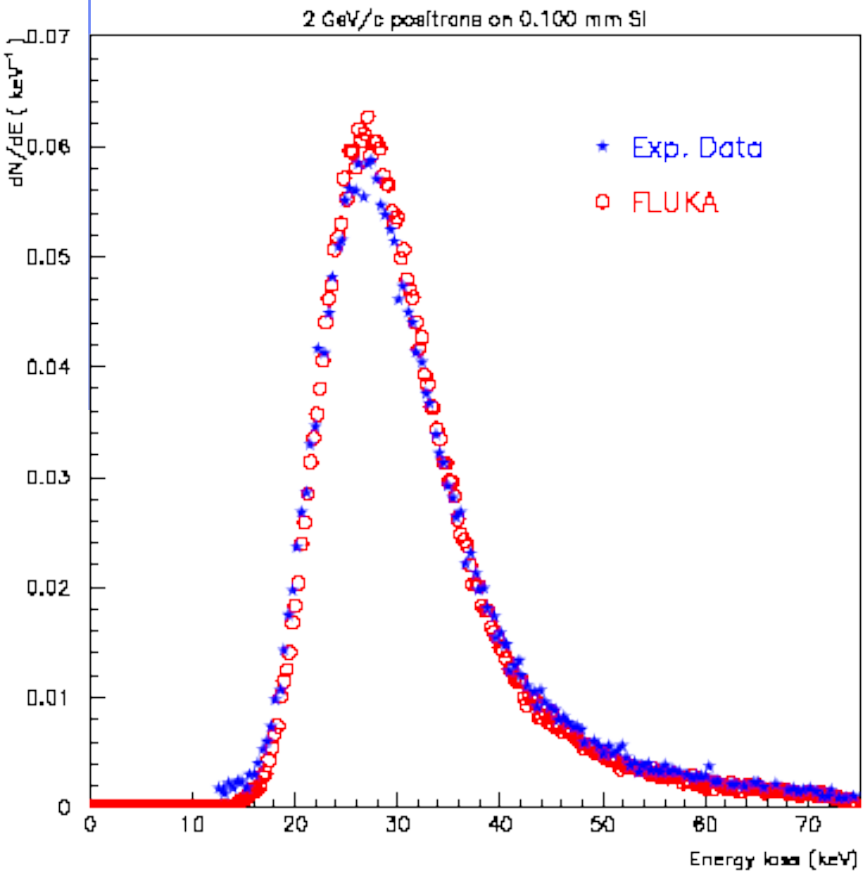
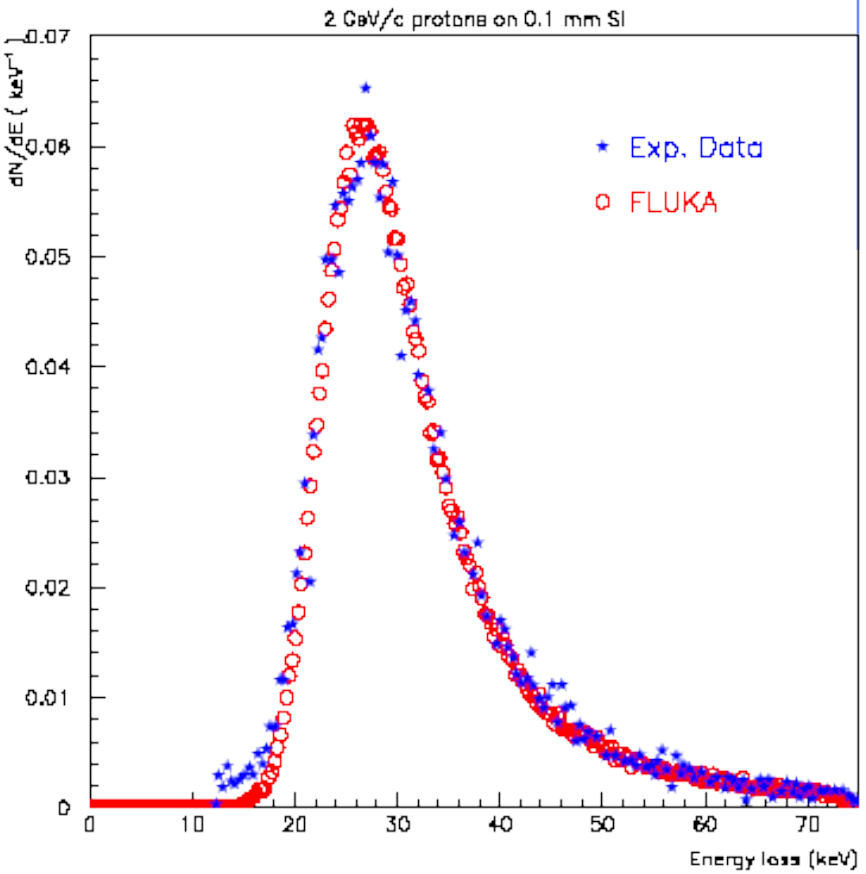


A few examples

Energy loss distributions





Experimental [1] and calculated energy loss distributions for 2 GeV/c positrons (left) and protons (right) traversing 100μm of Si

[1] J.Bak et al. NPB288, 681 (1987)

Same scheme for all charged projectiles

As discussed above, ionization energy loss scheme in FLUKA is set up in such a way that it is valid for all projectiles:

- Electrons/positrons
- Charged hadrons
- Muons
- Heavy Ions

δ

All share the same approach!

… but some extra features are needed for Heavy Ions

Heavy ions

Description of energy losses is more involved.

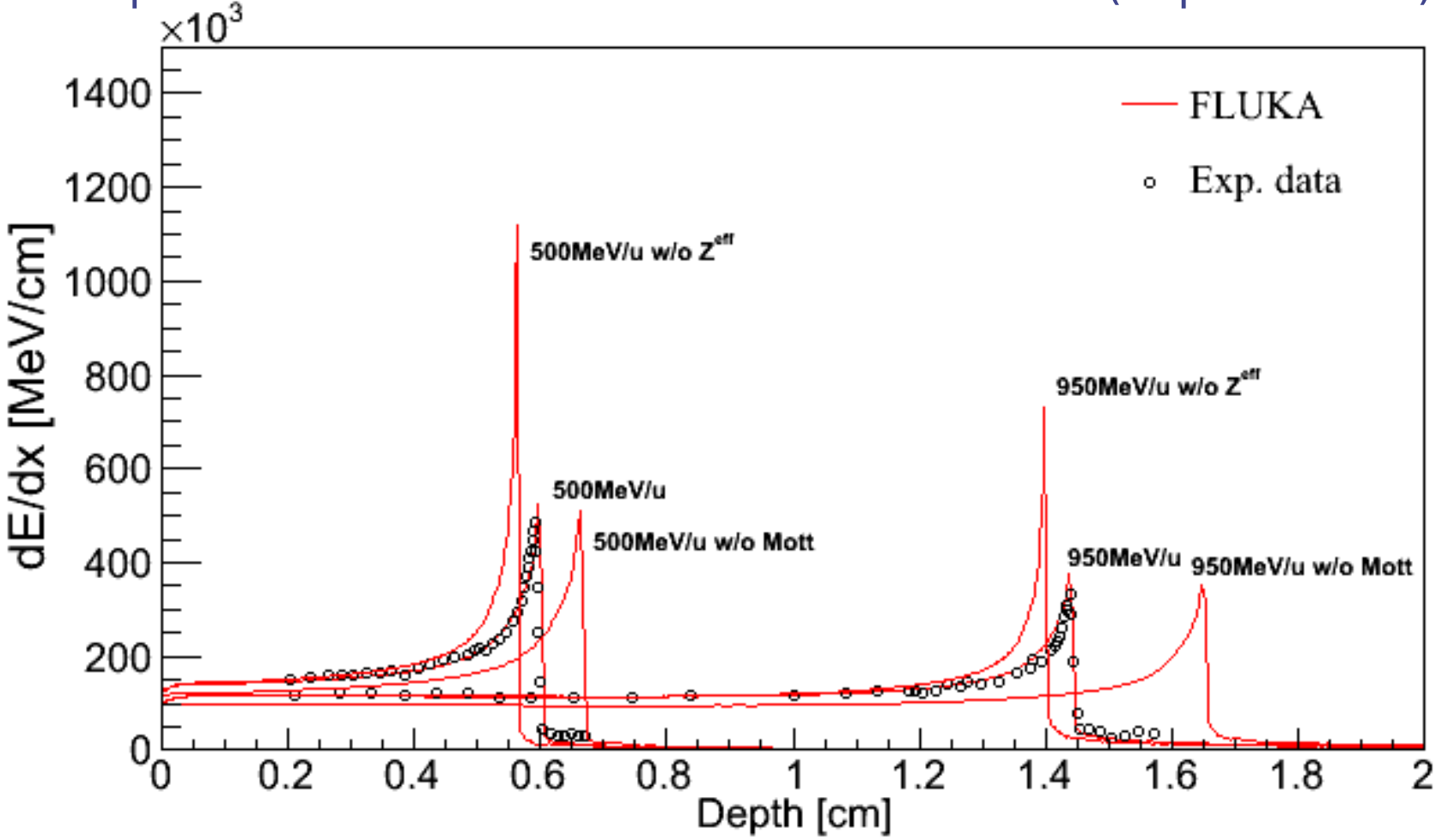
In addition to “normal” first Born approximation (Bethe-Bloch formula)

- Effective charge (up-to-date parameterizations)
- Charge exchange effects (dominant at low energies, ad-hoc model developed for FLUKA)
- Mott cross section.
- Nuclear form factors (of projectile ion!).
- Direct e+/e- production.

Heavy ions

Without discussing the corrections, we show their effect and how things can go wrong if care is not taken:

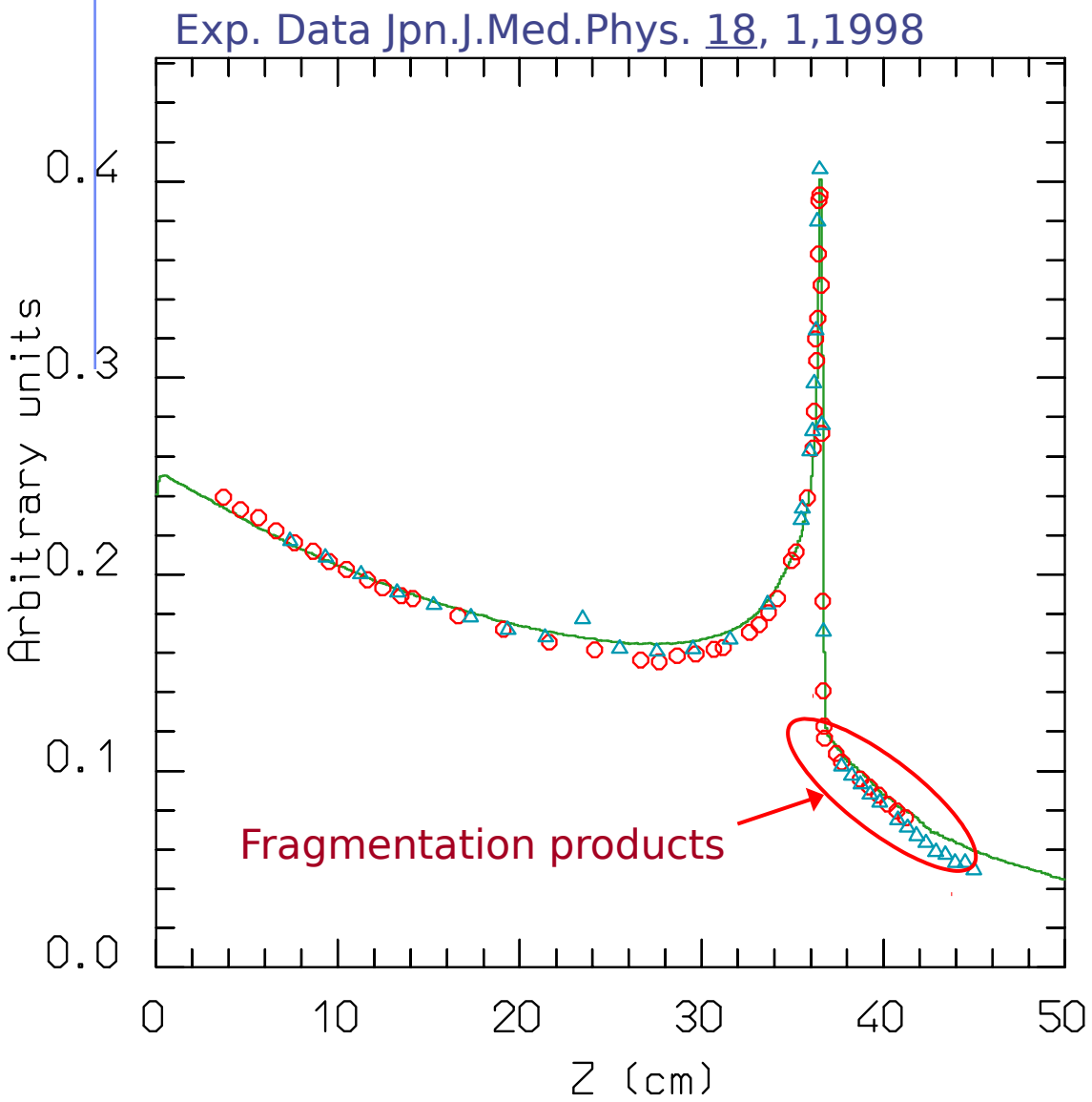
Depth-dose distribution of ^{238}U beam in steel (exp data GSI).



Exaggerated case (wouldn't be as dramatic for ^{12}C)

Bragg peak: ^{20}Ne @ 670 MeV/n

A few examples of energy deposition by heavy ions in FLUKA

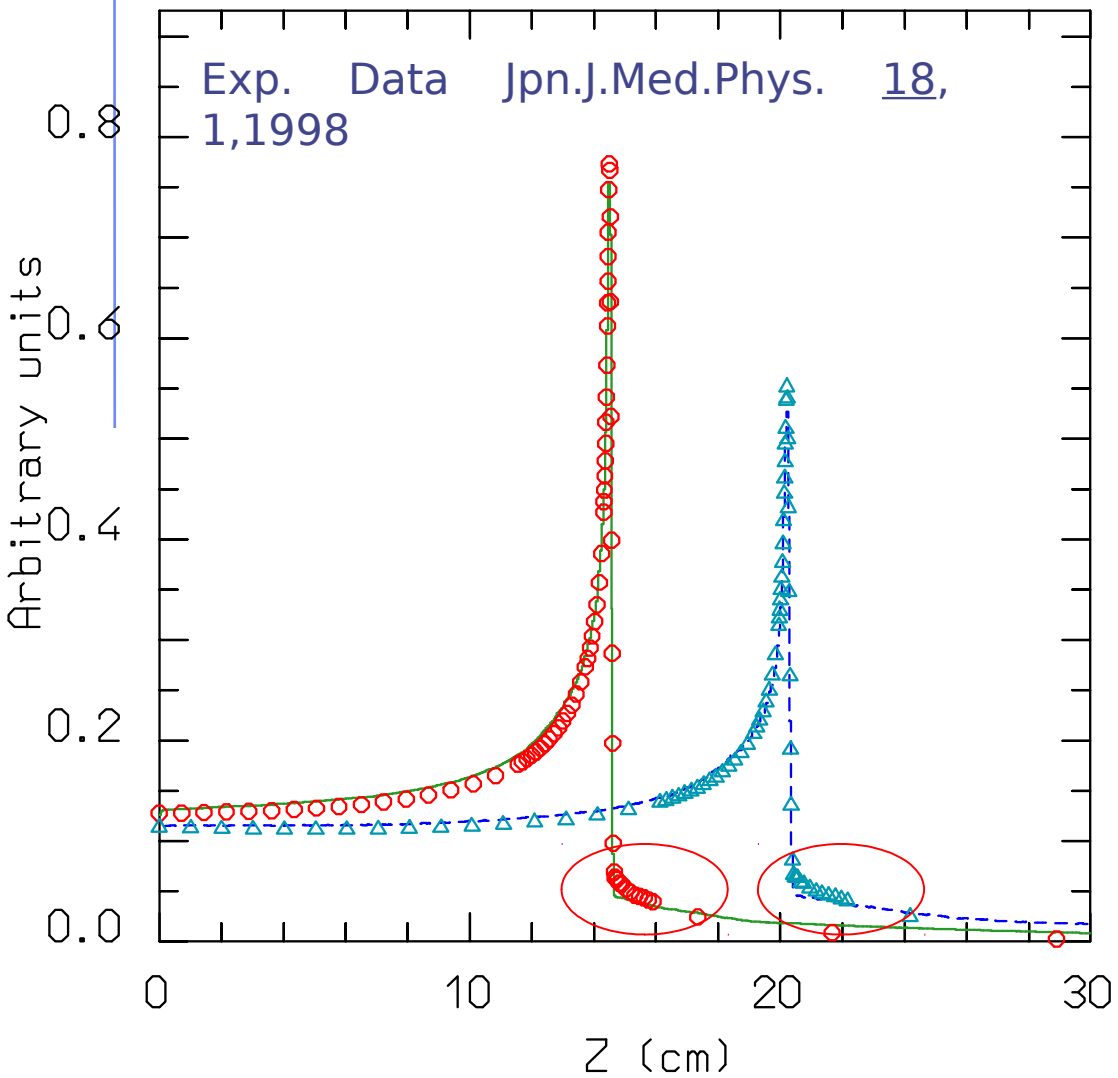


Dose vs depth distribution for 670 MeV/n ^{20}Ne ions on a water phantom.

Solid line is the FLUKA prediction. The symbols are exp data from LBL and GSI.

Tail due to fragmentation products (talk tomorrow).

Idem for ^{12}C



Dose vs depth distribution for 270 and 330 MeV/n ^{12}C ions on a water phantom.

The full green and dashed blue lines are the FLUKA predictions.

The symbols are exp data from GSI.

Nuclear stopping power

- Besides collisions with target electrons, charged projectiles undergo Coulomb scattering with atomic nuclei
- The resulting energy losses, called nuclear stopping power, are smaller than the atomic ones, but are important for
  - Heavy particles (i.e. ions)
  - Damage to materials:
    - Non-Ionizing Energy Loss (NIEL)
    - Displacements per Atom (DPA)

Scoring built-in.

1/4 - Summary

- We have discussed two separate treatments for ionization energy losses in FLUKA: discrete vs continuous.
- Discrete losses (above delta production threshold) sampled individually.
- Continuous losses described effectively along particle step. First 6 moments of energy-loss distribution reproduced thanks to FLUKA's fresh approach via cumulants of dσ/dT.
- Approach is set up in such a way that it works for all charged projectiles considered in FLUKA.
- Extra effort for ions leads to good agreement with exp.

2/4 - Transport thresholds

Transport threshold

For practical reasons, in a MC simulation we do not follow particles until they stop.

In practice, we follow particles until their energy drops to/below a preset transport threshold

Transport threshold: Kinetic energy below which a particle track is no longer sampled.

What happens with the particle's energy?

Particle (and its energy) is deposited on the spot (for electrons) or ranged out (for heavier projectiles).

Particle transport threshold

```
*  ..+....1....+....2....+....3....+....4....+....5....+....6....+....7..
PART-THR       Thresh      Part1      Part2      Step
```

PART-THR Type: Momentum p: Part: to Part: Step:

Fluka name	Fluka number
4-HELIUM (1)	-6
3-HELIUM (1)	-5
TRITON (1)	-4
DEUTERON (1)	-3
HEAVYION (1)	-2
OPTIPHOT	-1
RAY (2)	0
PROTON	1
APROTON	2
ELECTRON	3
POSITRON	4
NEUTRIE	5
ANEUTRIE	6
PHOTON	7
NEUTRON	8
ANEUTRON	9
MUON+	10
MUON-	11
KAONLONG	12
PION+	13
PION-	14
KAON+	15
KAON-	16
LAMBDA	17
ALAMBDA	18
KAONSHRT	19
SIGMA-	20
SIGMA+	21
SIGMAZER	22
PIZERO	23
KAONZERO	24
AKAONZER	25

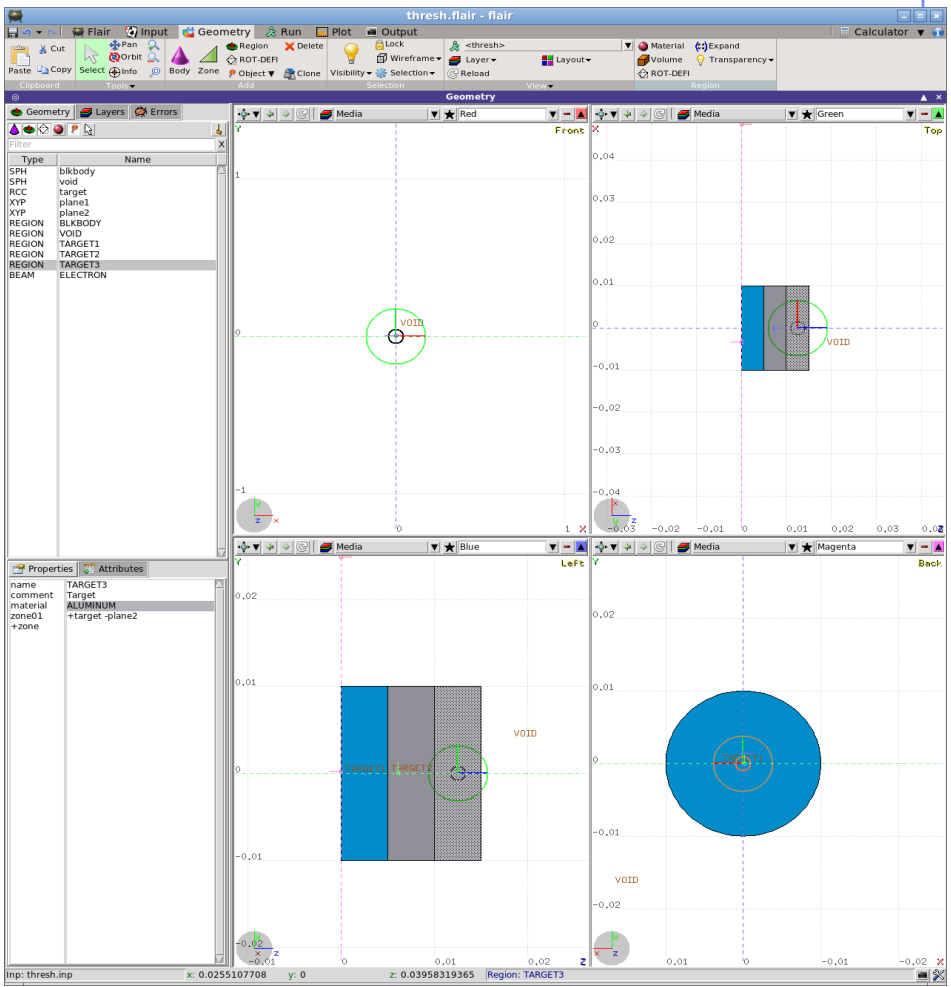
- Hadron and muon transport thresholds are set with PART-THR
- The neutron threshold (rounded to closest group boundary), recommended to leave at the default value (1 x 10^{-5} eV)
- For photons, electrons, and positrons: EMFCUT (see the manual for details).

Threshold tuning example

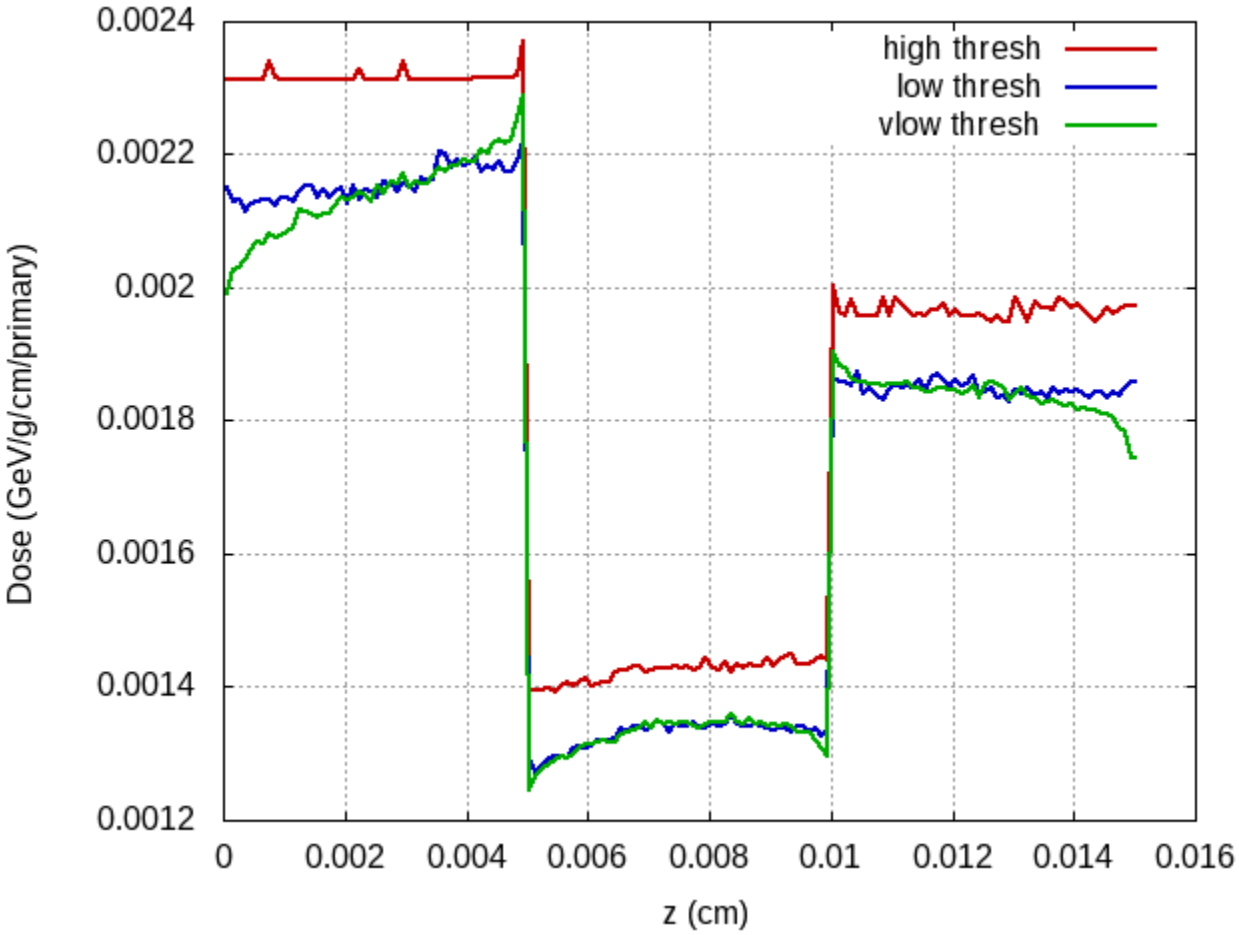
3 thin layers: water, lead, aluminum (50 um each)

10 MeV electron beam from the left

Thresholds: 10 keV, 100 keV, 1 MeV



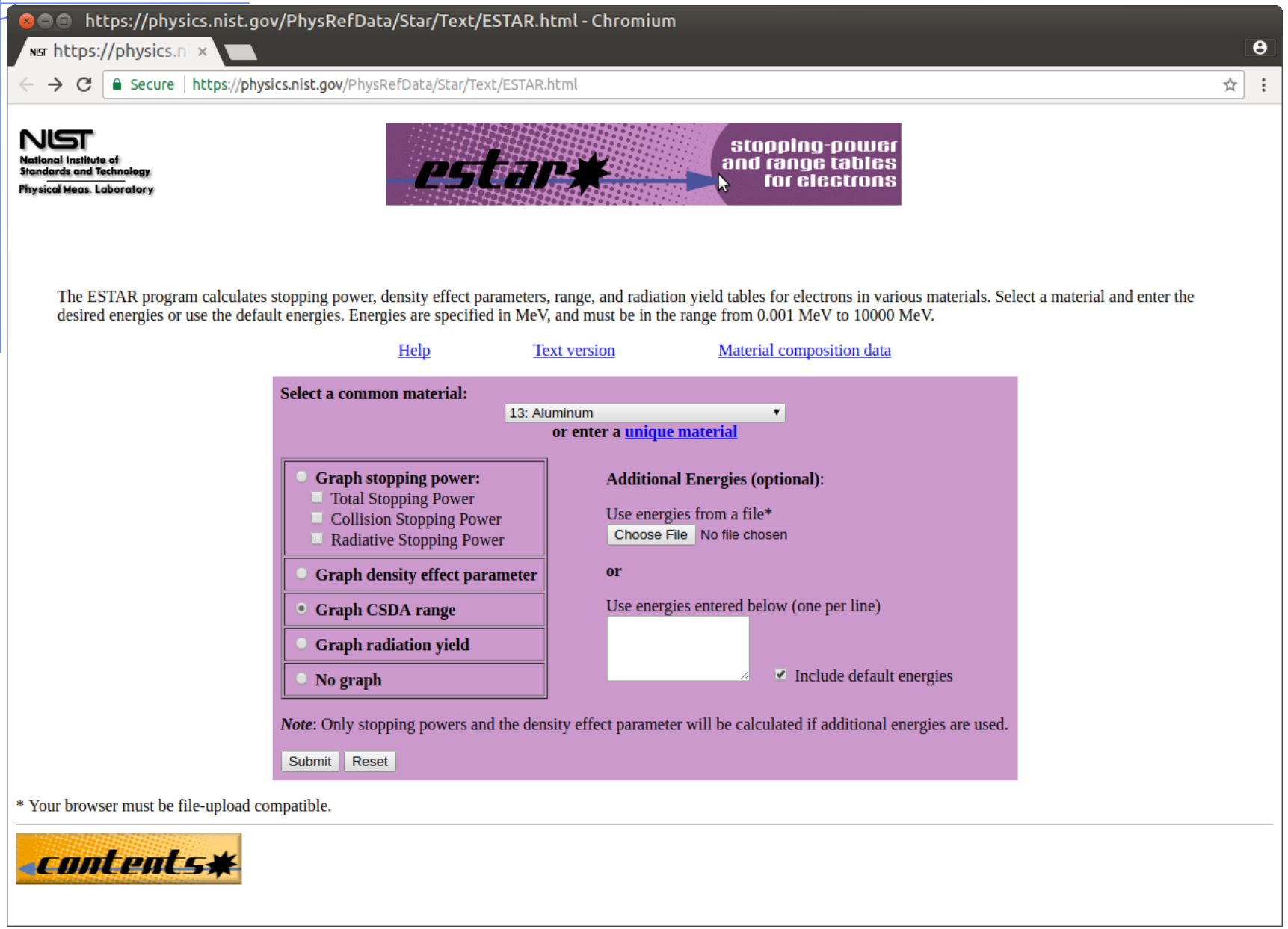
Threshold tuning: exercise care!



The 10 keV threshold is most accurate.
The 100 keV threshold is a good compromise if you just want an average value.
The 1 MeV threshold is too coarse an approximation.

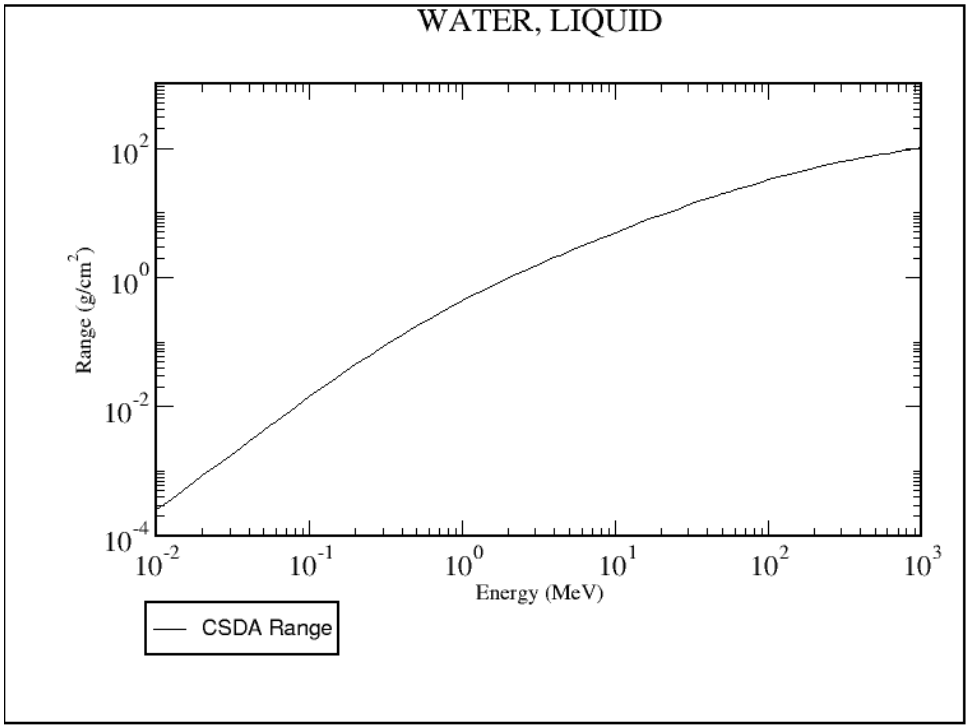
General guideline: inspiration from CSDA range

CSDA range


https://physics.nist.gov/PhysRefData/Star/Text/ESTAR.html - Chromium
https://physics.n
Secure | https://physics.nist.gov/PhysRefData/Star/Text/ESTAR.html
NIST
National Institute of Standards and Technology
Physical Meas. Laboratory
estar
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

CSDA range - Electrons in water

Water density: 1 g/cm^3 → We may directly read Range in cm



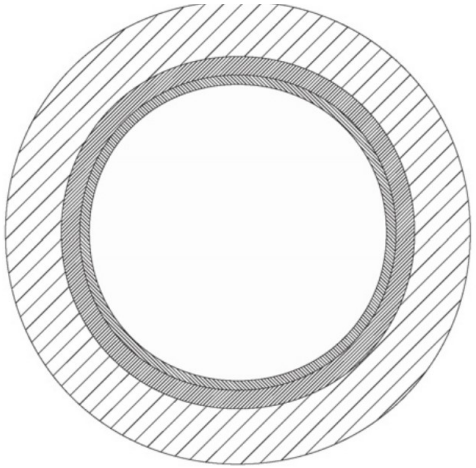
1-MeV electron can travel O(1 mm) = 1000 um
Depositing them on the spot in a ~50 um geometry is asking too much...

10 keV electron travels O(2 10^(-4)) cm = 2 um → depositing them is fine

However: if you're working with larger geometries or coarser scoring grids, can be OK!

Another example : TEPC

(T.T. Boehlen et al, Phys. Med. Biol. **56 (2011) 6545)**



Tissue-equivalent proportional counter (TEPC)

Spherical volume of ~12.7 mm diameter.

Filled with low pressure gas ~ tissue equivalent (ICRU 83)

Anode through center of sphere (surrounded by helical grid) collects charge deposited by passing ion beam as a function of impact parameter.

Idea: measure energy (and derived quantities) imparted by ions (and delta rays).

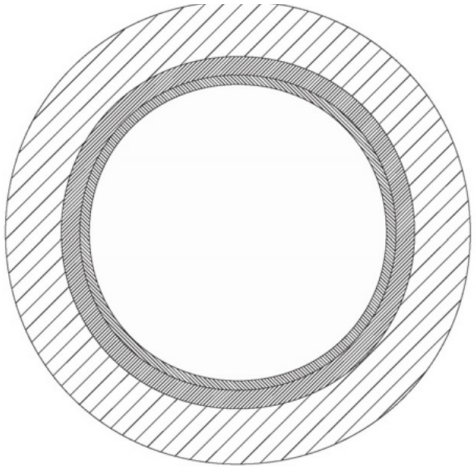
Interesting for dosimetry….

… and also a perfect opportunity for testing FLUKA ionization scheme (!)

Another example : TEPC

(T.T. Boehlen et al, Phys. Med. Biol. **56 (2011) 6545)**

- Measurements with a spherical TEPC
  - sensitive volume filled with a tissue-equivalent gas
  - Deposited dose was measured as a function of impact parameter.
- Measurements simulated with FLUKA
  - Low transport thresholds in inner volume (1 keV and, for testing only, 150 eV)



Validation with TEPC measurements

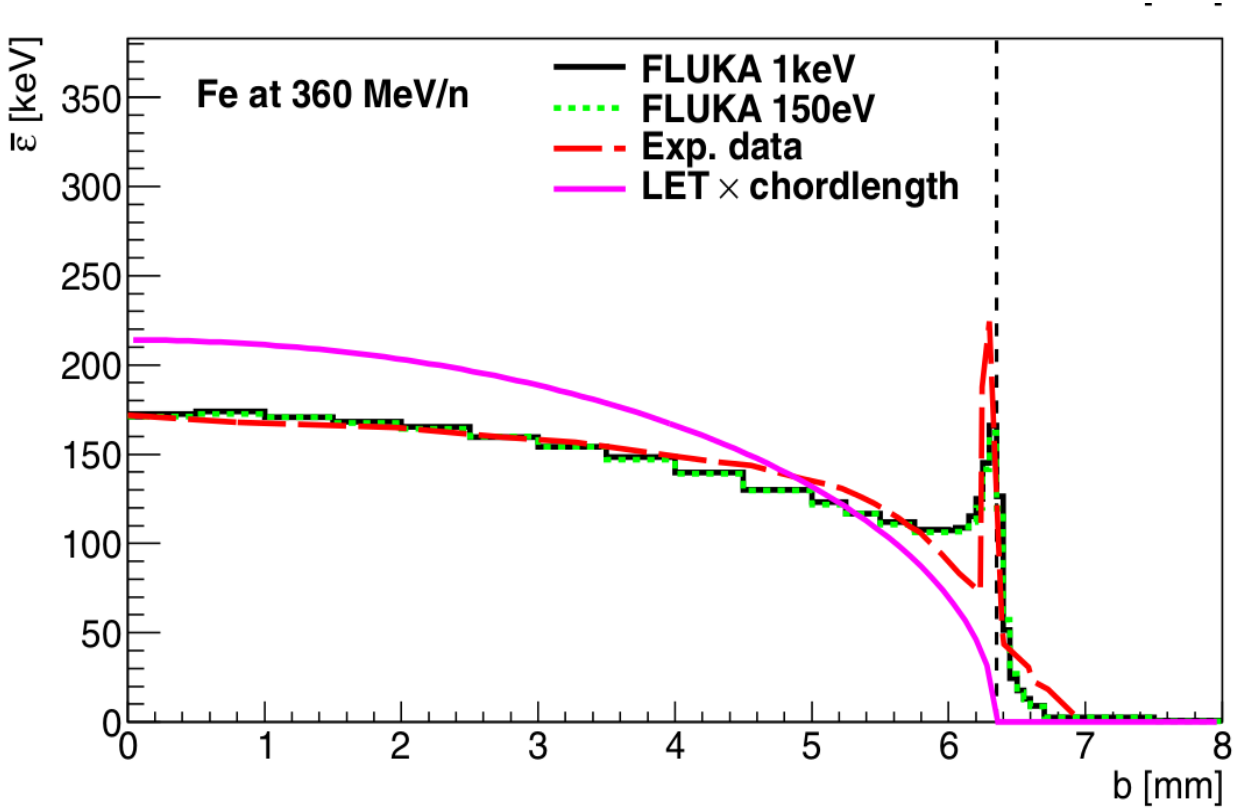


Figure 3. FLUKA simulations and measurements of the mean imparted energy $\bar{\varepsilon}$ in the TEPC cavity as a function of the impact parameter b on the detector for Ne ions at 210 MeV/n (Guetersloh *et al* 2004) and for Fe ions at 360 MeV/n (Gersey *et al* 2002). Simulations with a delta-ray production and transport threshold of 150 eV and 1 keV are shown. The unrestricted LET times the chord-length in the cavity is also shown for reference. The cavity–wall interface at 6.35 mm is marked by a vertical dashed black line.

3/4: Multiple Coulomb scattering

Description of elastic (potential) scattering with screened atomic nuclei

The problem

Besides ionization energy losses, charged particles undergo Coulomb scattering by (screened) atomic nuclei.

These collisions are also frequent.

It is often impractical to sample them all individually.

One needs effective scheme to sample global effect of Coulomb collisions along a step.

Formally: what is the distribution of angles after a given step length? What does the spatial distribution look like?

Approach: specify dxs in individual collision and solve transport equation (with reasonable approx) to obtain distribution of angles after a traveled path length.

Single scattering cross section

At the heart: assume that in a single Coulomb collision the dxs is:

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

i.e., Rutherford dxs with screening parameter accounting for:
- projectile and target atomic number.
- fraction of atomic electrons contributing to screening.

For ele/posi: additional spin-relativistic terms.
For all projectiles: possibility of accounting for nuclear form factors.

(Both imply multiplicative factors above).

Advantage: can be integrated analytically for any projectile/material.

Multiple scattering distribution

Angular distribution after a given step length?

Molière obtained it from transport equation with approximations:

- Small-angle approximation to the single-scattering cross section.
- Number of collisions is large enough (above say 10 or 20).
- ...which leads to a **minimum applicable step length (!!!!)**

Advantage: expressions are simple and depend only parametrically on projectile charge and material properties (!).

Just to see what it looks like, distribution of angles after path length t:

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

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

Main idea: every time that the projectile takes a step t, we sample the aggregate deflection from F_{Mol}.

Care gone into MCS scheme

MCS presented before allows one to sample the accumulated deflection as a function of step length.

BUT THIS IS NOT THE FULL STORY.

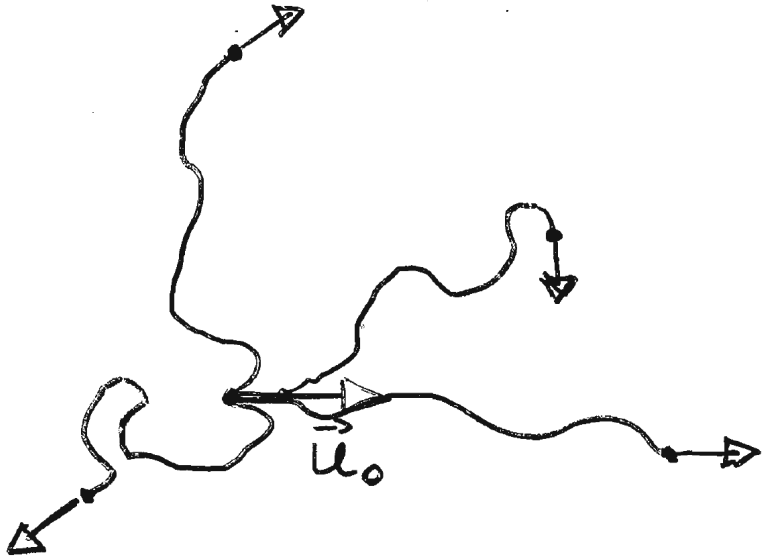
Additional machinery is required to account for spatial distribution.

Actual step is not along straight line: trajectories are “corrugated”

→ Path length correction (shortening which accounts for wiggliness)

→ Corrections in place to account for lateral displacement

→ Truncation of the step at boundaries



The FLUKA MCS

- Care is taken to maintain relationships among various quantities (correlations):

  scattering angle ↔ longitudinal displacement
  longitudinal displacement ↔ lateral displacement
  Path length correction ↔ lateral deflection

- Optionally, spin-relativistic corrections (1st or 2nd Born approximation for ele/posi), MULSOPT.

- Optionally effect of nucleus finite size (form factors) can be included (MULSOPT).

- Careful geometry tracking near boundaries.

- MCS is able to coexist with transport in magnetic fields

Switching to single scattering

- Molière theory breaks down for too short path lengths: in very thin layers, wires, or gases, it does not apply.
- In FLUKA, it is possible to switch from multiple scattering algorithm to single scattering in defined materials (control number of single-scattering steps via MULSOPT).
- Cross section as given by Molière (for consistency)

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

- Integrated analytically without approximations
- Nuclear and spin-relativistic corrections are applied a posteriori.

Combined result of model effort

- As a result, FLUKA can correctly simulate electron backscattering even at very low energies and in most cases without switching off the condensed history transport (a real challenge for an algorithm based on Moliere theory!)

- The sophisticated treatment of boundaries allows also to deal successfully with **gases**, **very thin regions** and **interfaces**;

- The same algorithm is used for charged hadrons and muons (!).

Example: electron backscattering

From light to heavy materials.
From relatively low to relatively high energy.

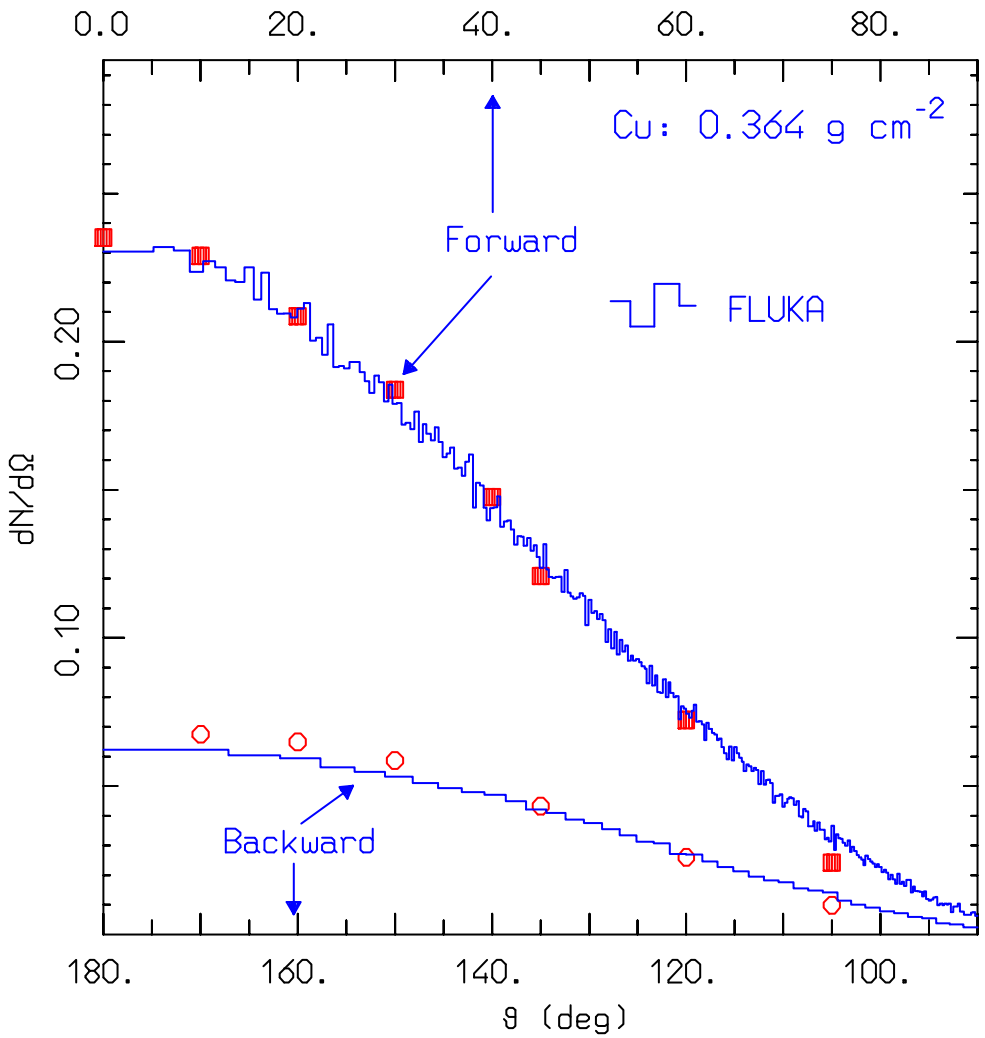
Energy (keV)	Material	Experim. (Drescher et al 1970)	FLUKA Single scattering	FLUKA Multiple scattering	CPU time single/mult ratio
9.3	Be	0.050	0.044	0.40	2.73
	Cu	0.313	0.328	0.292	1.12
	Au	0.478	0.517		1.00
102.2	Cu	0.291	0.307	0.288	3.00
	Au	0.513	0.502	0.469	1.59

Fraction of normally incident electrons backscattered out of a surface.
All statistical errors are less than 1%.

NB: last column. Single-scattering at higher energies would lead to much longer times!

Molière: example

A bit more interesting in angle-resolved terms:



1.75-MeV electrons on 0.364g/cm^2 layer of Cu foil

Transmitted (forward) and backscattered (backward) electron angular distributions

Dots: measured
Curves: FLUKA

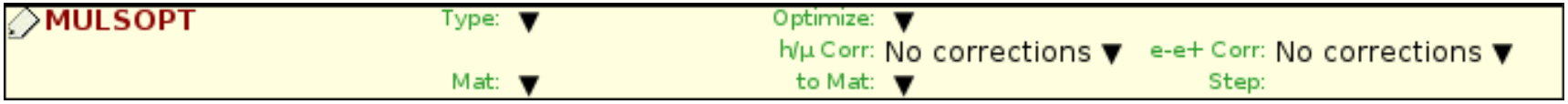
User control of MCS

- There are situations where MCS based on Molière theory (despite all efforts) is not applicable: transport in residual gas, interactions in thin geometries like wire scanners or thin slabs, electron spectroscopies at low energies, microdosimetry, etc.

- FLUKA allows user to control various MCS parameters, as well as to switch to detailed single scattering if needed (CPU demanding, but affordable and accurate e.g. at low electron energies, ***can be tuned x material!).***

- Relevant FLUKA card (to be used on a per-material basis):

```
* ..+....1....+....2....+....3....+....4....+....5....+....6....+....7..
MULSOPT        Flag1      Flag2      Flag3       Mat1       Mat2       StepSDUM
```

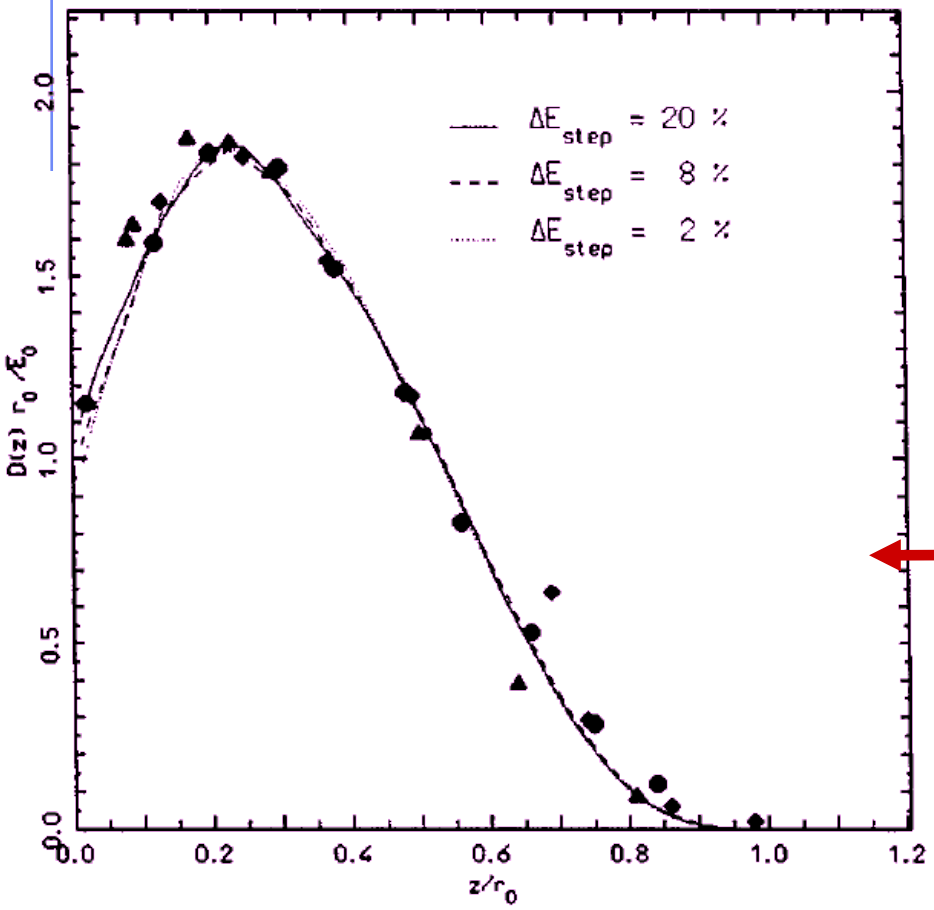


- Details in FLUKA manual, but essentially:
  - Switch to single scattering mode.
  - Spin-relativistic corrections and nucl size effects.

Maximum step size

Step size is fixed by the corresponding percentage energy loss of the particle

Thanks to FLUKA mcs and boundary treatment, results are stable vs. (reasonable) step size.
First step is where step size matters most.



Comparison of calculated and experimental depth-dose profiles, for 0.5 MeV e^- on Al, with three different step sizes. (2%, 8%, 20%)
Symbols: experimental data.
r_0 is the csda range

Step size settings for special cases

For typical applications the default 20% fractional energy loss is fine.

For special problems (i.e. thin slabs, microdosimetry, etc) 5-10% is preferred. Stability of results wrt step size should be checked.

If really needed, for EM:

```
* ..+....1....+....2....+....3....+....4....+....5....+....6....+....7..
EMFFIX          Mat1   DEstep1       Mat2   DEstep2       Mat3   DEstep3
```

For Had/μ

```
* ..+....1....+....2....+....3....+....4....+....5....+....6....+....7..
FLUKAFIX      DEstep                          Mat1      Mat2      Step
```

3/4: Summary

- We have given a general overview of FLUKA's approach to multiple Coulomb scattering.
- Based on the Moliere theory, with additional effort to maintain various correlations and careful treatment near boundaries.
- Possibility to switch to single-scattering mode for delicate situations.
- Even for electron backscattering the model performs well!

Cheat Sheet

Some of the ionization, transport, and MCS cards:

DELTARAY – Modify δ-ray production parameters (hadrons, muons)
PART-THR - Set particle transport threshold (hadrons, muons)
EMFCUT – Set δ-ray production and transport threshold (e^-,e^+)

STERNHEI - Ionization potential and density effect
MAT-PROP parameters customization

EMFFIX - Set step size control for electrons/positrons
FLUKAFIX – Set step size control for hadrons/muons

4/4: Biasing

Biasing - Overview

General concepts:

Analog vs. biased Monte Carlo calculation

Biasing options

(Just a few of those available in FLUKA)

Importance biasing
Leading particle biasing
Multiplicity tuning
Biasing mean-free paths
- **decay lengths biasing**
- **hadronic inelastic interaction lengths**

Additional information:
User-written biasing
Weight Windows

Analog Monte Carlo simulations

- Samples particle histories from actual phase space distributions
- Predicts average quantities, standard deviation (uncertainties), and higher statistical moments.
- Preserves correlations and reproduces fluctuations (provided the physics is correct…)
- Can be used as a “black box”

BUT

- Can be inefficient (slow convergence).
- Fails to predict important contributions due to rare events

Importance biasing

- Simplest, safest, and easiest to use of all biasing techniques

- importance biasing combines *two techniques*:

  Surface Splitting
  Russian Roulette

The user assigns a relative importance I to each geometry region (actual absolute value doesn’t matter).

The higher the interest/urgency in obtaining results in a region, the higher the importance to assign.

Moving into region with higher I

Surface Splitting

A particle crosses a region boundary, coming from a region of importance I_1 and entering a region of *higher* importance $I_2 > I_1$:

- the particle is replaced on average by $n=I_2/I_1$ identical particles with the same characteristics
- the statistical weight of each "daughter" is multiplied by $I_1/I_2<1$

WARNING: If I_2/I_1 is too large, excessive splitting may occur with codes which do not provide an appropriate protection .

An internal limit in FLUKA prevents excessive splitting if I_2/I_1 is too large (> 5), a problem found in many biased codes.

Moving into region with lower I

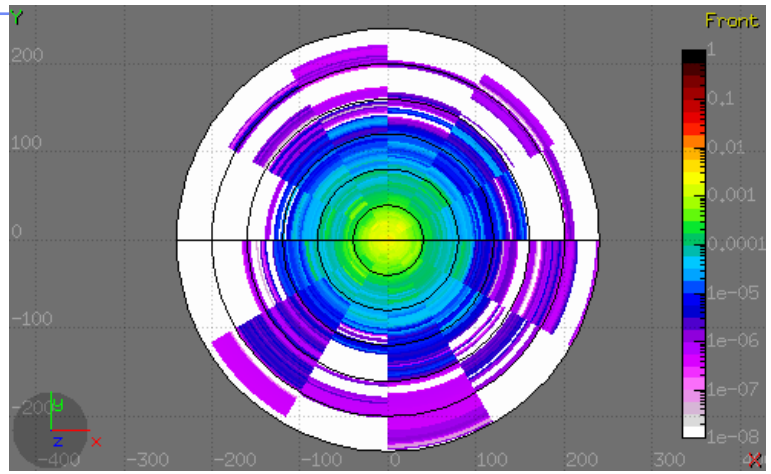
Russian Roulette

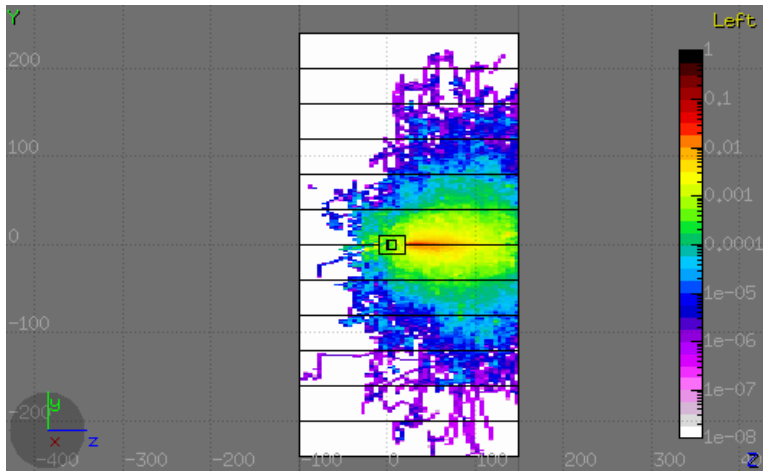
A particle crosses a region boundary, coming from a region of importance I_1 and entering a region of *lower* importance $I_2 < I_1$:

- the particle is submitted to a random survival test: with a chance I_2/I_1 the particle survives with its weight increased by a factor I_1/I_2
- with a chance $(1 - I_2/I_1)$ the particle is killed

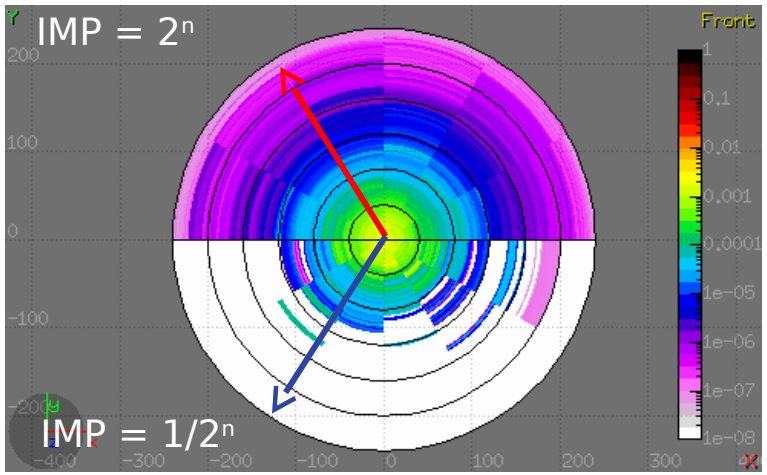
3.5-GeV proton on water/Al/Pb +shielding

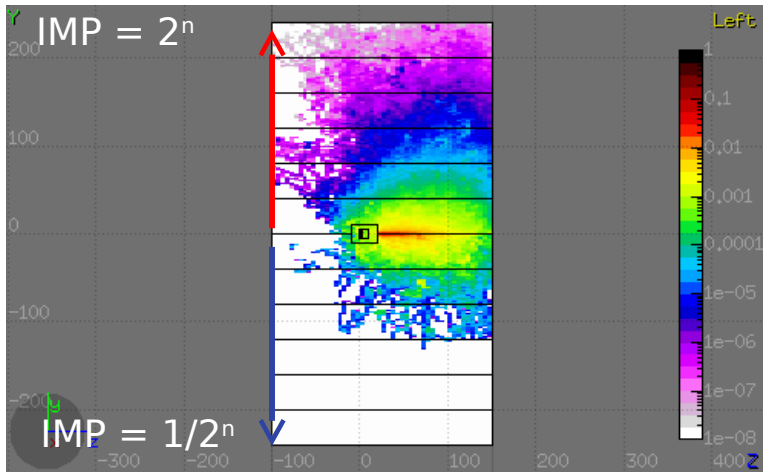
No BIAS





Region Importance Biasing





5 cycles, 1e4 primaries each. Importance biasing is commonly used to maintain a uniform particle population, compensating for attenuation due to absorption or distance.

Biased Monte Carlo simulations

- Samples from artificial distributions and applies a weight to the particles to correct for the bias
- Same mean with smaller variance, *i.e.*, faster convergence

BUT

- Cannot reproduce correlations and fluctuations

- Requires physical judgment, experience and a good understanding of the problem (it is not a “black box”!)
- In general, the user needs to do a series of test runs in order to optimize biasing parameters
- balance between user’s time and CPU time

Main biasing input cards

BIASING

1) region importance biasing (surface splitting or Russian Roulette)

2) multiplicity tuning at hadronic interactions

EMF-BIAS

leading particle biasing for e+, e- and photon interactions

LAM-BIAS

mean free path biasing (decay length biasing, hadronic interaction length biasing)

Time allowing:

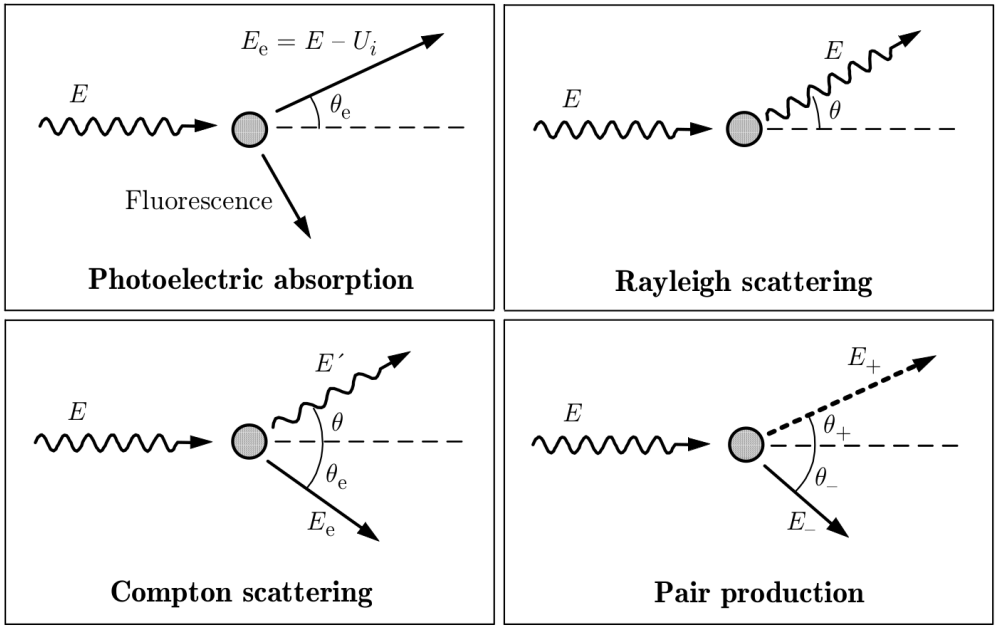
An anticipated example (Scoring lecture tomorrow!)

To give a hint on powerful and flexible built-in scoring capabilities of FLUKA

Brief reminder anticipating last example

We use the opportunity to follow up on previous FLUKA modelling talk.

From yesterday's lecture on PENELOPE, relevant processes < 1 GeV:



Also accounted for in FLUKA.

Reminder from previous lecture on FLUKA models:
photonuclear reactions, muon+- production, high-energy corrections to pair production, etc.

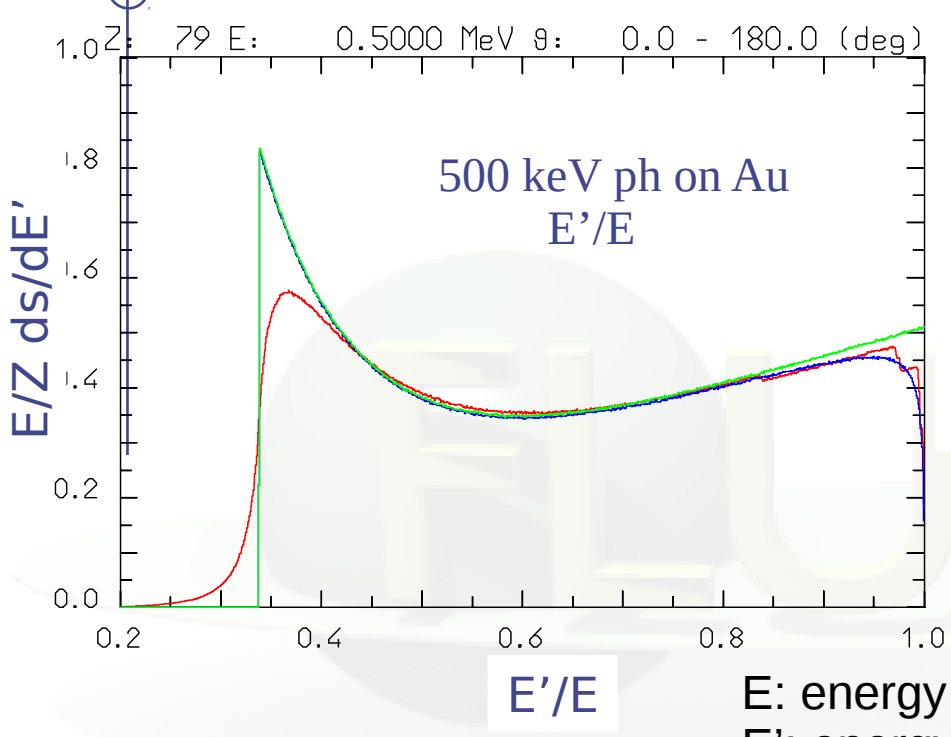
Not for this school, but keep in mind the tool is at your disposal.

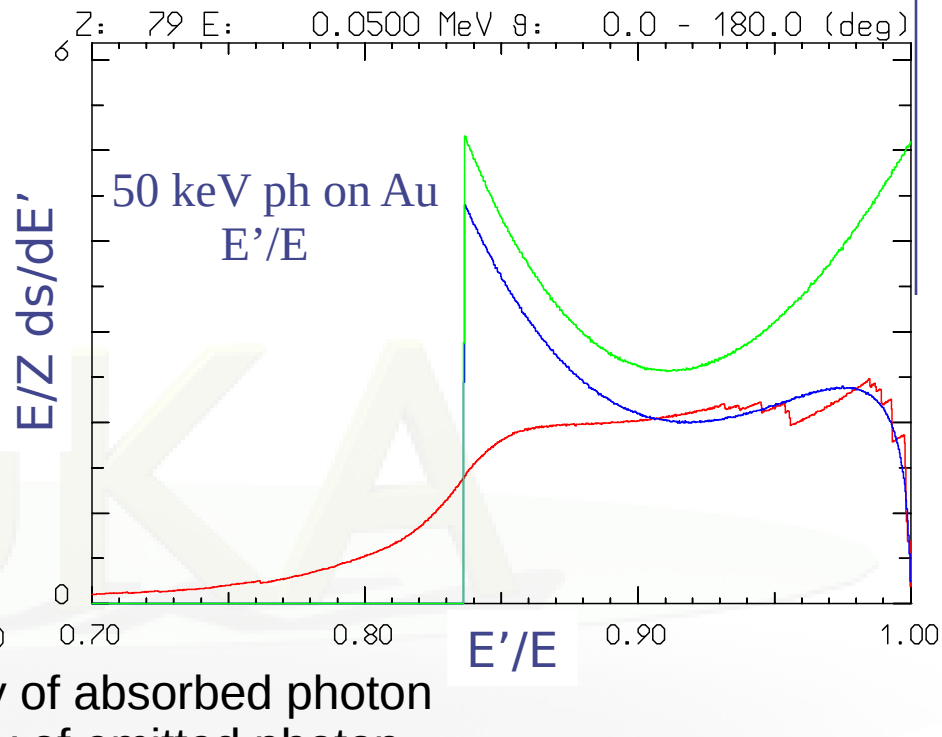
Compton and annihilation on bound e^-

E.g. similarly detailed treatment in FLUKA of Compton scattering
(relevant for example at the end of this session)

- **Bound electron momentum distributions** parameterized out of available (relativistic) Hartee-Fock calculations for all (sub)shells for all elements
- **Fermi momentum distribution** for conduction electrons in **metals**
- **Explicit bound-electron – photon kinematics for Compton scattering,** with full account for energy, momentum conservation (since 2008).
- Same machinery for **positron annihilation** at rest: **(quasi) first-principle based acolinearity** description (next release!)

Diff xs examples





E: energy of absorbed photon
E': energy of emitted photon

Assuming electrons free and at rest (green). Threshold from kinematics.
NOT REALISTIC! Target e^- are actually bound and follow an atomic momentum distribution.

First degree of sophistication: consider "form factors" (blue). Gives average account of bin

More realistic account: atomic momenta distribution for each subshell. At E'~E shell structure clearly visible.

Anti-coincidence Compton shield

Gamma spectroscopy:

- Detector: high purity Ge semiconductor

- Limit of detection governed by two factors:
  - detector efficiency: larger if larger detector used, but price limit.
  - background: due to Compton scattering (reduces contrib from main photopeak into the background). The lower the energy of the peak, the more difficult it is to distinguish from the background.

Idea: reduce background by filtering out Compton-scattered photons (!).

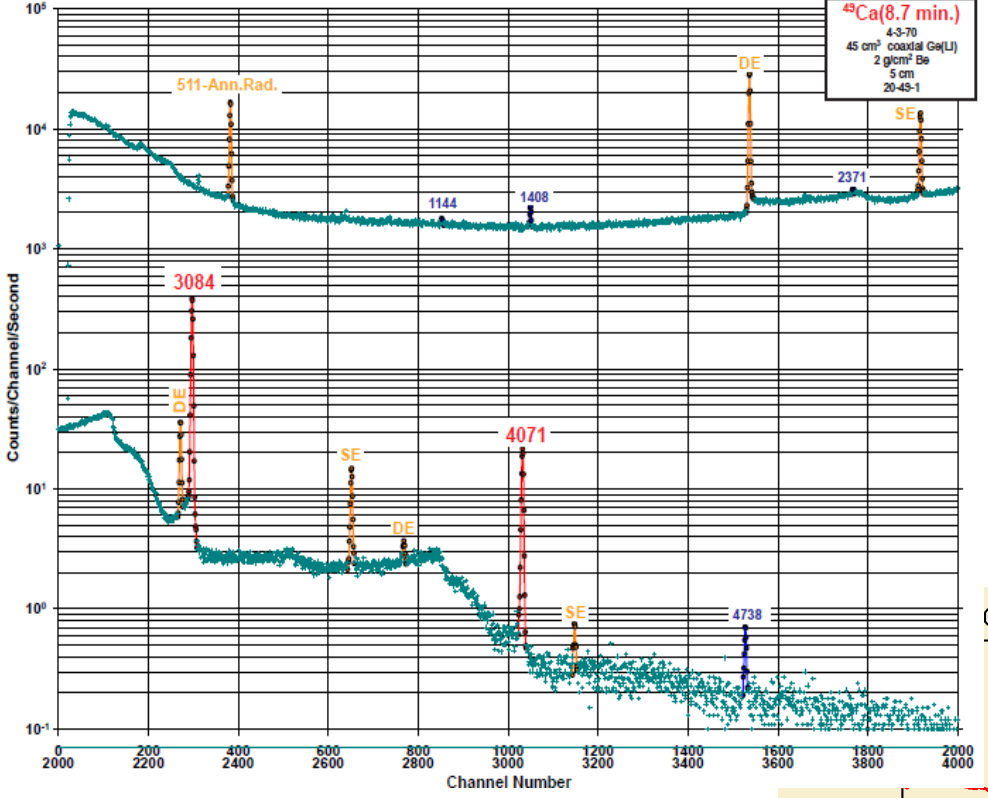
Surround Ge detector with something larger/cheaper: BGO (bismuth germanium oxide).

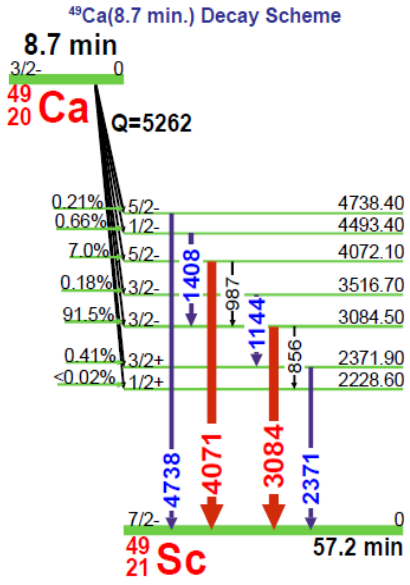
Discard coincident events in both detectors → measure in anti-coincidence.

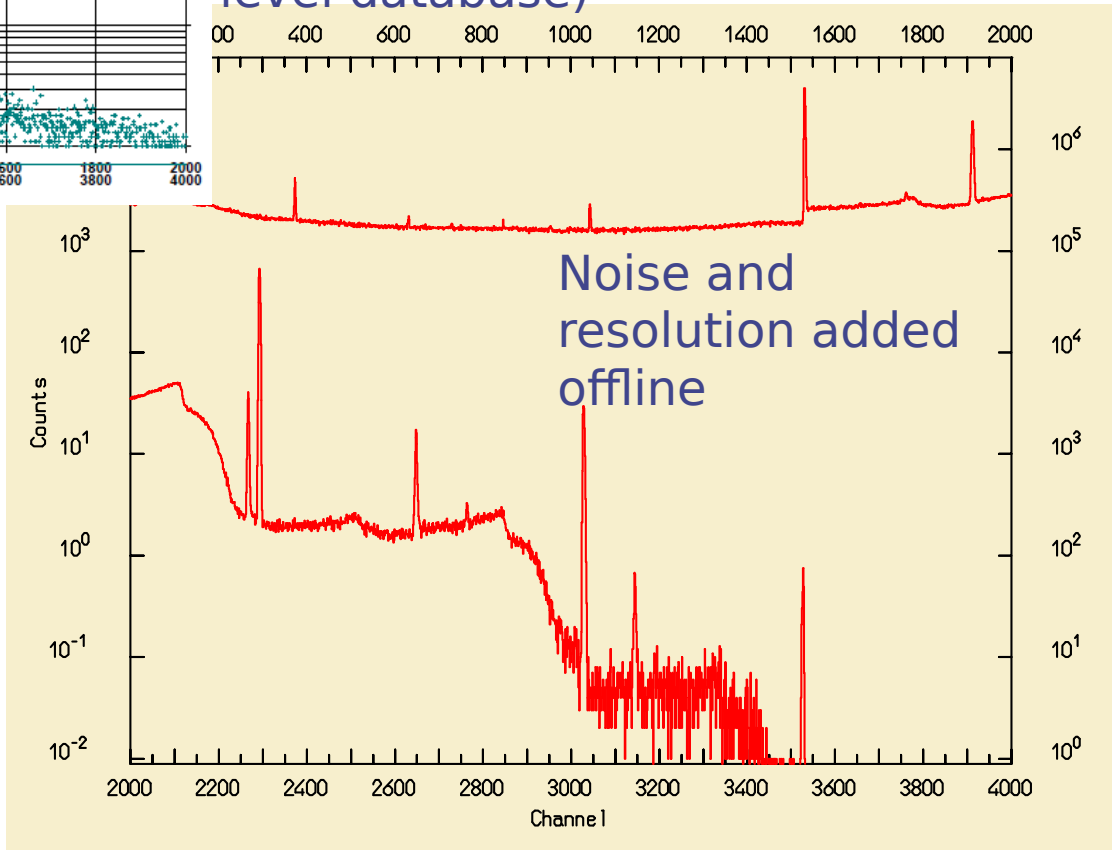
Example of gamma spectrum in Ge(Li)

Data from Gamma Ray Spectrum Catalogue http://id.inel.gov/gamma

In Fluka : direct simulation of nuclear decay with correlated photon cascade (decay and nucl level database)





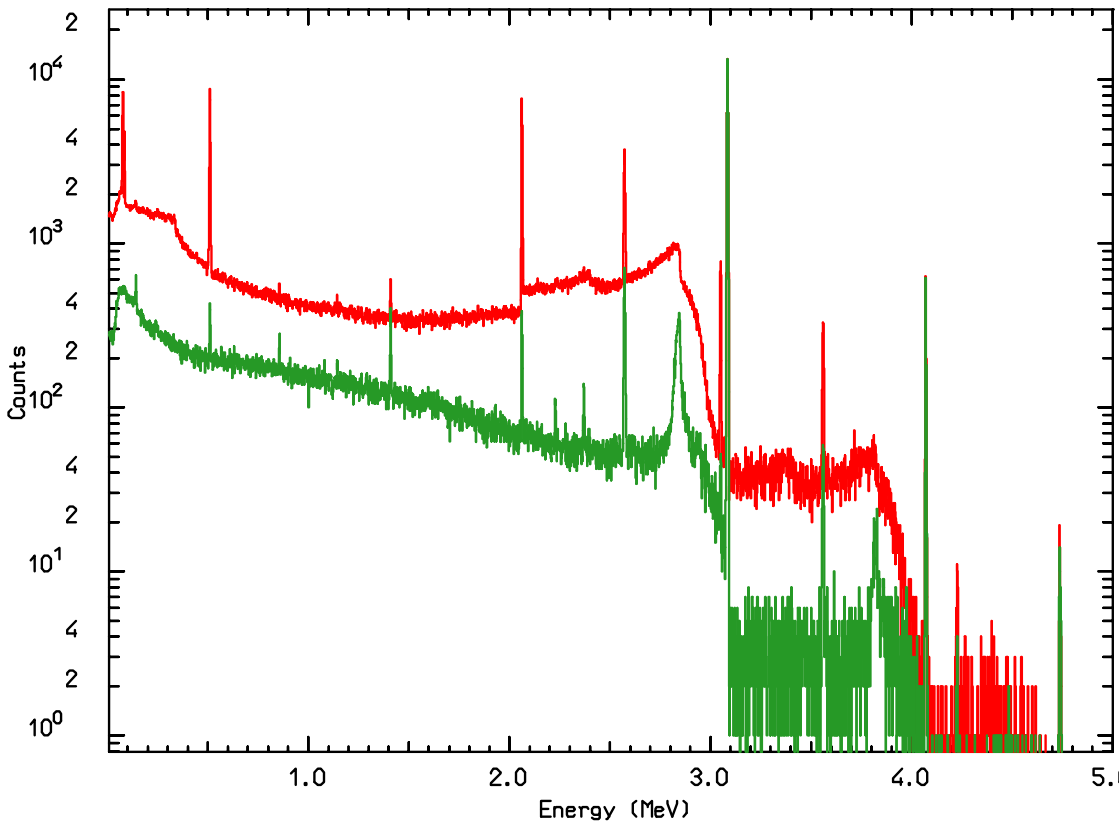


A la FLUKA

FLUKA has built-in energy deposition scoring for events occurring in coincidence/anticoincidence among various regions.

```
* ..+....1....+....2....+....3....+....4....+....5....+....6....+....7..
DETECT         NChann      Emin       Emax  TriggEne  Coi/Anti    Region  NAME
*
```

+Region: detector
-Region: trigger



Summary

We will give a general overview of a few topics:

- **Ionization**: energy loss of charged projectiles in collisions with electrons of medium.

- **Multiple Coulomb scattering**: deflections of charged projectiles with screened Coulomb potential of nuclei.

- **Transport**: general picture + thresholds.

- **Biasing:** a few notions + example.

- **Anticipated scoring example:** Compton anti-coinc shield

Backup slides

Preliminaries: cumulants

Probability density function: f(x)

Characteristic function:

$$\phi_X(t) \equiv \left\langle \mathrm{e}^{\mathrm{i}tX} \right\rangle = \int_{-\infty}^{\infty} \mathrm{d}x \; \mathrm{e}^{\mathrm{i}tx} p_X(x)$$

Cumulant generating function:

$$\psi_X(t) \equiv \ln \phi_X(t)$$

Cumulants:

$$K_k \equiv \left\langle X^k \right\rangle_c = \frac{1}{\mathrm{i}^k} \left. \frac{\partial^k \psi_X(t)}{\partial t^k} \right|_{t=0}$$

Goudsmit & Saunderson 1/2

Given dxs in single interaction: $f_1(\theta) = \frac{1}{\sigma}\frac{\mathrm{d}\sigma}{\mathrm{d}(\cos\theta)}$

Expand in Legendre pol: $f_1(\theta) = \sum_{\ell=0}^{\infty} \frac{2\ell+1}{4\pi} g_\ell \, P_\ell(\cos\theta)$

Distrib after n collisions: $f_n(\mathbf{\Omega}) = \sum_{\ell=0}^{\infty} \sqrt{\frac{2\ell+1}{4\pi}} (g_\ell)^n Y_{\ell 0}(\mathbf{\Omega})$

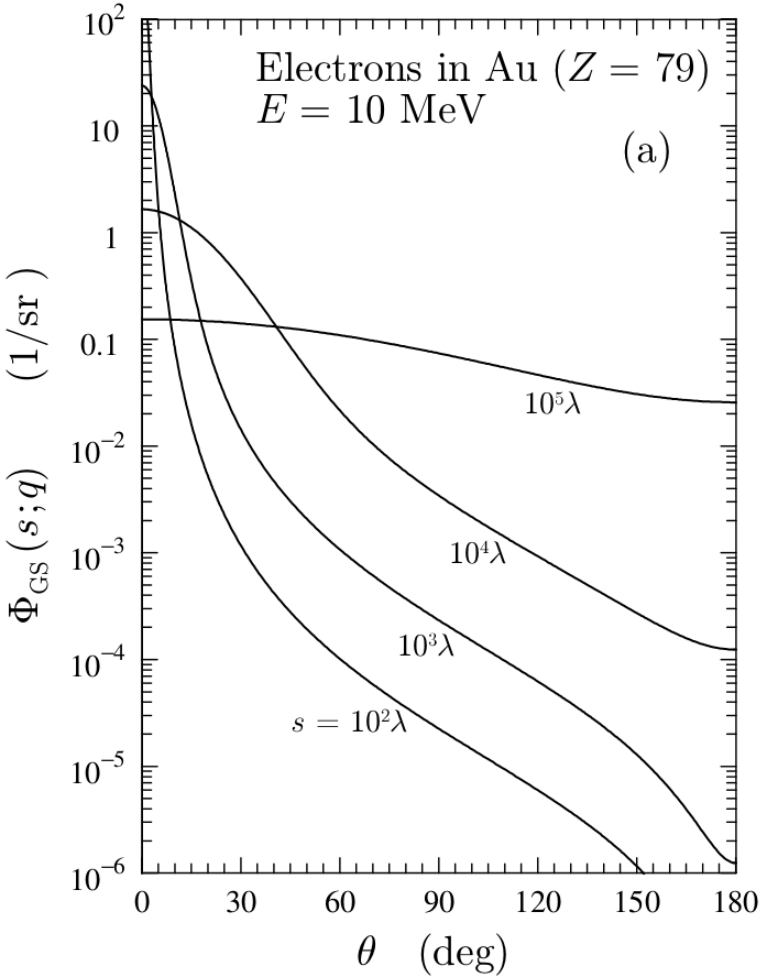
If num col is Poisson distrib: $P(n) = \exp(-s/\lambda)\frac{(s/\lambda)^n}{n!}$

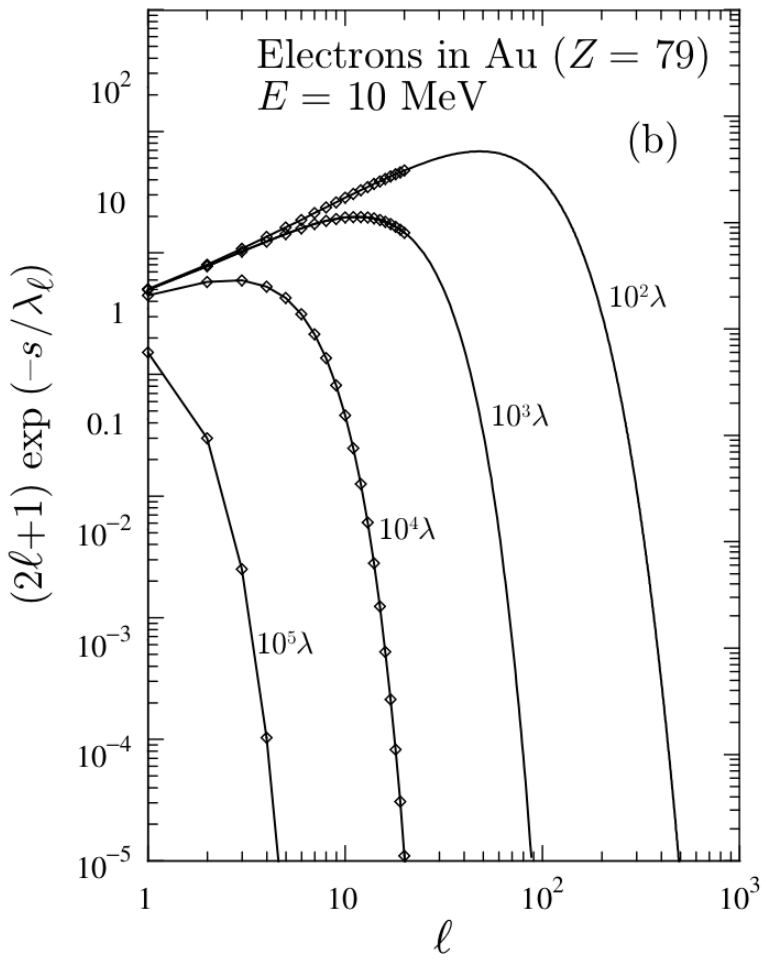
Goudsmit & Saunderson (1939),
Distribution of angles after a path length s:

$$\Phi_{\mathrm{GS}}(s;\mathbf{\Omega}) = \sum_{n=0}^{\infty} P(n) f_n(\mathbf{\Omega}) = \sum_{\ell=0}^{\infty} \sqrt{\frac{2\ell+1}{4\pi}} \left[\exp(-s/\lambda) \sum_{n=0}^{\infty} \frac{(s/\lambda)^n}{n!} (g_\ell)^n \right] Y_{\ell 0}(\mathbf{\Omega})$$

Main idea: given step length s, sample deflection from GS.

Goudsmit & Saunderson 2/2





Note 1: only realistic for the shorter path lengths (no losses).

Note 2: forward peaked for short paths s.

Note 3: large no. of contributions for short paths s.

Main GS pros and cons // Moliere

GS pros:

- valid for any distribution (as long as Legendre expandable)

GS cons:

- numerically intensive
- large number of terms for intermediate and small steps.
- too tedious for small steps, near boundaries, etc

Alternative: Moliere approach, ~GS for an easily integrable dxs.

$$\frac{d\sigma_{Mol}}{d\Omega} \approx \frac{d\bar{\sigma}_{Mol\,small}}{d\Omega_{small}} = \frac{4z^2Z^2r_e^2m_e^2c^4}{\beta^4E^2\theta^4} \times \frac{\theta^4}{(\theta^2+\chi_a^2)^2}$$

Additional pproximations:

→ Small deflections assumed in the derivation

→ Path length must be longer than ~4 MFPs (GS would need lots of terms!)

Additional factors not shown: spin-rel corr, nuclear form factors.

Example : TEPC (T.T. Boehlen et al, Phys. Med. Biol. **56 (2011) 6545)**

- Tissue-equivalent proportional counters (TEPC) measure the imparted energy ε and derived quantities such as the lineal energy y in volumes which mimic dimensions and medium characteristics of a mammalian cell nucleus (ICRU 1983) and are one of the principal instruments used in microdosimetry.
- They respond to ions passing the sensitive volume of the TEPC as well as to delta-rays from ions passing close to the sensitive volume which penetrate the cavity.
- Fluka compared with several measurements with a spherical TEPC
  - sensitive volume filled with a tissue-equivalent gas
  - inner diameter of 12.7mm.
  - Gas pressure adapted to simulate tissue of diameters between *1.0 and 3.0µm.*
  - An anode wire extends through the center of the cavity, surrounded by a helical grid which forms a uniform field close to the wire
  - The cavity is surrounded by conductive tissue-equivalent plastic with a thickness between 1.27 and 3*.7mm.*

Validation with TEPC measurements

Verifying adequacy of FLUKA energy loss straggling, delta ray generation/transport and MCS in microscopic volumes.

IOP PUBLISHING PHYSICS IN MEDICINE AND BIOLOGY

Phys. Med. Biol. **56** (2011) 6545–6561 doi:10.1088/0031-9155/56/20/002

FLUKA simulations of the response of tissue-equivalent proportional counters to ion beams for applications in hadron therapy and space

T T Böhlen[1,2], M Dosanjh[1], A Ferrari[1], I Gudowska[2] and A Mairani[3]

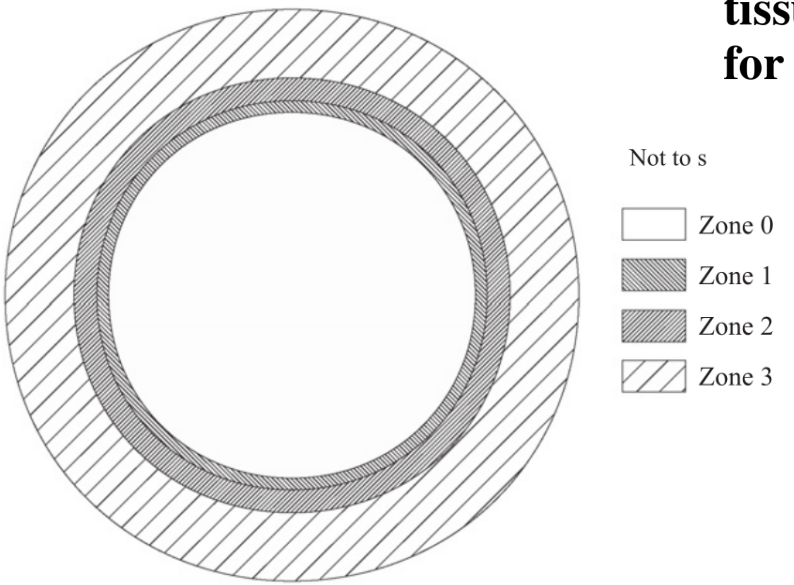


Figure 1. Production and transport threshold settings for delta-rays for the TEPC used for simulations with FLUKA. Inside the cavity (Zone 0) and in the 3-μm-thick inner layer of the plastic wall (Zone 1), the thresholds were lowered to 1 keV for the presented simulations (if not stated explicitly differently). In the adjacent plastic layer of 197 μm, the thresholds were set to 10 keV (Zone 2). In the rest of the plastic wall (Zone 3) and the remaining geometry, the default thresholds of 100 keV were set.

CSDA range of electrons in mat:

100 keV → 126 um
10 keV → 2.2 um

https://www.nasa.gov/mission_pages/station/research/experiments/TEPC.html

Reduce variance or CPU time ?

A Figure of merit of a statistical estimator

Computer cost of MC estimator = s^2 x t

(s^2 = Variance, t =CPU time per primary particle)

- some biasing techniques are aiming at reducing s (Russian roulette), others at reducing t (Surface splitting).
- often reducing s increases t, and *viceversa*
- therefore, minimizing $s^2 x\ t$ means to reduce s at a faster rate than t increases or *viceversa*
- the choice depends on the problem, and sometimes a combination of several techniques is most effective
- bad judgment, or excessive “forcing” on one of the two variables can have unintended consequences on the other one, making computer cost explode