蘭州大學
LANZHOU UNIVERSITY

Ionization and Transport

23rd FLUKA Beginner's Course
Lanzhou University
Lanzhou, China
June 2-7, 2024

Overview:

We will briefly discuss the following interaction mechanisms of charged projectiles traversing a material:

- **Ionization losses**: energy loss in collisions with target electrons

(Coulomb interaction of the charged projectile with atomic electrons leading to excitation or ionization. *Energy deposition; Radiation Damage; Detectors…*)

- **Collisions** of charged projectiles with (screened) Coulomb potential of nuclei → (Multiple) Coulomb scattering (part 3 of this Lecture)

(Small deflections of the projectile trajectory, unless close encounter. *Trajectories; Beam Spreading; Shielding*)

In addition to giving a glimpse of FLUKA's approach to these interaction mechanisms (and FLUKA options governing them), we address here the concept of *transport thresholds* and transport in magnetic and *electric* fields.

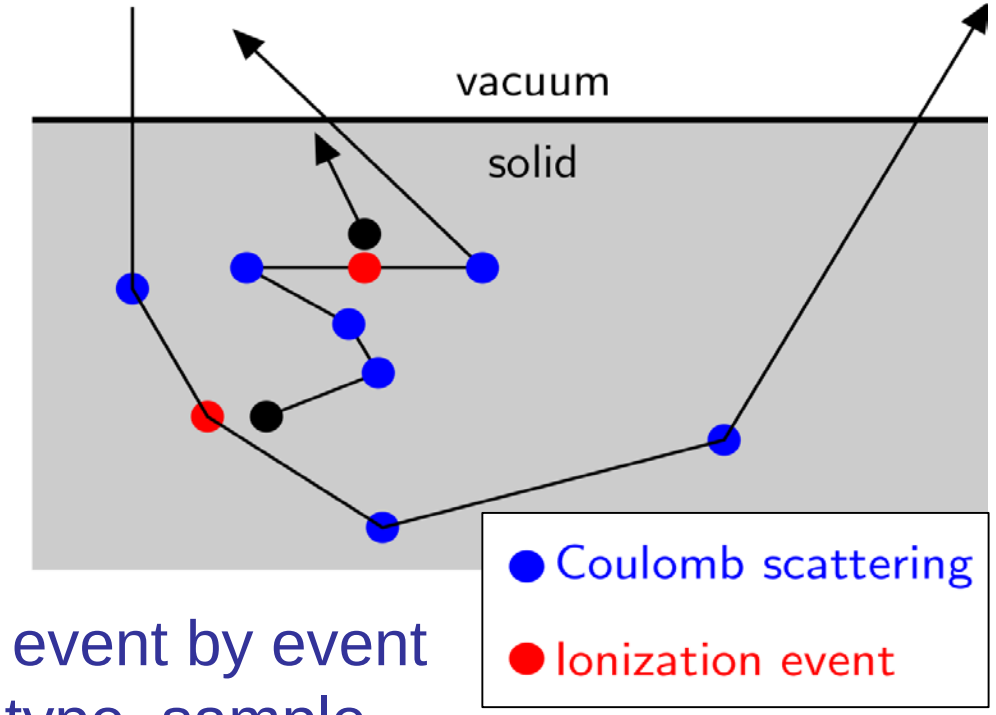
In a "detailed" Monte Carlo simulation

MC: simulate ensemble of particle trajectories + statistical analysis of desired observables (= what we want to score).

For each type of event:

- differential cross section (dxs)
- → energy loss T, deflection angle.

e.g., ionization losses and Coulomb scattering with target atoms



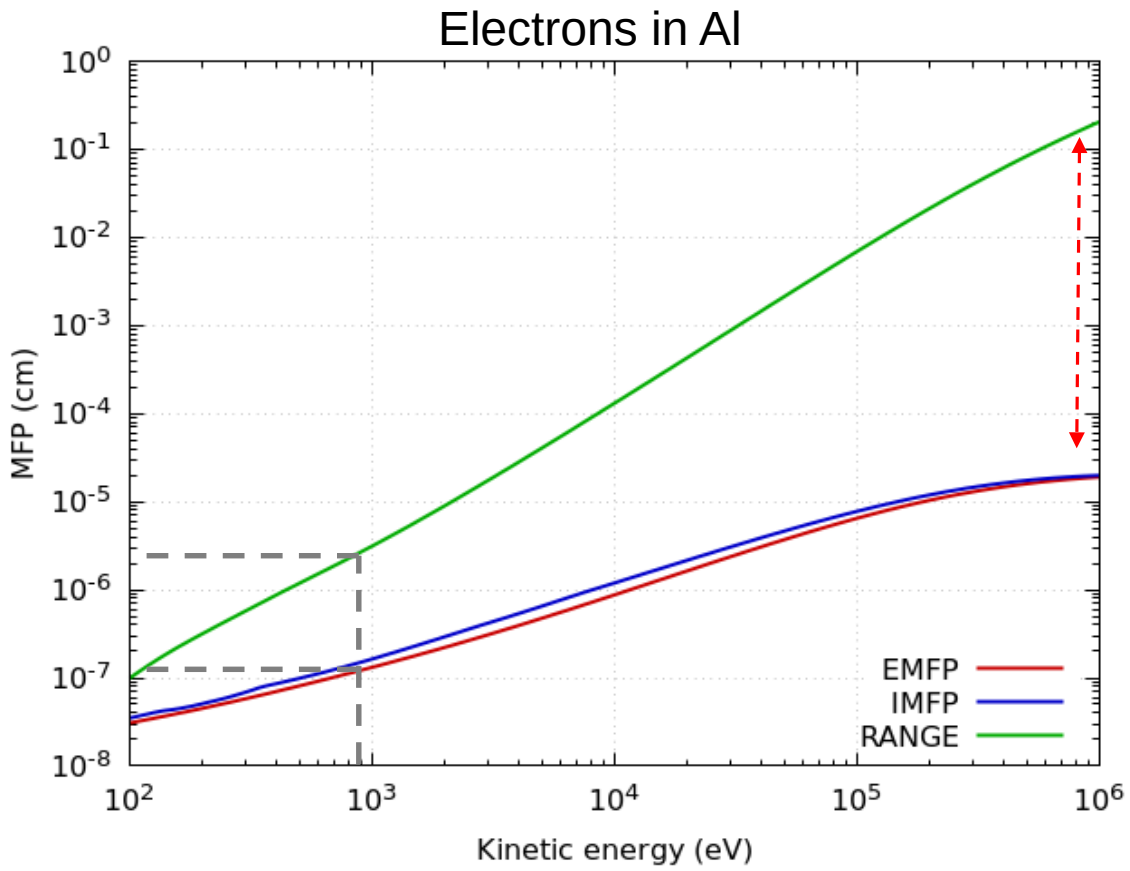
Ideally one would simulate each particle trajectory event by event (detailed simulation): take step, decide interaction type, sample from dxs, update energy/direction… and loop.

In a "detailed" Monte Carlo simulation

…is this feasible in practice?

Estimate number of ionization losses

Rough estimate of number of ionization losses to sample per primary: range/IMFP



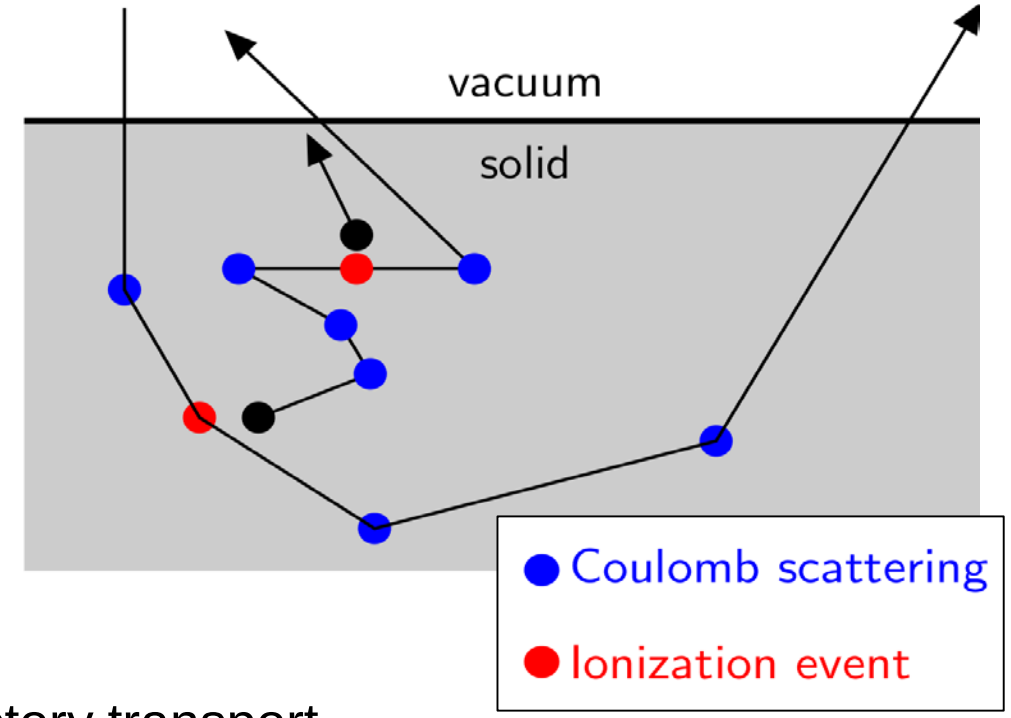
***E*MFP**: *elastic* mean free path

***I*MFP**: *inelastic* mean free path

For a 1-MeV e^-: **range/IMFP ~ 2000** events (!) → **Too many to simulate explicitly**

A more practical approach

- **"Condensed history"** simulation schemes are a practical necessity to keep CPU time within acceptable bounds
- Main idea in scheme adopted in FLUKA and most other codes:
  - Sample ionization losses explicitly only when the effect is large
  - Account for global effect of *small losses* in an effective way according to the Bethe-Bloch theory (to be briefly discussed here) along each particle step



In this session: brief overview of FLUKA's condensed history transport scheme for ionization (as well as multiple Coulomb scattering).

Ionization and excitation energy losses

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

Bethe – Bloch formula with corrections:

Spin 0 (spin 1/2 is similar):

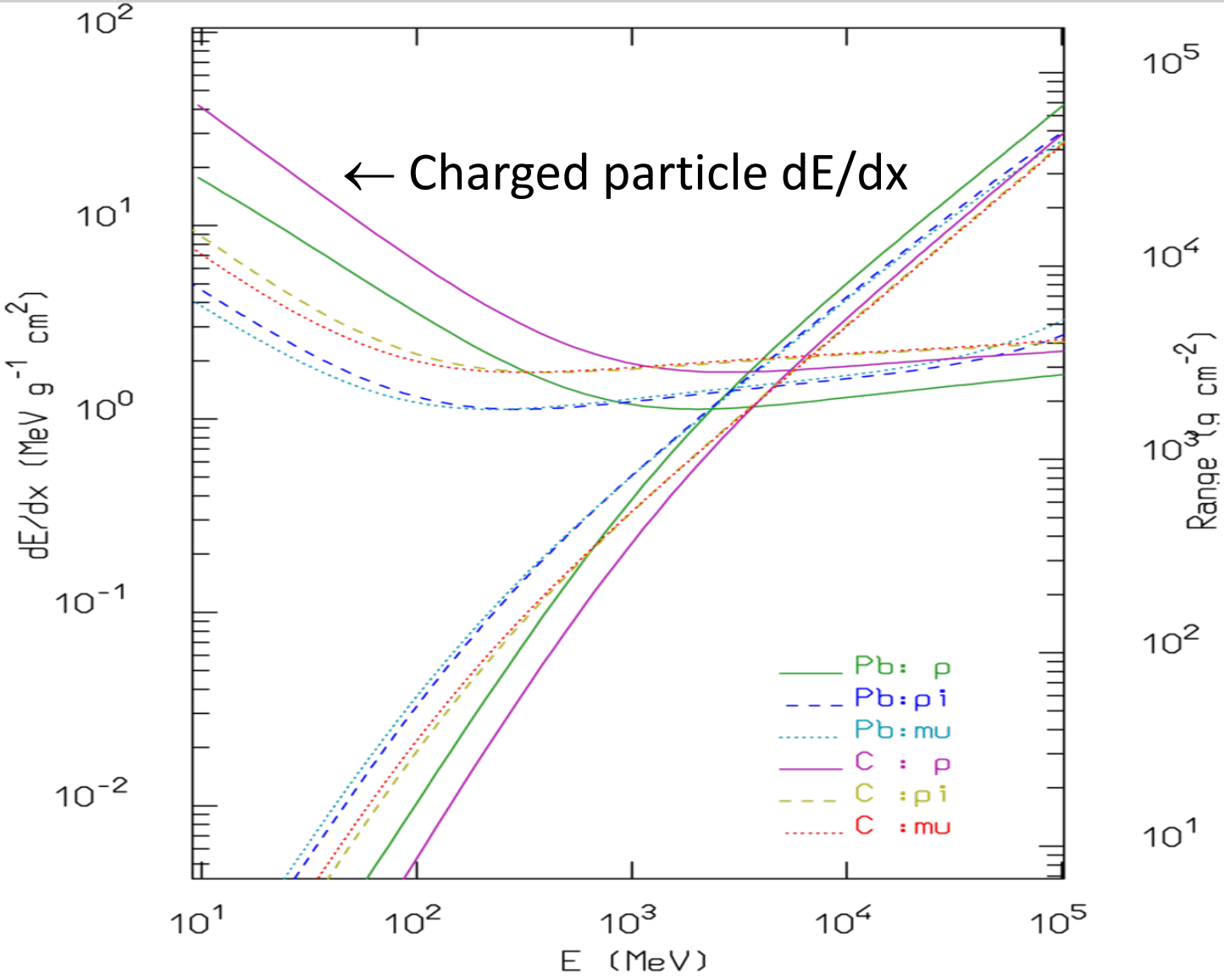
~ln $\beta^4\gamma^4$ relativistic rise

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

- 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)

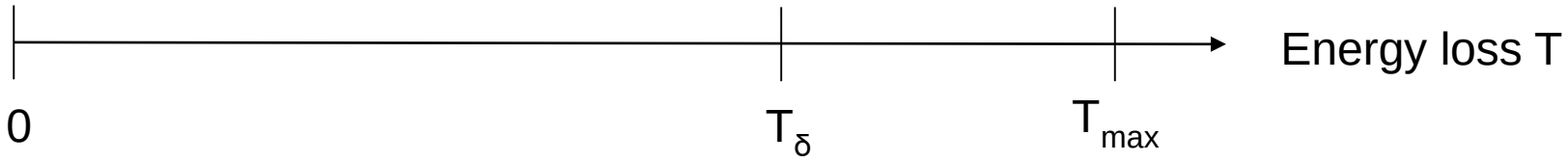
- (Bethe formula derived within 1st Born approximation: 1st-order perturbation theory and plane waves, assuming $v>>v_e$). It includes "distant" and "close" (δ-ray, knock-on electrons) collisions
- To improve shortcomings, a series of corrections are used:
  - δ : density correction
  - C : is the shell correction, important at low energies
  - L_1 : Barkas correction (z^3)
  - L_2 : Bloch (z^4) correction
  - G : Mott corrections

Example of dE/dx:

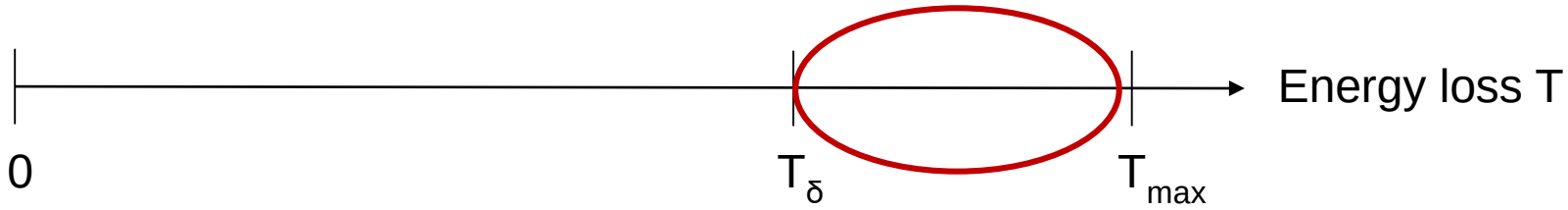


Ionization energy losses in FLUKA

2 different treatments: small vs large energy losses.



$T>T_\delta$: Discrete losses ('exact' method)



- 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?

$T>T_\delta$: detailed sampling

Depending on projectile, ***discrete*** energy losses are sampled from:

$$\left(\frac{d\sigma}{dT_e}\right)_0 = \frac{2\pi r_e^2}{\beta^2}\frac{m_e c^2}{T_e^2}\left[1-\beta^2\frac{T_e}{T_{max}}\right]$$

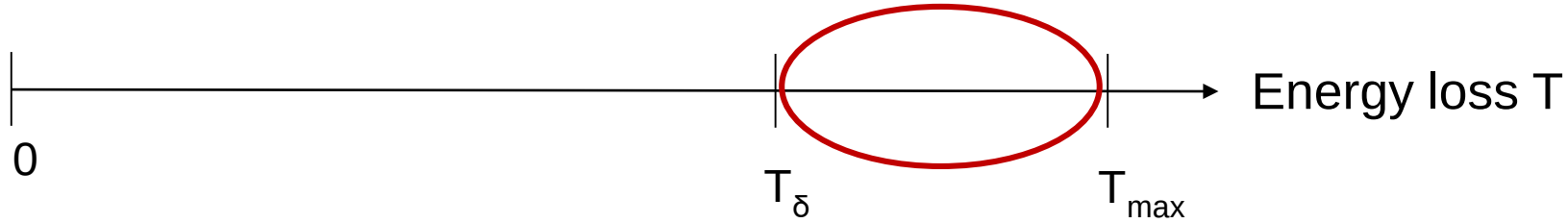
$$\left(\frac{d\sigma}{dT_e}\right)_{\frac{1}{2}} = \frac{2\pi r_e^2}{\beta^2}\frac{m_e c^2}{T_e^2}\left[1-\beta^2\frac{T_e}{T_{max}}+\frac{1}{2}\left(\frac{T_e}{T_0+Mc^2}\right)^2\right]$$

Specific expressions:

- Møller scattering (e^-)
- Bhabha scattering (e^+)
- Mott cross section for heavy ions

- T_e is sampled from these differential cross section according to projectile type
- All moments reproduced: average energy loss, fluctuations, etc.
- Energy and momentum exactly conserved

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 later):
  - e^-, e^+: EMFCUT card with PROD-CUT SDUM;
    (see note after MCS for WHAT(3)=FUDGEM)

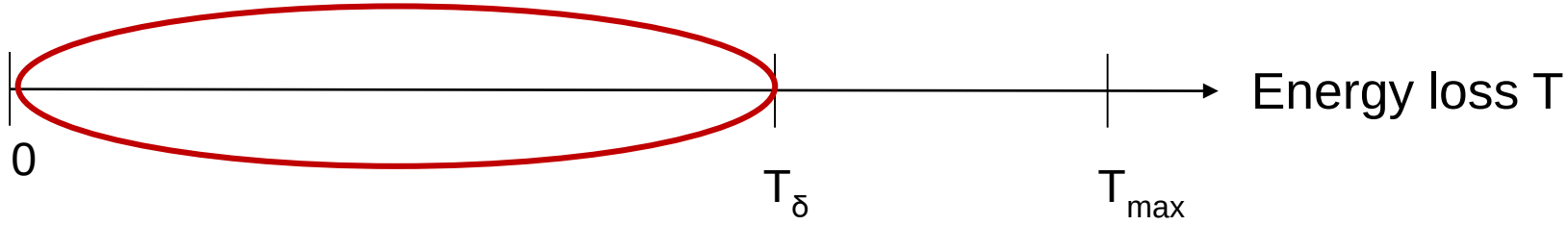
```
* ..+....1....+....2....+....3....+....4....+....5....+....6....+....7..
EMFCUT     ElePosiTh   WHAT(2)   WHAT(3)      Mat1       Mat2       StepPROD-CUT
```

  - Charged hadrons/muons: set by DELTARAY card: on stdout

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

δ_{Thresh}	production threshold (from materials Mat1 to Mat2)
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 ($T<T_\delta$)



- Below T_δ: Small losses are frequent → too much CPU to sample them individually
- Approach: account for the *aggregate effect of these small losses* below the δ-ray production threshold as a continuous energy loss at each particle step according to restricted Bethe-Bloch
- 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 including excitation/ionization (next slide)
  - and by applying energy loss fluctuations on top to account for the stochastic nature of energy loss (next slide+2)
- 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 restricted to $T<T_\delta$

Spin 0 (spin 1/2 is similar):

$$\left(\frac{dE}{dx}\right)_{0T_\delta} = \frac{2\pi n_e r_e^2 m_e c^2 z^2}{\beta^2}\left[\ln\left(\frac{2m_e c^2 \beta^2 T_\delta}{I^2(1-\beta^2)}\right)\right.$$
$$\left. -\beta^2\left(1+\frac{T_\delta}{T_{\max}}\right)+2zL_1(\beta)+2z^2L_2(\beta)-2\frac{C}{Z}-\delta\ +G\left(T_\delta\right)\right]$$

Equivalent expressions exist for e^-/e^+:

FLUKA's approach to loss fluctuations

- Aggregate energy loss in a step is sum of n individual losses T~dσ/dT, where n~Poisson and dσ/dT is the distribution of energy losses for each charged projectile.
- Mathematical machinery: sampling aggregate energy loss distribution in a step from the cumulants of T dσ/dT (see extra slides):

- Cumulants and all necessary integrals can be calculated analytically and exactly *a priori* (minimal CPU time penalty).
- 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

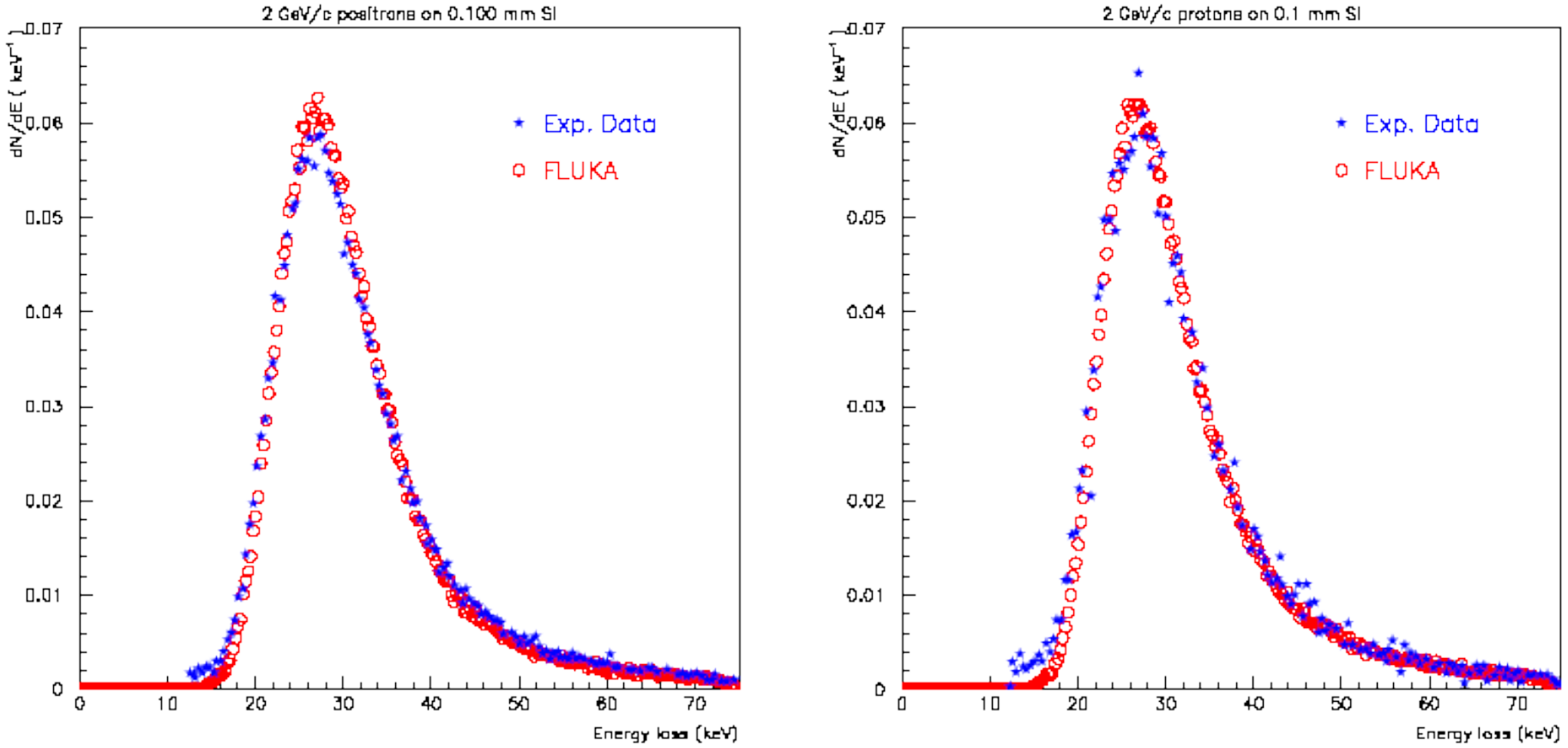
Energy-dependence in step and material parameters

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

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

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

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 charged projectiles*:

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

All share the same approach!

*)… but some extra features are needed for Heavy Ions (next slide)

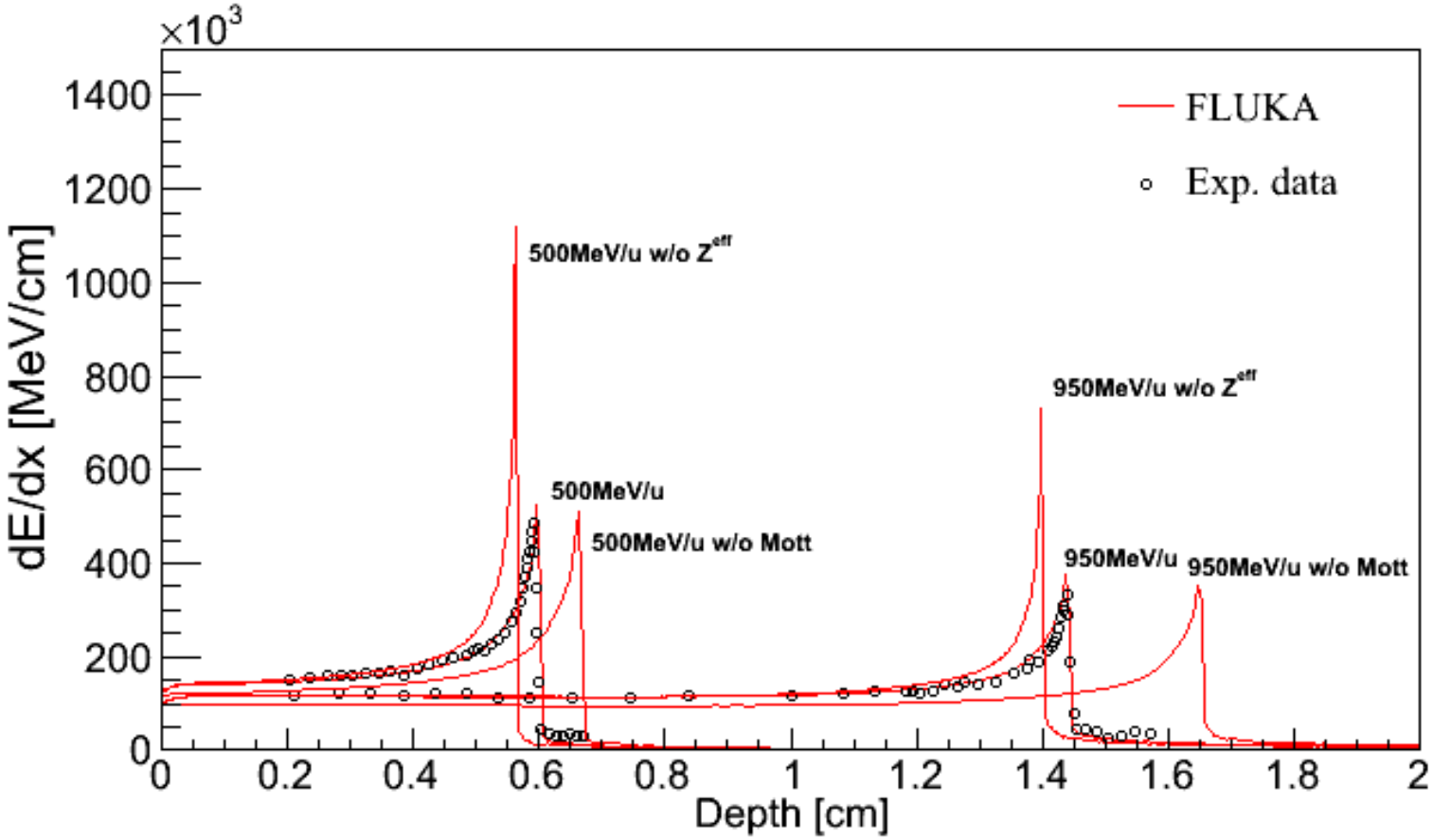
Heavy ions

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

- Effective charge (up-to-date parameterizations)
- … and related charge exchange effects (dominant at low energies, ad-hoc model developed for FLUKA)
- Mott cross section
- Nuclear form factors (of projectile ion!) (not discussed today)
- Direct e^+/e^- production (see PHYSICS with SDUM=IONBRPAI, not discussed today)

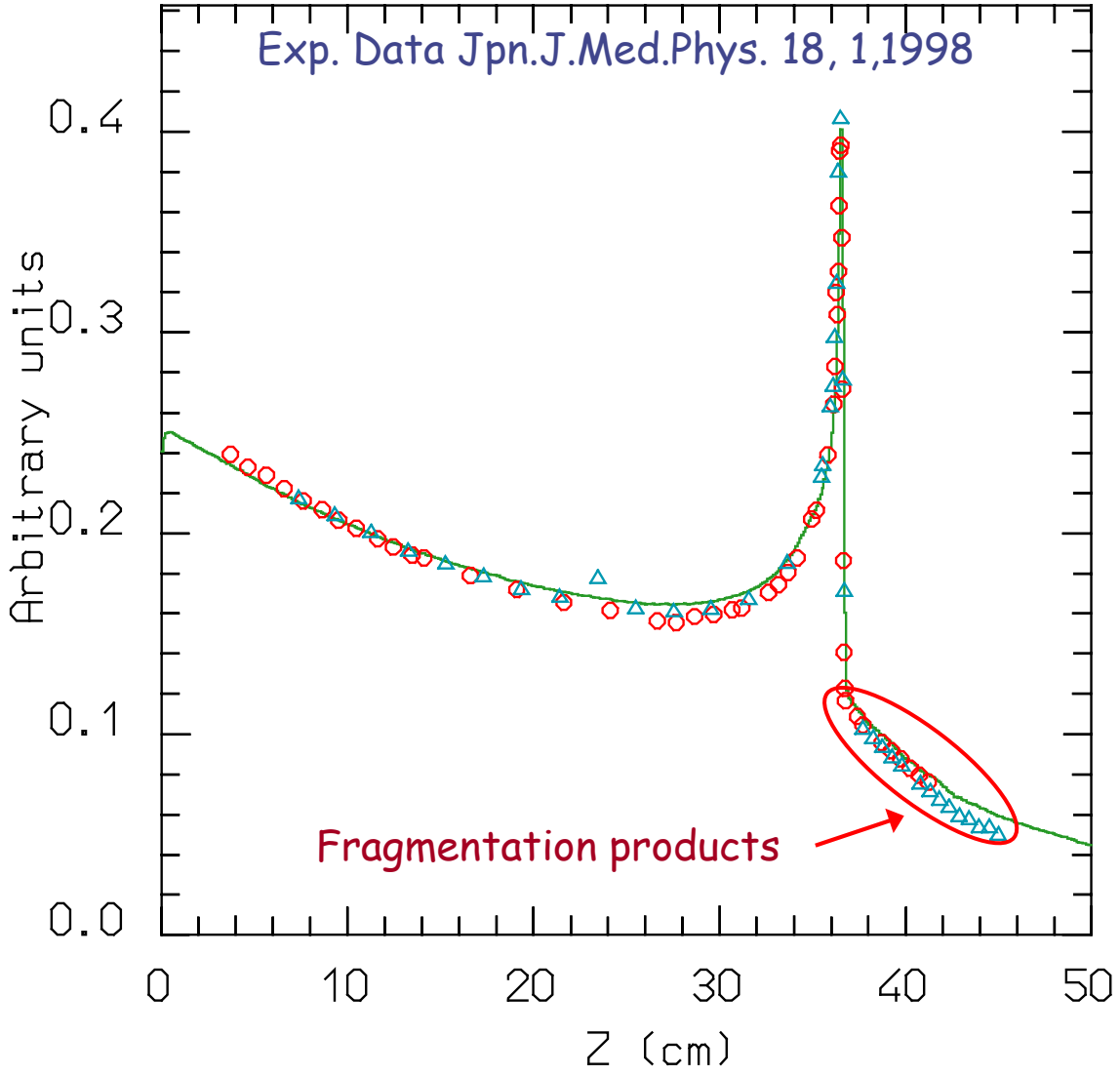
Heavy ions - example

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



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

Heavy Ions – example: ^{20}Ne @ 670 MeV/n

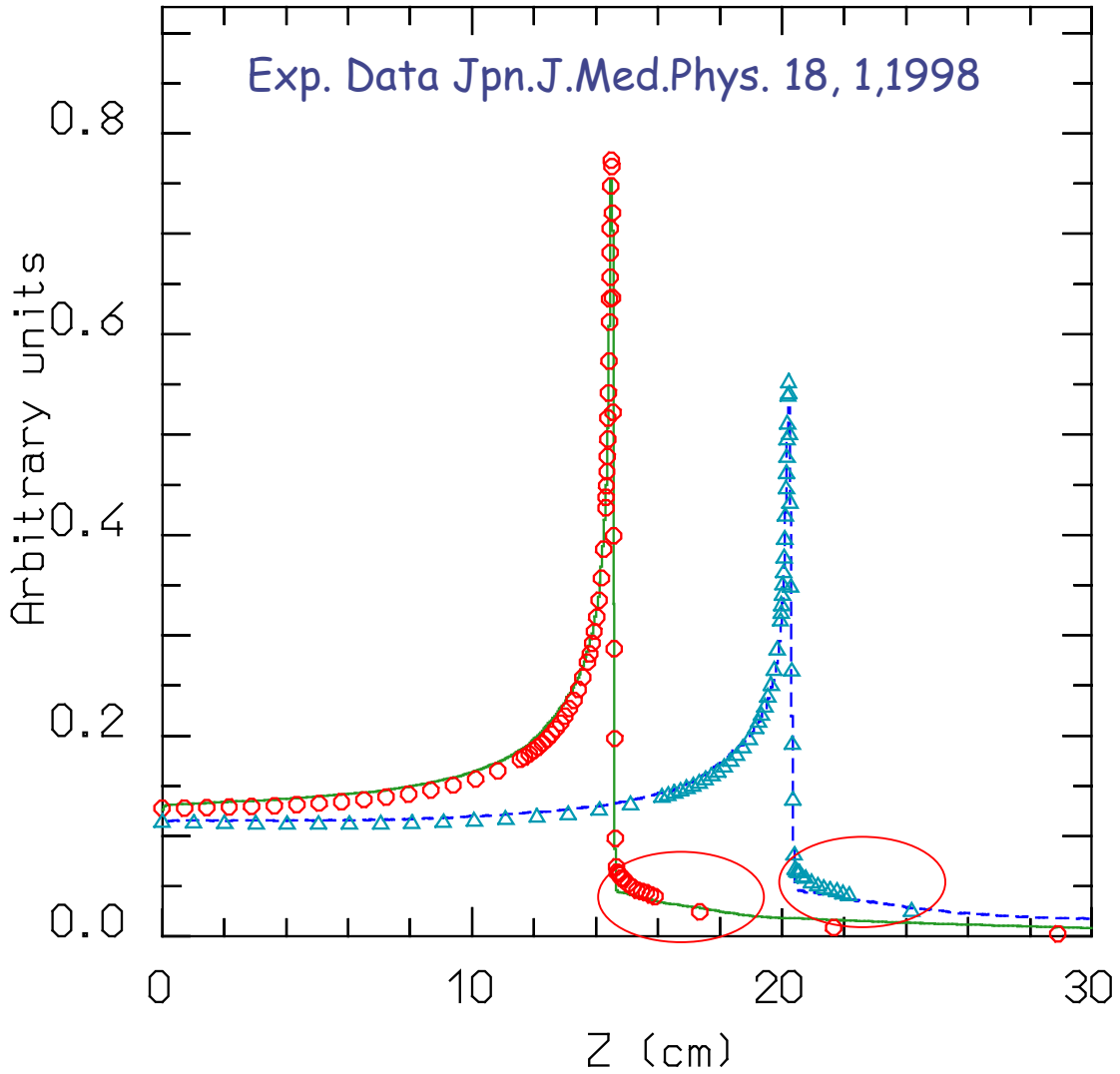


Dose vs depth distribution for 670 MeV/n ^{20}Ne ions on a water phantom.

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

Tail due to fragmentation products

Heavy Ions – example: ^{12}C @ 270 & 330 MeV/n



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 experimental data from GSI.

Summary

- We have discussed two separate treatments for ionization energy losses in FLUKA: discrete vs continuous
- Above delta production threshold: losses sampled individually, i.e., discrete losses
- Continuous losses described effectively along particle step. First 6 moments of energy-loss distribution reproduced thanks to FLUKA's approach via cumulants of $T d\sigma/dT$
- Approach is set up in such a way that it works for all charged projectiles considered in FLUKA
- Special corrections for ions leads to good agreement with experiments

2/4 - Transport thresholds

Transport threshold

In a MC simulation particles are not tracked until they “have lost all their kinetic energy”, but until their energy drops to/below a preset transport threshold

When a particle’s energy drops below threshold, what happens?
It is deposited on the spot (for electrons) or ranged out (for heavier projectiles).

EMFCUT card (without SDUM): energy transport threshold for electrons/positrons/gammas can be set REGION BY REGION.

EMFCUT	e±Thresh	γThresh	0.0	Reg1	Reg2	Step

[WHAT(3) not used]

Transport thresholds (non-EM)


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

PART-THR : allows setting transport threshold for hadrons, ions, muons and neutrinos globally for the entire geometry setup

Can be individually set for different particle types, or for all particles

Neutrons are special → The neutron threshold, recommended to leave at the default value (1E-14 GeV). Careful to reset if you set threshold from-to in a range containing neutron

Heavy ion transport thresholds are derived from that of a He^4 ion, scaling with ratio of atomic weight ion/He^4

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

How to set threshold values?

- The thresholds have default settings, depending on the SDUM selected on the DEFAULTS card (examine manual)
- ***DO NOT RELY*** on them, choose those which are best suited for your problem (see next slides)
- Guidelines to set threshold energies?

Threshold settings: examples

Set transport threshold for all hadrons and $\mu^{\pm}$ to 1 MeV…

```
PART-THR  -.001  4-HELIUM  @LASTPAR
```

… except for neutrons (set at 10^{-5} eV)

```
PART-THR  -1E-14  NEUTRON  NEUTRON
```

Activate δ-ray production above 100 keV for all materials

```
DELTARAY  0.0001                  3.       @LASTMAT
```

Produce secondary e^- and γ above 100 and keV in EM cascades (all mat.)

```
EMFCUT    -1.E-4  1.E-5      1.   3.       @LASTMAT          PROD-CUT
```

Transport $e^{\pm}$ and γ above 100 and keV in EM cascades (all regions)

```
EMFCUT    -1.E-4  1.E-5           1.       @LASTREG
```

- Hadron thresholds: little-to-moderate impact on CPU
- δ ray threshold: moderate-to-heavy impact on CPU
- γ thresholds: little-to-moderate impact on CPU
- $e^{\pm}$ thresholds: heavy impact on CPU

How to set threshold values? General guidelines

- **Threshold energies:**
  - It depends on the "granularity" of the geometry and/or of the scoring mesh.
  - Consider the interest in a given region
  - Compromise with CPU time
- **In practice :** compare the dimensions of the "problem" with the range of particles at the threshold energy. Energy/range tables are very useful (see for instance http://physics.nist.gov)
  - ❖ Warning 1: to reproduce correctly electronic equilibrium, neighboring regions should have the same electron energy (***NOT range in cm***) threshold. To be kept in mind for sampling calorimeters
  - ❖ Warning 2: Photon thresholds should be lower than electron thresholds (photons travel farther)
  - ❖ Warning 3: ***low thresholds for e-/e+/gammas are CPU eaters***
- **Delta-ray production threshold:**
  - *production threshold* < *transport threshold* → CPU wasted in producing and dumping particles on the spot
  - *production threshold* > *transport threshold* → the latter is increased

Electron/Photon transport thresholds in the .out file


```
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, given in MeV

Other particle transport thresholds


```
 === 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/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, given in MeV

3/4: Multiple Coulomb scattering

Description of Coulomb 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 an effective scheme to sample the 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

From single Scattering Cross Section to Molière mcs

At the heart of the approach: assume that in a single Coulomb collision the differential cross section 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 differential cross section *with screening parameter* χ_a
Advantage: can be integrated analytically for any projectile/material

Using this formula, Molière obtained the Angular distribution after a given step length from transport equation with approximations:

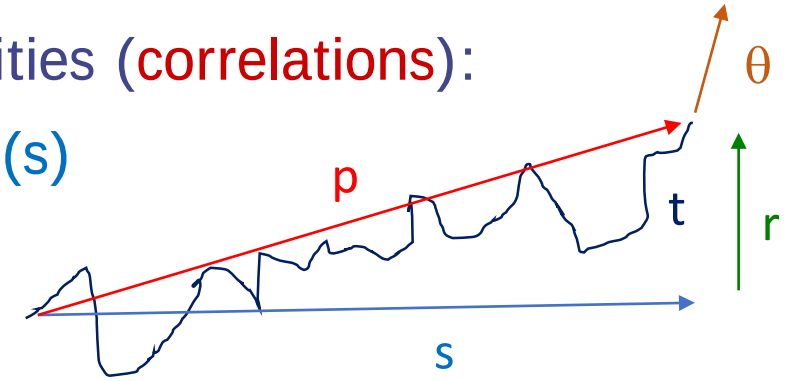
- Small-angle approximation to the single-scattering cross section
- Number of collisions is large enough (above say 10 or 20)
- ... which leads to a **minimum applicable step length (!!!!)**

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

The FLUKA MCS

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

  scattering angle (θ) ↔ longitudinal displacement (s)
  longitudinal displacement (s) ↔ lateral displacement (r)
  Path length correction (s/t) ↔ lateral deflection

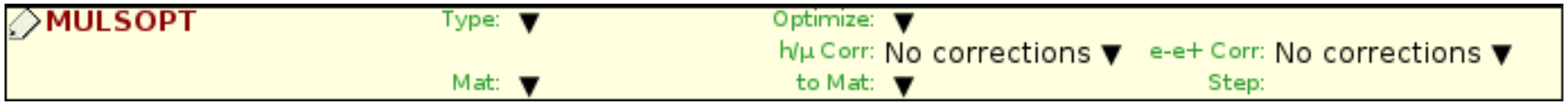


- Careful geometry tracking near boundaries
- MCS is able to coexist with transport in magnetic fields

User control of MCS (MULSOPT)

- 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 users 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):

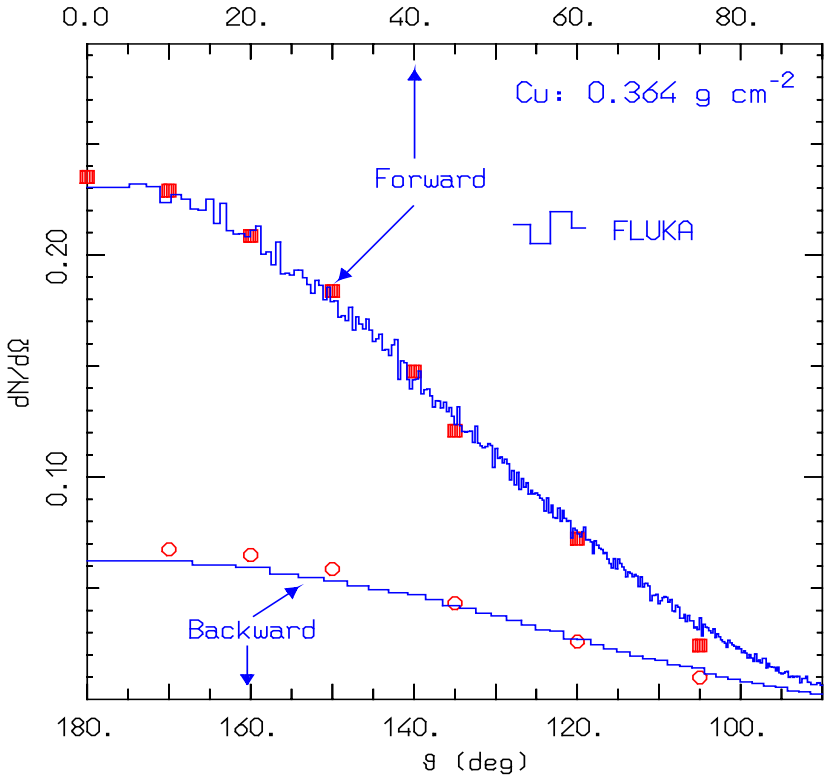
```
* ..+....1....+....2....+....3....+....4....+....5....+....6....+....7..
MULSOPT        Flag1      Flag2      Flag3       Mat1       Mat2       StepSDUM
```



- Details in FLUKA manual, but essentially:
  - Switch to single scattering mode, globally or just close to boundaries
  - Spin-relativistic corrections and nuclear finite size effects.

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!)



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

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

The FUDGEM parameter

In EMFCUT with SDUM=PROD-CUT, WHAT(3) accounts for the fraction of atomic electron contribution to MCS.

In Rutherford xs: $Z^2 \rightarrow Z(Z+f)$ f=WHAT(3)

A value of 10^{-5} is fine for very low delta-ray production thresholds: the contribution of atomic electrons is accounted for via explicit secondary electron production. Low means much lower than typical atomic shell binding energies (several 10s of keV). Practical hint: for $T_\delta \geq 10$ keV set to 1

For higher secondary electron production thresholds (i.e., >100 keV), if WHAT(3)<<1, there would be a fraction of atomic electrons not contributing to scattering. WHAT(3) should be set to 1.

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

A finite value should be entered for WHAT(3), otherwise an error message will occur

*** Atomic electron contribution to MCS for material …. Set to zero. Are you sure?****

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 demanding situations like electron backscattering the model performs well!

Options summary:

Some of the ionization, transport, and MCS cards:

EMFCUT – Set δ-ray production and transport threshold (e^-, e^+)
DELTARAY – Modify δ-ray production parameters (hadrons, muons)
IONFLUCT – Control the energy loss fluctuations *(for expert)*
MULSOPT - Control multiple/single scattering
PART-THR - Set particle transport threshold (hadrons, muons)

STERNHEI - Ionization potential and density effect
MAT-PROP – Material parameter customization

4/4 – Transport in electric and magnetic fields

Magnetic field tracking in FLUKA

FLUKA allows for tracking in arbitrarily complex magnetic fields (and electric fields in vacuum or gases).

Electric/Magnetic field tracking is performed by iterations until a given accuracy when crossing a boundary is achieved.

Meaningful user input is required when setting up the parameters defining the tracking accuracy.

Furthermore, when tracking in magnetic fields, FLUKA accounts for:

- The decrease of the particle momentum due to energy losses along a given step and hence the corresponding decrease of its curvature radius. Since FLUKA allows for fairly large (up to 20%) fractional energy losses per step, this correction is important in order to prevent excessive tracking inaccuracies to build up, or force to use very small steps
- The precession of the MCS **final direction** around the particle direction: this is critical in order to **preserve** the various **correlations** embedded in the FLUKA advanced MCS algorithm
- The precession of a (possible) particle polarization around its direction of motion: this matters only when polarization of charged particles is a issue (mostly for muons in Fluka)

NOTE: FLUKA does not generate synchrotron radiation from accelerated charged particles in a coupled way, but it can compute synchrotron radiation via SOURCE cards

How to define a magnetic (or electric field)

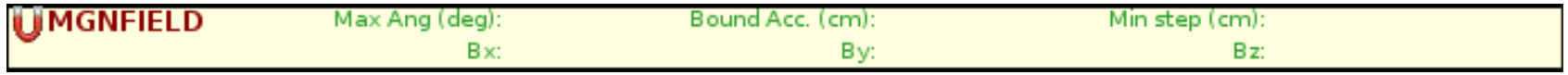
- Declare the regions with field in the ASSIGNMAT card (what(5))

Note: fields can be set independently for prompt and/or residual radiation

- Set field/precision with the card MGNFIELD (or ELCFIELD) card

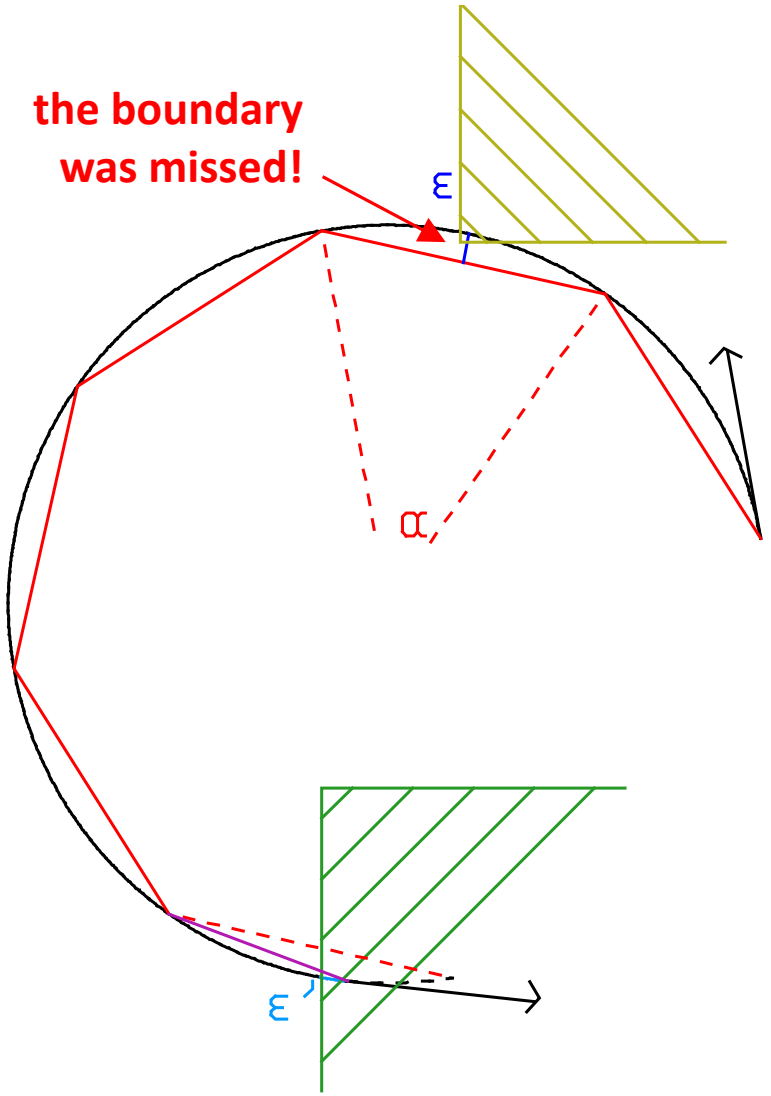
```
* ..+....1....+....2....+....3....+....4....+....5....+....6....+....7..
ELCFIELD            α          ε       Smin         Ex         Ey         Ez
```

```
* ..+....1....+....2....+....3....+....4....+....5....+....6....+....7..
MGNFIELD            α          ε       Smin         Bx         By         Bz
```



- If the field is UNIFORM, set its components (in Tesla or MV/m) in $\{B_x\ B_y\ B_z\}$ (or $\{E_x\ E_y\ E_z\}$)
- If not, leave $B_x=B_y=B_z=0$ (or $E_x=E_y=E_z=0$) and return the electric/magnetic field pointwise through the user routine MAGFLD (or ELEFLD)
- α, ε, S_{min} control the precision of the tracking, (see next slides). They can be overridden / complemented by the STEPSIZE card - Note: different defaults for MGNFIELD and ELCFIELD

Magnetic field tracking in FLUKA



The true step (black) is approximated by linear sub-steps. Sub-step length and boundary crossing iteration are governed by the required tracking precision

The red line is the path actually followed,
the magenta segment is the last substep, shortened because of a boundary crossing

- α= max. tracking angle [degrees]; <30 recommended
- **ε = maximum permissible error [cm] in geometry intersections (must be set << local dimensions)**

The end point is ALWAYS on the true path, generally NOT exactly on the boundary, but at a distance < ε ' from the true boundary crossing (light blue arc)

Electric/Magnetic field tracking in FLUKA – new algorithm


```
* ..+....1....+....2....+....3....+....4....+....5....+....6....+....7..
MGNFIELD          α         ε      Smin        Bx        By        BzRu
```

- For uniform magnetic fields, the previous algorithm has the particle going along cords of the circle
- For *non-uniform fields* (which would need to be programmed by means of a user-routine), in vacuum or gas, a more precise tracking algorithm based on Runge-Kutta-Gill 4th is recommended.

```
* ..+....1....+....2....+....3....+....4....+....5....+....6....+....7..
MGNFIELD          α         ε      Smin        Bx        By        BzRuRUNGKUTT
```

- The Runge-Kutta Gill tracking is activated by setting SDUM card of MGNFIELD to 'RUNGKUTT'
- NOTE#1: If electric fields are present (via ELCFIELD card), the Runge-Kutta Gill tracking is used ***automatically*** regardless of MGNFIELD SDUM card
- NOTE#2: ELCFIELD has no SDUM options currently available

Thanks for your attention!

Extra slides

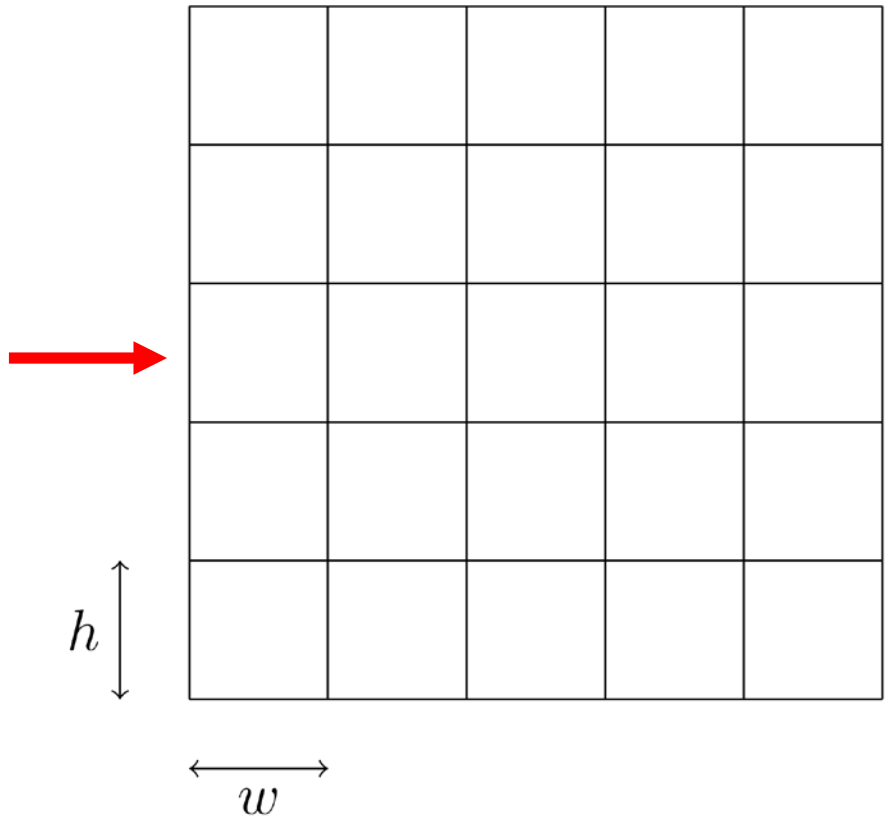
Example of setting threshold

Example (Thresholds)

- Suppose a geometry or scoring grid with dimensions h x w ~ 50 microns
- Let 10-MeV electrons impinge from the left

What are appropriate threshold values?

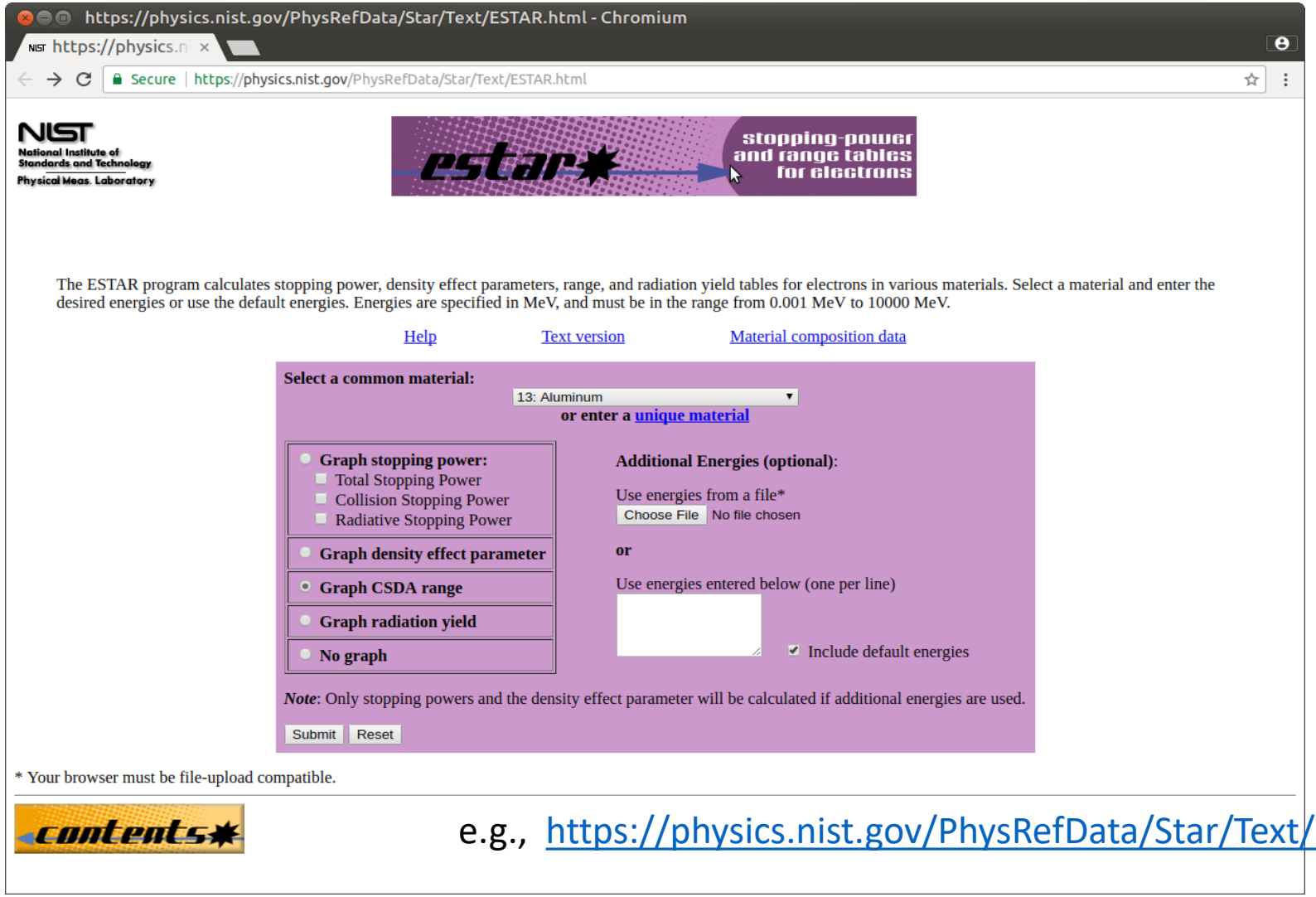
Naively: track electrons as long as they can travel farther than one bin width.



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

(beware of foils, wire scanners, etc. !)

Examine the particle's range



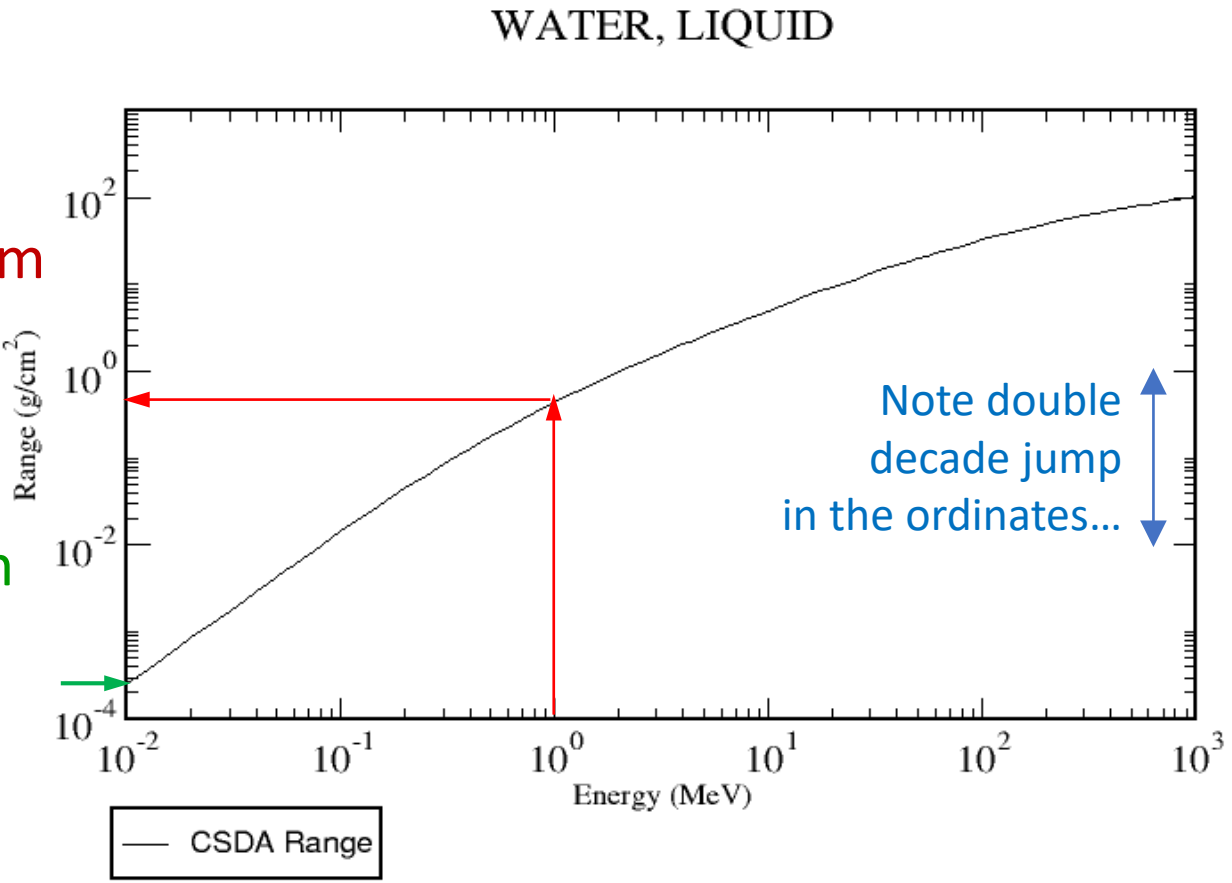
e.g., https://physics.nist.gov/PhysRefData/Star/Text/ESTAR.html

Range for electrons in water

Transport threshold at 1 MeV? → 1-MeV e^-
Range is ~0.7 g/cm^3 → 7000 um
Depositing/killing them on the spot in a ~50 um geometry is asking too much...

Transport threshold at 10 keV? → 10-keV e^-
range is O(10^{-4}) cm = O(1 um) Depositing them on the spot in a ~50 um geometry is fine, a bit Overkilling (CPU wasted)

If you're working with coarser geometries or scoring grids, higher thresholds can be OK!



(note: Water density: 1 g/cm^3 →
We may directly read range in cm)

Moliere distribution

Multiple (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, where χ is proportional to the deflection angle:

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

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

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

Example: Gas Bremsstrahlung

Gas Bremsstrahlung in FLUKA

In spite of the high or ultra-high vacuum in storage rings, residual gas molecules lead to an observable effect:

- Electrons impinging on them may lead to the emission of Bremsstrahlung photons.
- E.g. for GeV electrons → Bremsstrahlung photons up to ~GeV.
- Photons at these energies are much more penetrating than synchrotron light, which typically does not exceed O(100 keV).
- Thus, there is a radiation hazard.
- It is therefore important to make preliminary studies assessing the dose due to residual-gas Bremsstrahlung.

Gas Bremsstrahlung in FLUKA: MATERIAL / MULSOPT / EMFCUT

- We cannot do a simulation at the actual density corresponding to 10^{-9} mbar.
- Main idea: we do a simulation at an *artificially higher density*, and *linearly scale down the results a posteriori to the actual gas density*.
- At high densities, however, there are effects leading to the *angular broadening* of the electron beam which are not present at low densities (i.e., do not scale with density) and should be effectively switched off:

```
..+....1....+....2....+....3....+....4....+....5....+....6....+....7....+....8
Suppress multiple scattering in the air target
MULSOPT                    Type: ▾              Optimize: off ▾
 h/μ steps: 0          e-e+ steps: 0          h/μ Corr: No corrections ▾  e-e+ Corr: no MCS ▾
                            Mat: GAS ▾             to Mat: ▾                  Step: 0.
* ..+....1....+....2....+....3....+....4....+....5....+....6....+....7....+....8
* Suppress multiple scattering in the air target
MULSOPT         0.0        0.0        3.0        GAS                 0.
```

```
Suppress Moller scattering in the air target
EMFCUT                     Type: ELPO-THR ▾     e-e+ Brem: 0.0      γ Bhabha/Moller: 2.0
 Photonuc: 0.0                 Mat: GAS ▾            to Mat: ▾                Step: 0.0
* Suppress Moller scattering in the air target
EMFCUT          0.0        2.0        0.0        GAS                 0.0ELPO-THR
```

Gas Bremsstrahlung – example (I)

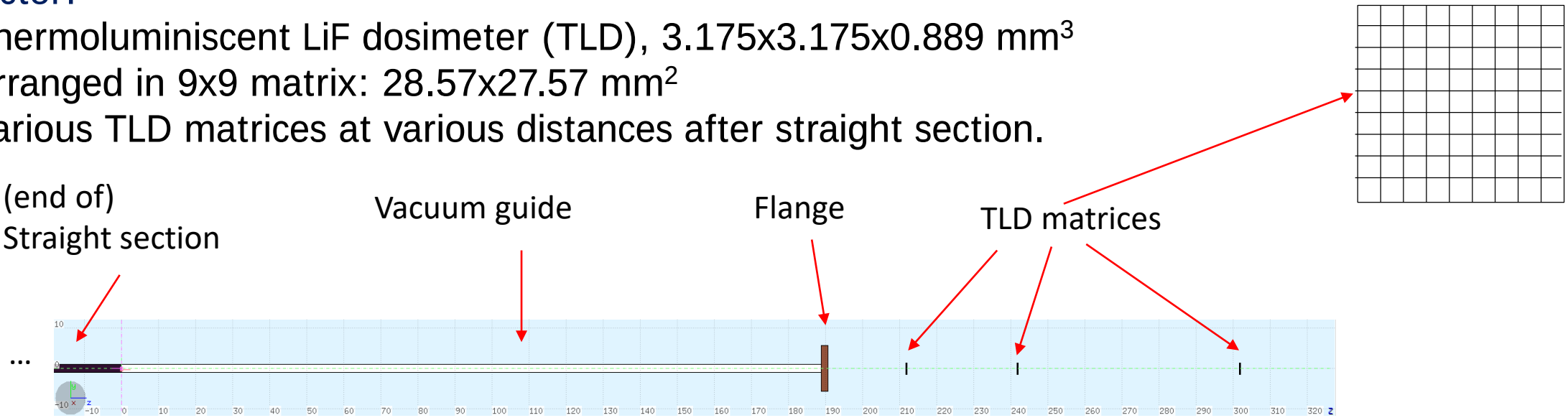
ADONE e^+e^- storage ring (INFN-Frascati, 1980s-1990s):

Relevant machine section for this example:

- 613.5 cm long straight section (residual gas at 10^{-9}-10^{-10} Torr)
- ...followed by a 190.7 cm long vacuum guide
- ...topped by a 1.87 cm thick stainless steel flange
- ...surrounded by air (atmospheric pressure).

The detector:

- Thermoluminiscent LiF dosimeter (TLD), 3.175x3.175x0.889 mm^3
- Arranged in 9x9 matrix: 28.57x27.57 mm^2
- Various TLD matrices at various distances after straight section.



Gas Bremsstrahlung – example (II)

Dose (measured vs FLUKA) at the TLD matrix 541.7 cm away from end of straight section:

Open circles: central row
... then pairwise away from central row

Exp issues: inhomogeneous pressure

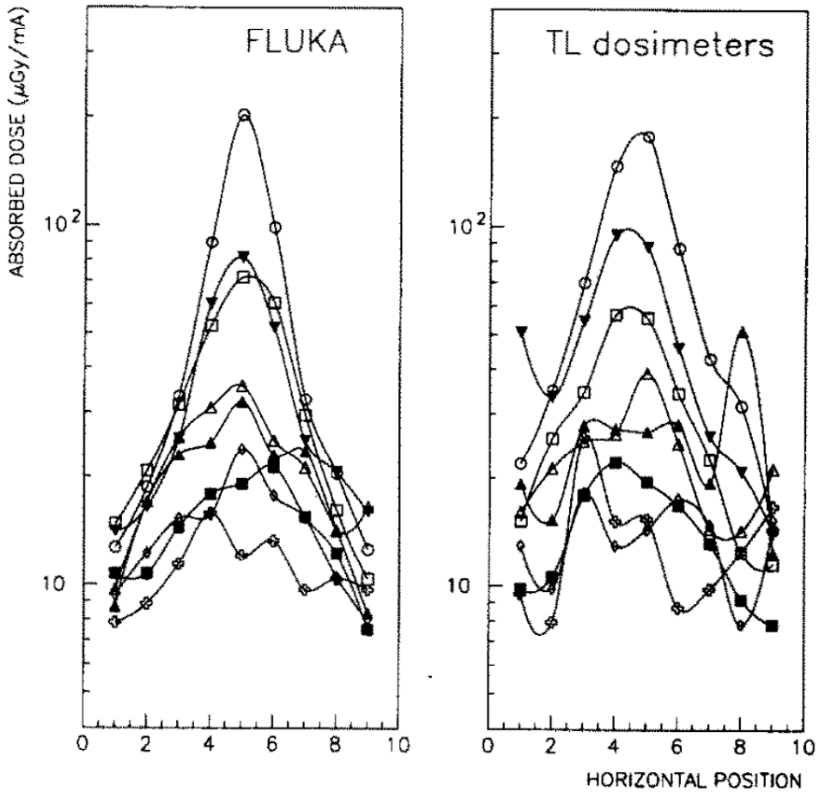


Fig. 2. Horizontal intensity distribution (in terms of absorbed dose), at 541.7 cm from the end of the straight section, as a function of horizontal position for various vertical positions of the TLDs, and comparison with the results of the simulation.

Relevant references with many more details:

Ferrari A. *et al., Nucl Instrum Meth B* **83** 518-524 (1993)
Esposito A. *et al., Nucl Instrum Meth B* **88** 345-349 (1994)

End