Ionization and Transport

20th FLUKA Beginners' Course

Stellenbosch University (South Africa)

May 28 – June 1, 2018

Overview

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

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

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

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 fields.

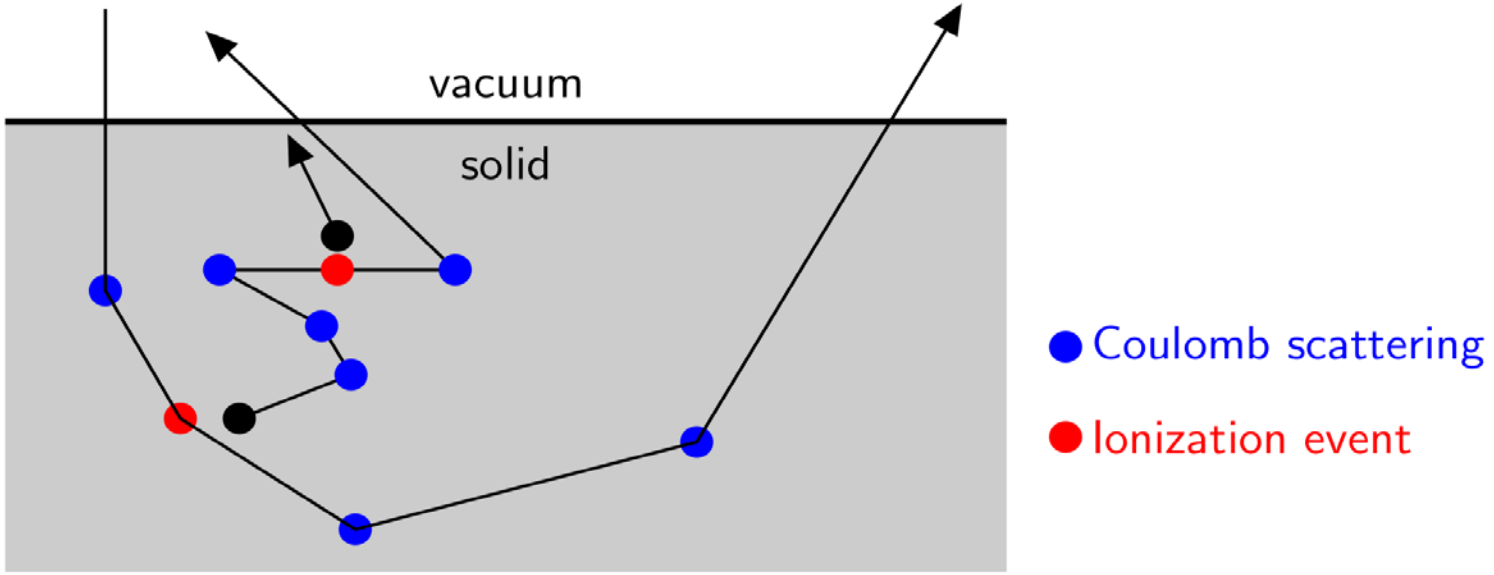
In a “detailed” Monte Carlo simulation

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

For each type of event: differential cross section (dxs)
→ energy loss T, deflection angle.

E.g. ionization losses and Coulomb scattering with target atoms

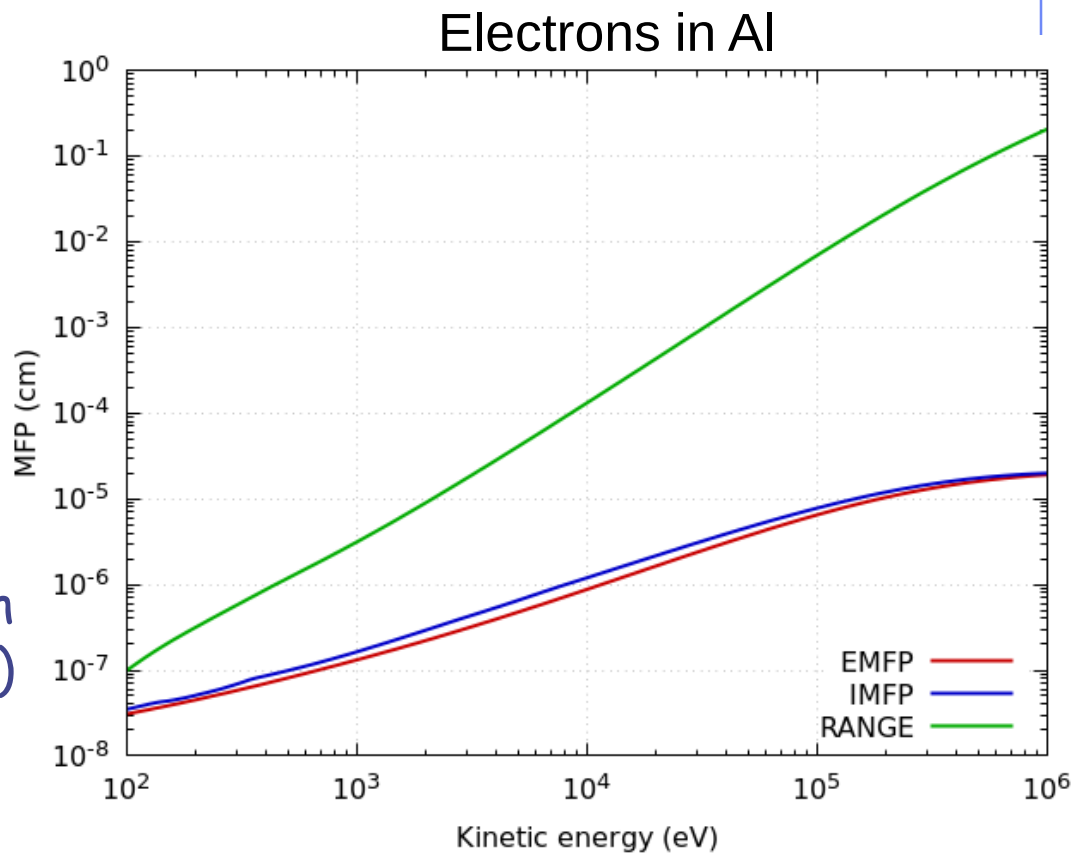
Ideally one would simulate each particle trajectory event by event (detailed simulation): take step, decide interaction type, sample from dxs, update ene/dir… and loop.



...is this feasible in practice?

Estimate number of ionization losses

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



IMFP: inelastic mean free path
(EMFP: elastic mean free path)

For a 1-MeV e^-: range/IMFP ~ **10000** events (!).

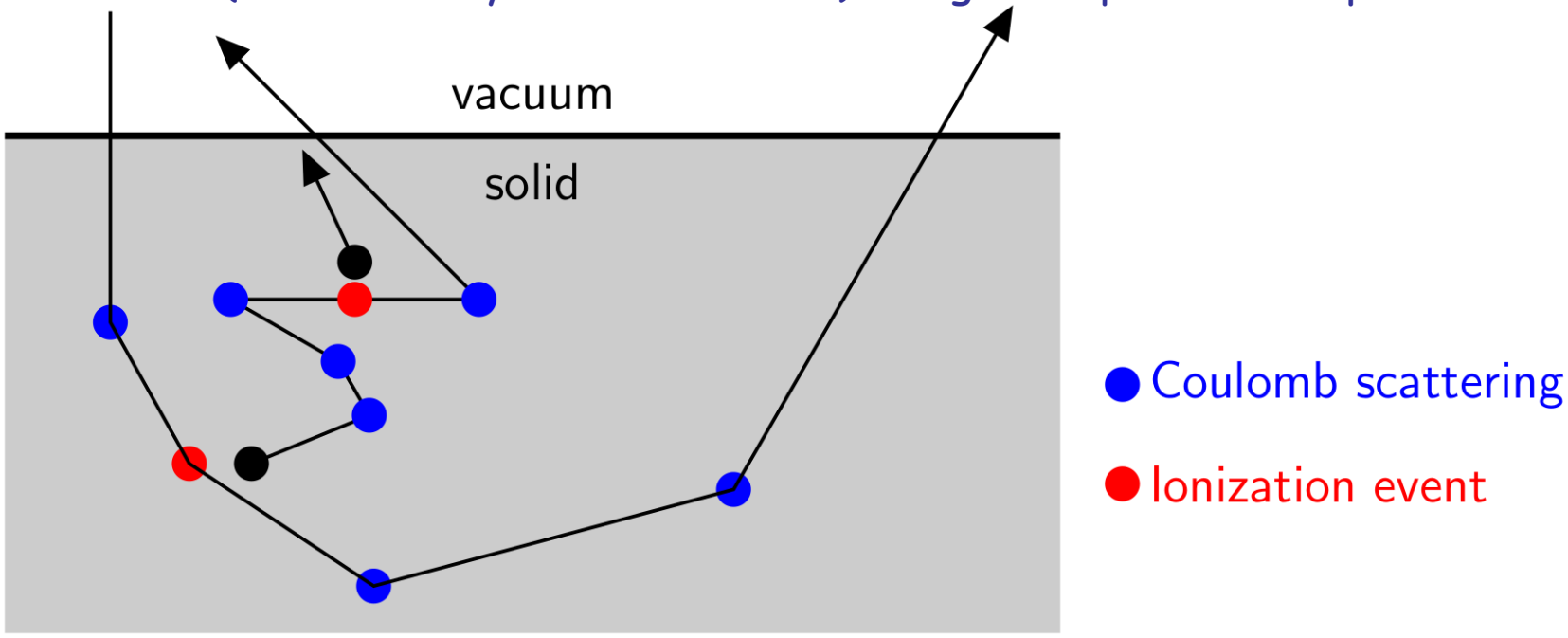
Too many to simulate explicitly.

A more practical approach

Condensed simulation schemes are a practical necessity to keep CPU time within acceptable bounds.

Main idea in scheme adopted in FLUKA:

- Sample ionization losses explicitly only when the effect is large
- Account for global effect of small losses in an effective way (to be briefly discussed here) along each particle step.



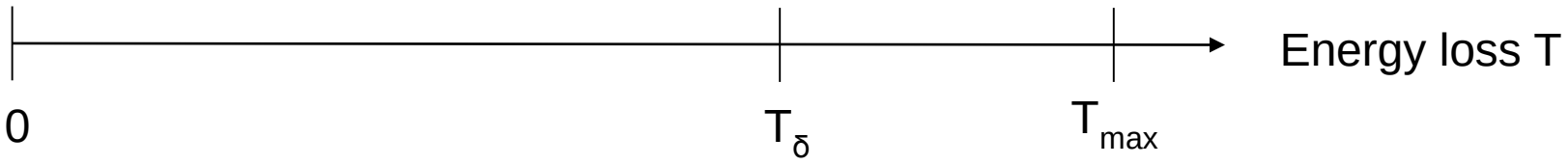
In this session: brief overview of FLUKA's condensed transport scheme for ionization (as well as multiple Coulomb scattering).

Ionization energy losses

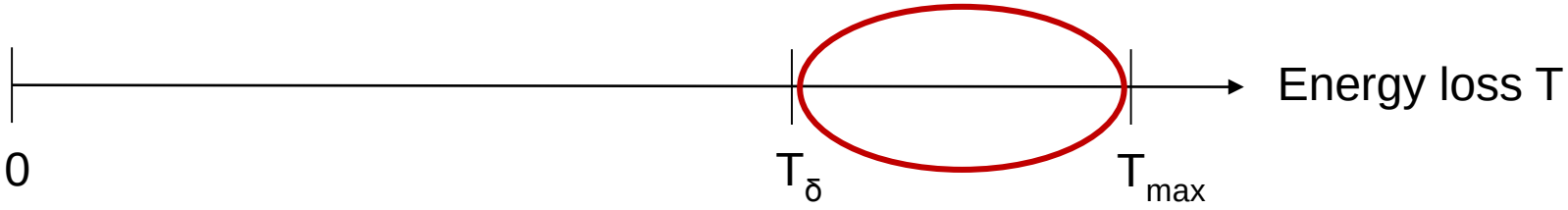
Energy losses of charged projectiles in collisions with the electrons of the medium

Ionization energy losses in FLUKA

2 different treatments: small vs large energy losses.



$T > T_\delta$: 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?

$T > T_\delta$: detailed sampling

Depending on projectile, discrete energy losses are sampled from:

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

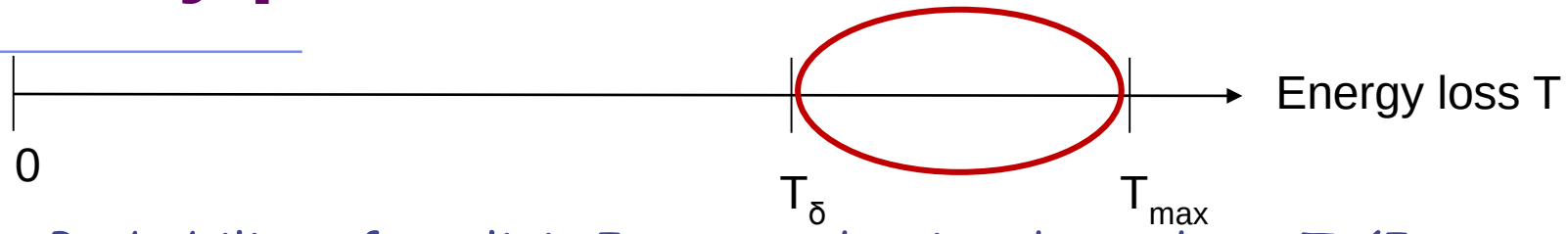
$$\left(\frac{d\sigma}{dT_e}\right)_{\frac{1}{2}} = \frac{2\pi r_e^2}{\beta^2}\frac{m_e c^2}{T_e^2}\left[1-\beta^2\frac{T_e}{T_{max}}+\frac{1}{2}\left(\frac{T_e}{T_0+Mc^2}\right)^2\right]$$

Specific expressions:

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

T 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, can be overridden (rule of thumb below):
  - Electrons,positrons: 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:

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

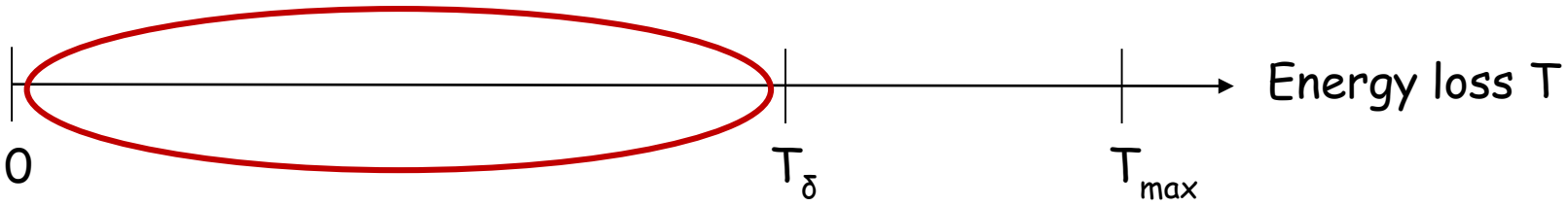
where:

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: 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 (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

Spin 0 (spin 1/2 is similar):

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

- 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 $v \gg v_e$)

- 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.

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 dσ/dT (see extra slides):

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

- 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

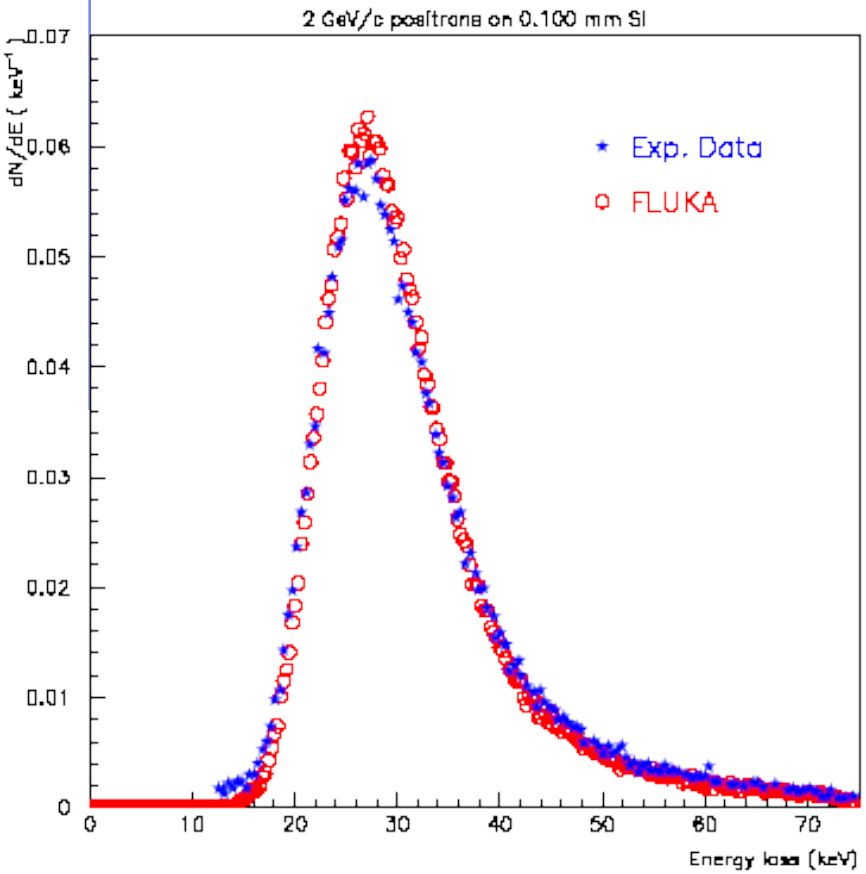
Energy-dependence in step and material parameters

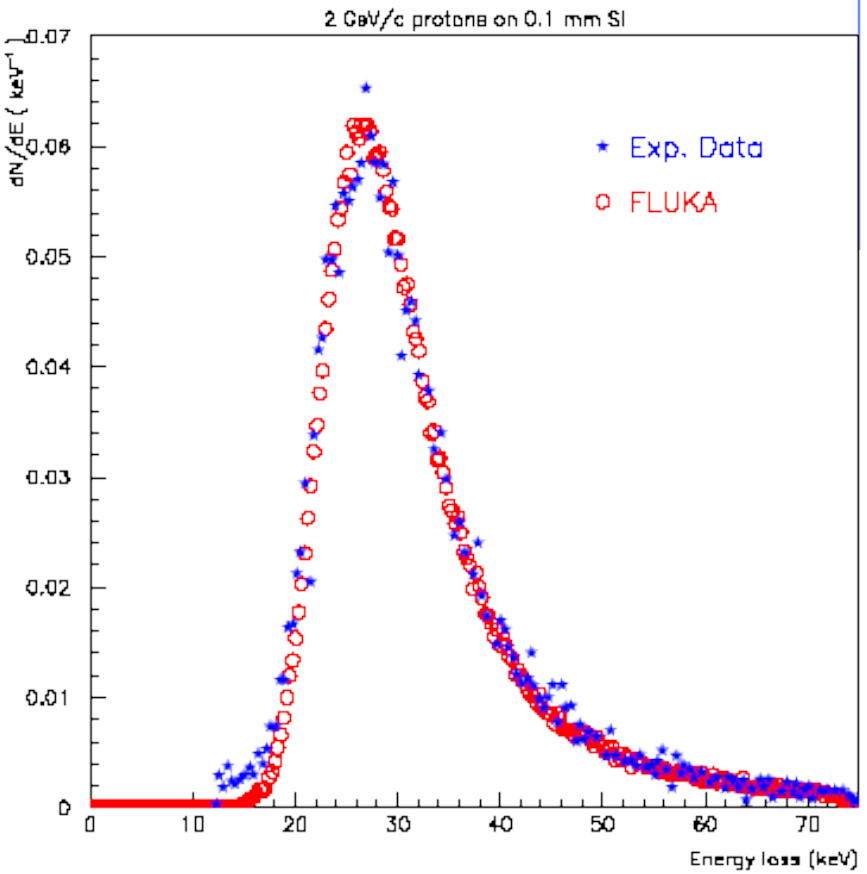
Below the δ-ray threshold, energy losses are treated as "continuous", with some **special features**:

- 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

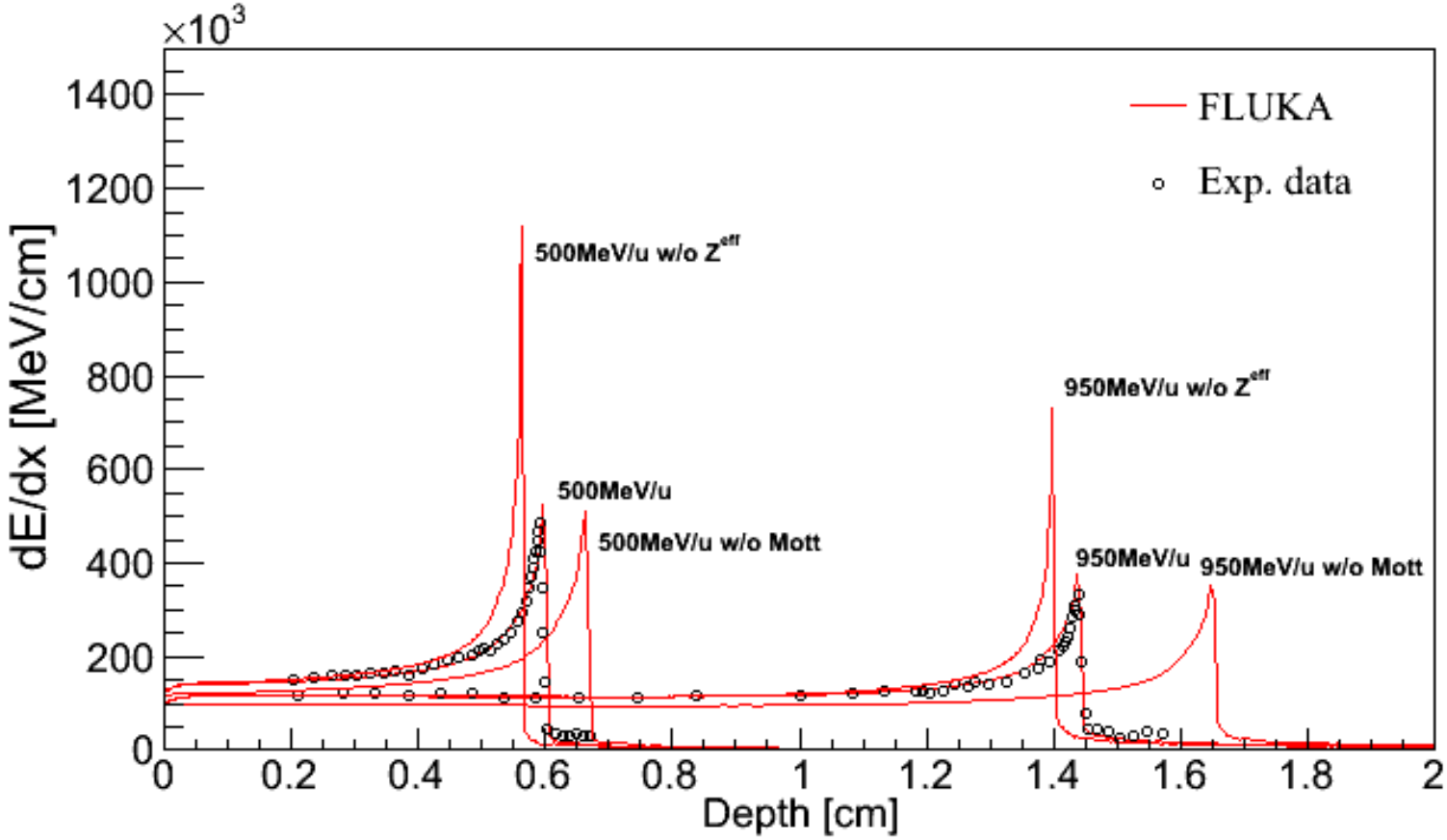
Heavy ions

- 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.

Ref: Uggerhoj U.I., *Matem.-fys. Meddelelser* **52** 699 (2006)

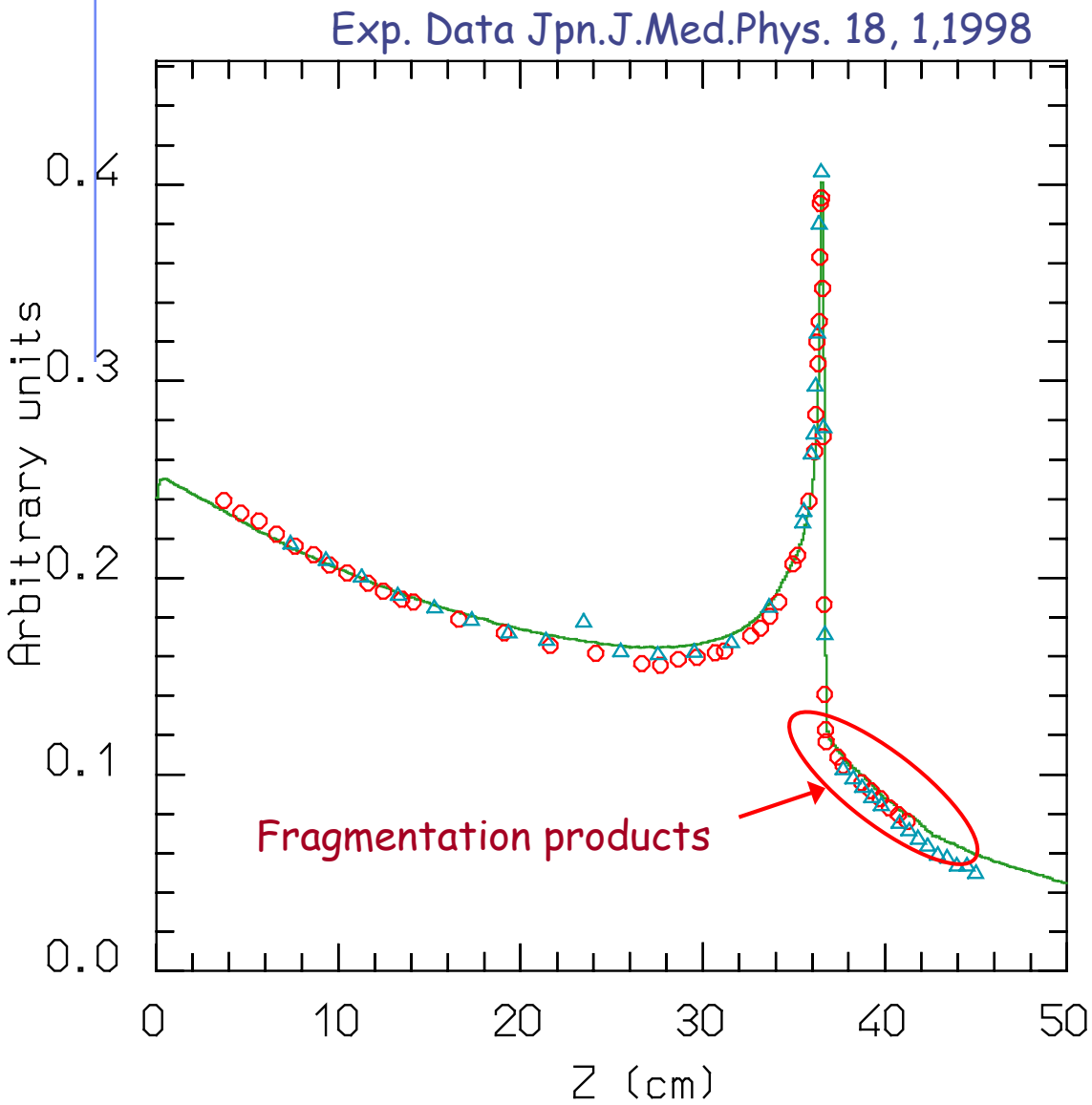
Heavy ions

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



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

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

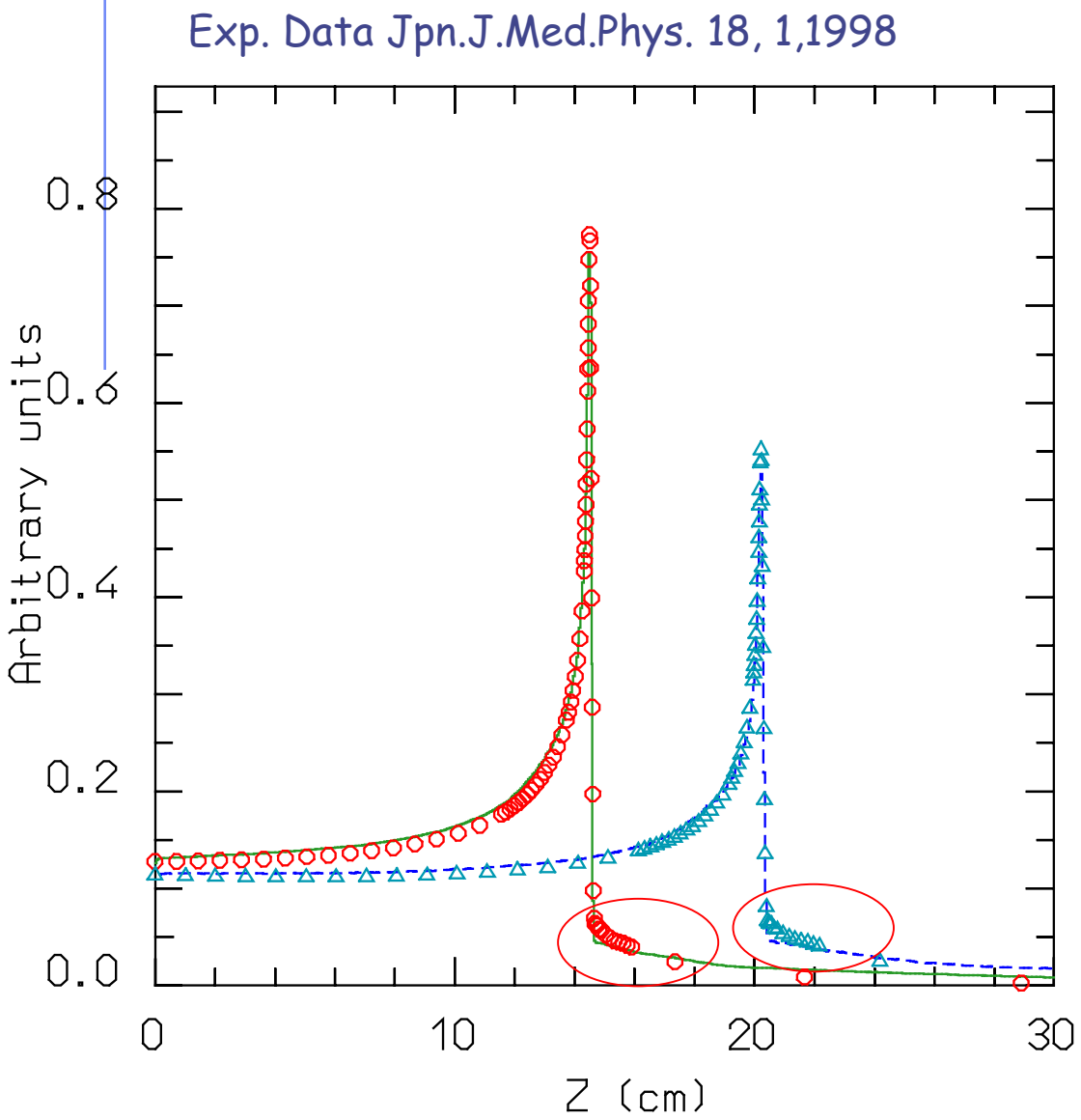


Dose vs depth distribution for 670 MeV/n ^{20}Ne ions on a water phantom.

Solid line is the FLUKA prediction. The symbols are 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.

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 approach via cumulants of $d\sigma/dT$.
- Approach is set up in such a way that it works for all charged projectiles considered in FLUKA.
- Dedicated effort for ions leads to good agreement with exp.

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	$e^{\pm}$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 card: allows to set 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 are special -> The neutron threshold (rounded to closest group boundary), recommended to leave at the default value (1 x 10^{-5} eV). Careful to reset if you set threshold from-to in a range containing neutron.

Heavy ion transport thresholds are derived from that of a He4 ion, scaling with ratio of atomic weight ion/He4.

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?

Example

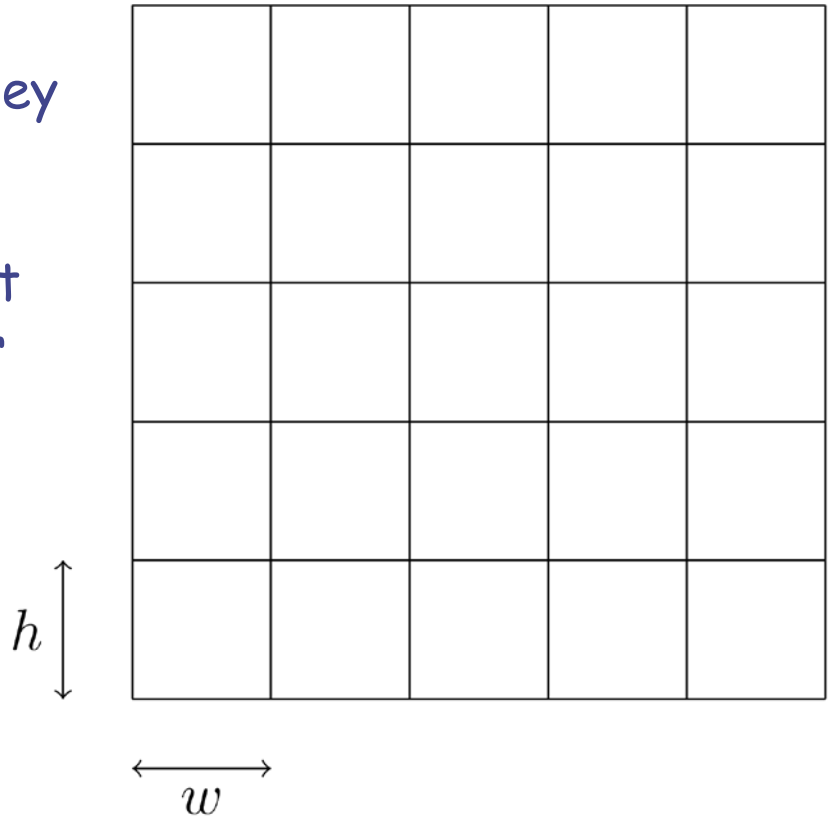
Suppose geometry or scoring grid with dimensions h,w ~ 50 microns

Let 10-MeV electrons impinge from the left.

What are appropriate threshold values?

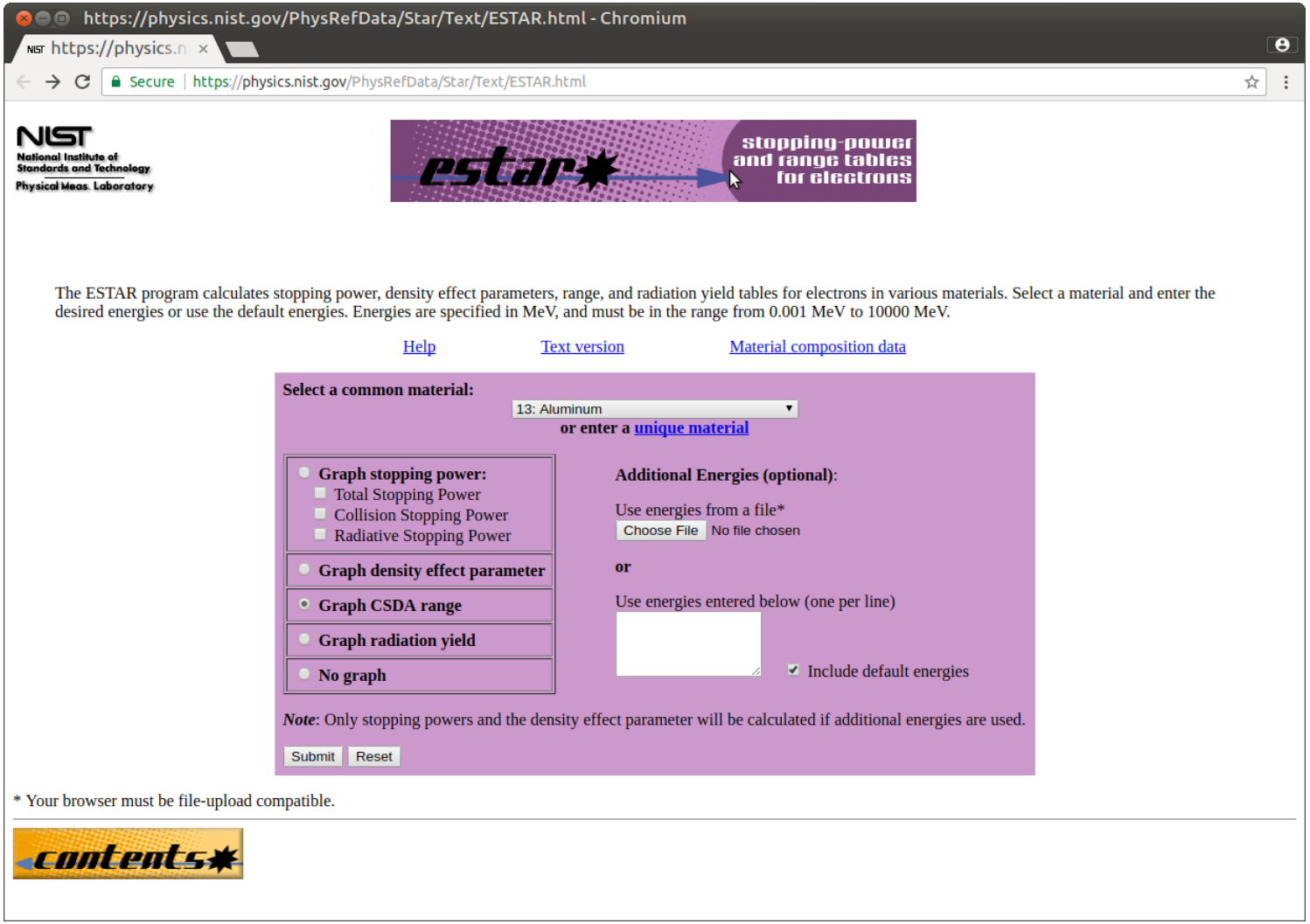
Naively: track electrons as long as they can travel farther than bin width.

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



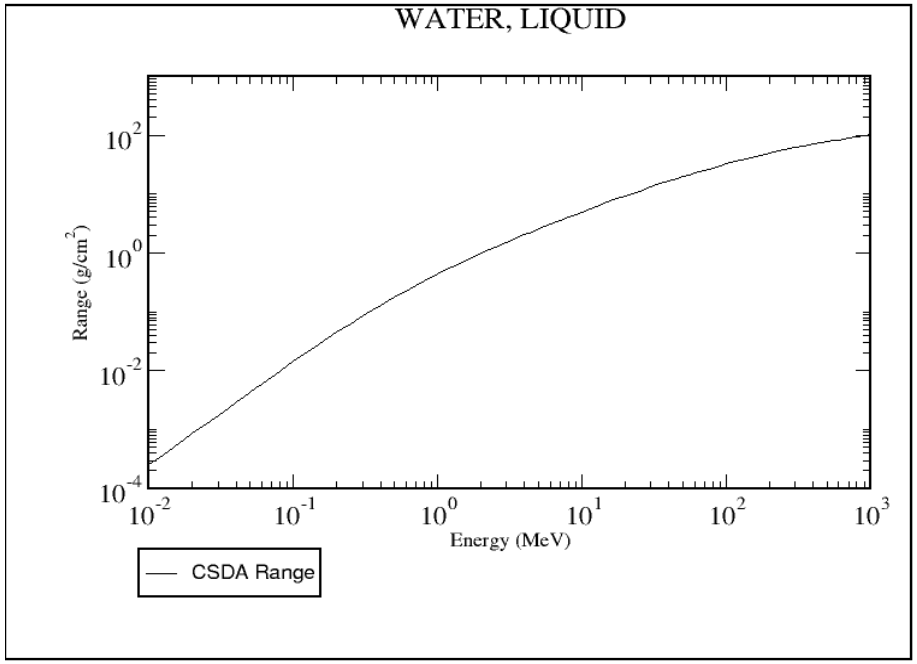
1) Examine range

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



Range for electrons in water

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



Note double decade jump in the ordinates…

Transport threshold at 1 MeV? → 1-MeV e^- Range is O(1 mm) = 1000 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

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

How to set threshold values?

- General guidelines to set threshold energies?
  - It depends on the “granularity” of the geometry and/or of the scoring mesh. Energy/range tables are very useful.
  - Consider the interest in a given region.
  - Warning 1: to reproduce correctly electronic equilibrium, neighboring regions should have the same electron energy (NOT range) threshold. To be kept in mind for sampling calorimeters
  - Warning 2 : Photon thresholds should be lower than electron thresholds (photons travel more)
  - Warning 3: ***low thresholds for e-/e+/gammas are CPU eaters***
- Delta-ray production threshold:
  - If production threshold < transport threshold: CPU wasted in producing and dumping particles on the spot
  - If 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 in output file

```
 === Particle transport thresholds:

Global cut-off kinetic energy for particle transport:  1.000E-04 GeV
The cut-off kinetic energy is superseded by individual particle thresholds if set


  Cut-off kinetic energy for 4-HELIUM transport:  1.000E-04 GeV

  Cut-off kinetic energy for 3-HELIUM transport:  1.000E-04 GeV

  Cut-off kinetic energy for TRITON   transport:  1.000E-04 GeV

  Cut-off kinetic energy for DEUTERON transport:  1.000E-04 GeV

  Cut-off kinetic energy for PROTON   transport:  1.000E-04 GeV

  Cut-off kinetic energy for APROTON  transport:  1.000E-04 GeV

  Cut-off kinetic energy for ELECTRON transport defined in the Emfcut card

  Cut-off kinetic energy for POSITRON transport defined in the Emfcut card

  Cut-off kinetic energy for NEUTRIE  transport:  0.000E+00 GeV

  Cut-off kinetic energy for ANEUTRIE transport:  0.000E+00 GeV

  Cut-off kinetic energy for PHOTON   transport defined in the Emfcut card

  Cut-off kinetic energy for NEUTRON  transport:  1.000E-14 GeV
```

Electron/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 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:

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

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

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

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

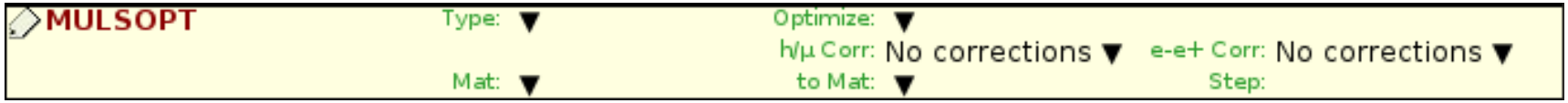
- Optionally, spin-relativistic corrections (1st or 2nd Born approximation for ele/posi), MULSOPT.
- Optionally effect of nucleus finite size (form factors) can be included (MULSOPT).
- Careful geometry tracking near boundaries.
- MCS is able to coexist with transport in magnetic fields

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):

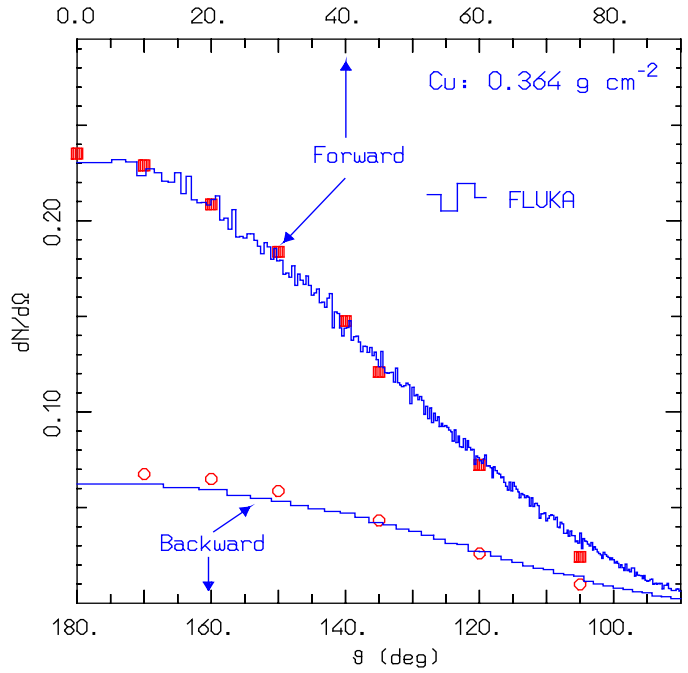
```
* ..+....1....+....2....+....3....+....4....+....5....+....6....+....7..
MULSOPT        Flag1     Flag2     Flag3      Mat1      Mat2      StepSDUM
```



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

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 (!).

FUDGEM

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

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

A value of 10^{-5} is fine for low delta-ray production thresholds: the contribution of atomic electrons is accounted for via ionization losses. Low means much lower than typical atomic shell binding energies (several 10s of keV).

For higher delta-ray production thresholds, 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:
*** 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!

Cheat Sheet

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)
PART-THR - Set particle transport threshold (hadrons, muons)

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

4/4 – Transport in magnetic fields

Magnetic field tracking in FLUKA

FLUKA allows for tracking in arbitrarily complex magnetic fields. 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.

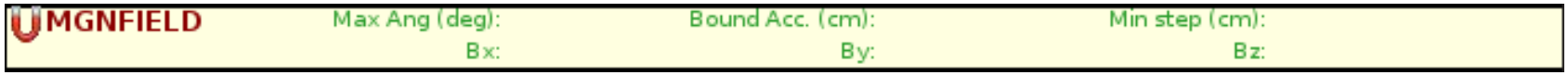
Furthermore, when tracking in magnetic fields FLUKA accounts for:

- 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)

How to define a magnetic field

- Declare the regions with field in the ASSIGNMAT card (what(5))
- Set field/precision with the card MGNFIELD:

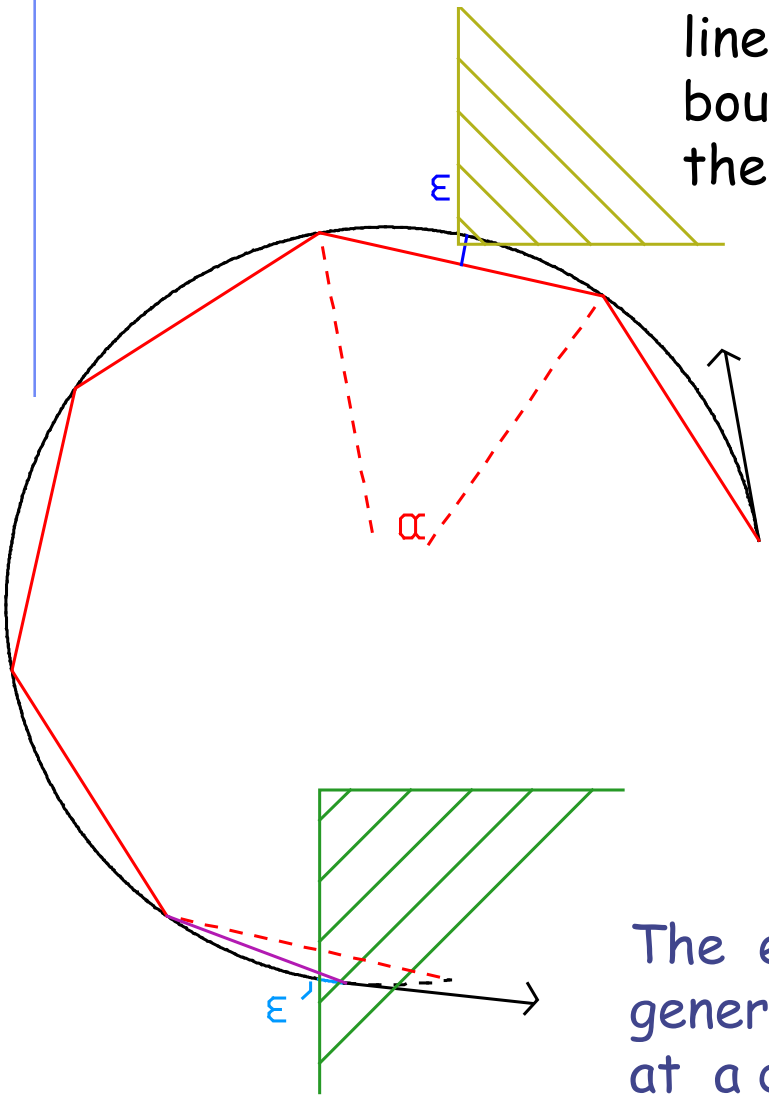
```
* ..+....1....+....2....+....3....+....4....+....5....+....6....+....7..
MGNFIELD            α           ε        Smin          Bx          By          Bz
```



- IF the field is UNIFORM set its components (tesla) in B_x, B_y, B_z
- If not, leave B_x=B_y= B_z=0 and provide a magnetic field pointwise through the user routine MAGFLD (see later)
- α, ε, Smin control the precision of the tracking, (see next slides). They can be overridden/complemented by the STEPSIZE card

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



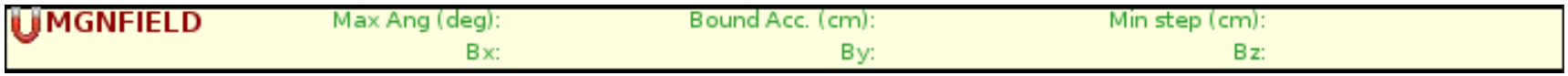
The red line is the path actually followed,
the magenta segment is the last substep, shortened because of a boundary crossing

- α= max. tracking angle (MGNFIELD)
- ε = **maximum permissible error in geometry intersections,**

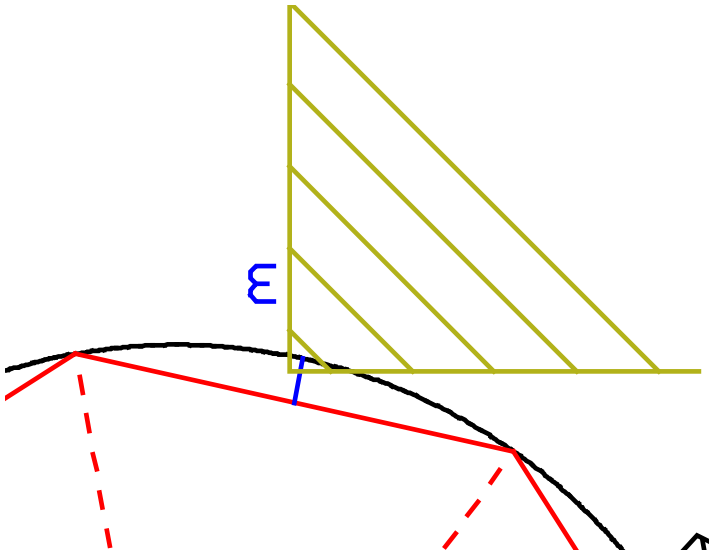
The end point is ALWAYS on the true path, generally NOT exactly on the boundary, but at a distance < ε' from the true boundary crossing (light blue arc)

Setting the tracking precision I

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



- α largest angle in degrees that a charged particle is allowed to travel in a single sub-step. Default = 57.0 (but a maximum of 30.0 is recommended!)
- ε upper limit to error of the boundary iteration in cm (ε' in fig.). It also sets the tracking error ε. Default = 0.05 cm



IF α and/or ε are too large, boundaries may be missed (as in the plot);
IF they are too small, CPU time explodes....
Both α and ε conditions are fulfilled during tracking.
→ Set them according to your problem
→ Tune ε by region with the STEPSIZE card
→ Be careful when very small regions exists in your setting : ε must be smaller than the region dimensions!

End

Additional material

Topics

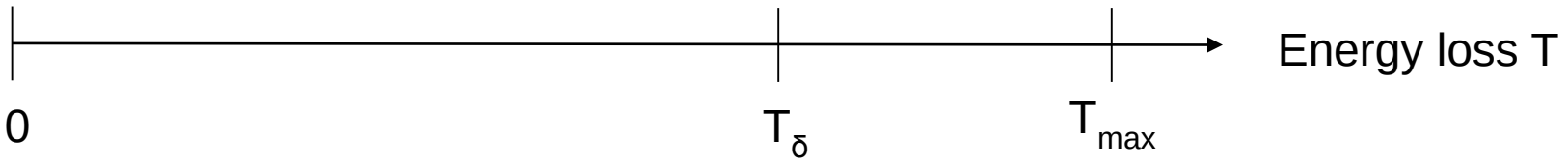
- General settings
- Interactions of leptons/photons
  - Photon interactions
    - Photoelectric
    - Compton
    - Rayleigh
    - Pair production
    - Photonuclear
    - Photomuon production
  - Electron/positron interactions
    - Bremsstrahlung
    - Scattering on electrons
  - Muon interactions
    - Bremsstrahlung
    - Pair production
    - Nuclear interactions
- Ionization energy losses
  - Continuous
  - Delta-ray production
- Transport
  - Multiple scattering
  - Single scattering

These are common to all charged particles, although traditionally associated with EM

  - Transport in Magnetic field

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. User tunable (!)***

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.

dpa: Displacements Per Atom

- FLUKA generalized particle name: DPA-SCO
- Is a measure of the amount of radiation damage in irradiated materials
  For example, 3 dpa means each atom in the material has been displaced from its site within the structural lattice of the material an average of 3 times
- Displacement damage can be induced by all particles produced in the hadronic cascade, including high energy photons.
  The latter, however, have to initiate a reaction producing charged particles, neutrons or ions.
- The dpa quantity is directly related with the total number of defects (or Frenkel pairs):

$$dpa = \frac{1}{\rho} \sum_i N_i N_F^i$$

ρ atoms/cm^3
$\mathbf{N_i}$ particles per interaction channel i
$\mathbf{N_f^i}$ Frenkel pairs per channel

Control of step size II

Step sizes are optimized by the DEFAULT settings. If the user REALLY needs to change them with:

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
```

DEstep should always be below 30%

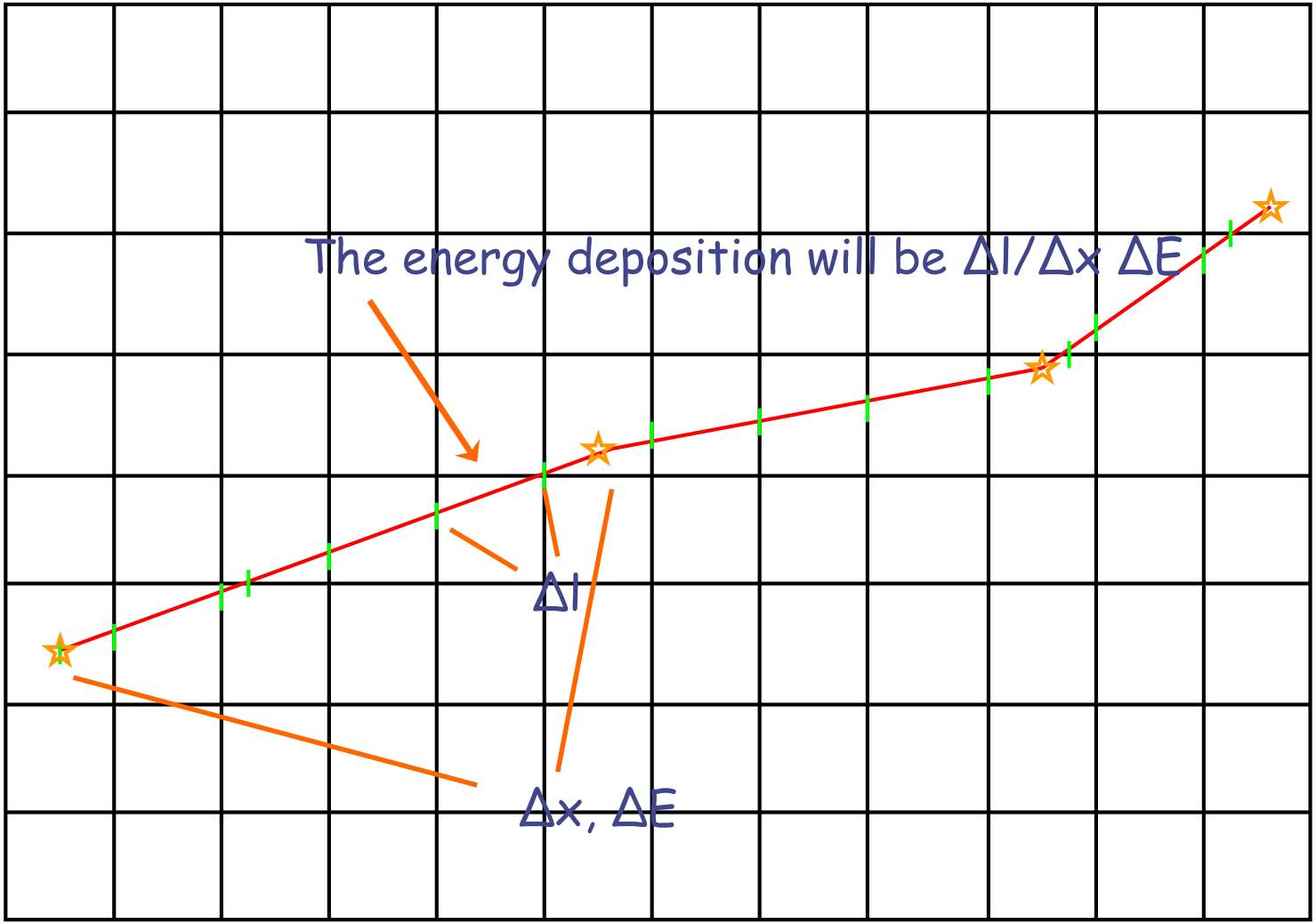
- In most routine problems, a 20% fraction energy loss gives satisfactory results. For dosimetry, 5-10% should be preferred.

WARNING : if a **magnetic field** is present, it is important to set also a maximum absolute step length and possibly a precision goal for boundary crossing by means of command STEPSIZE (see later)

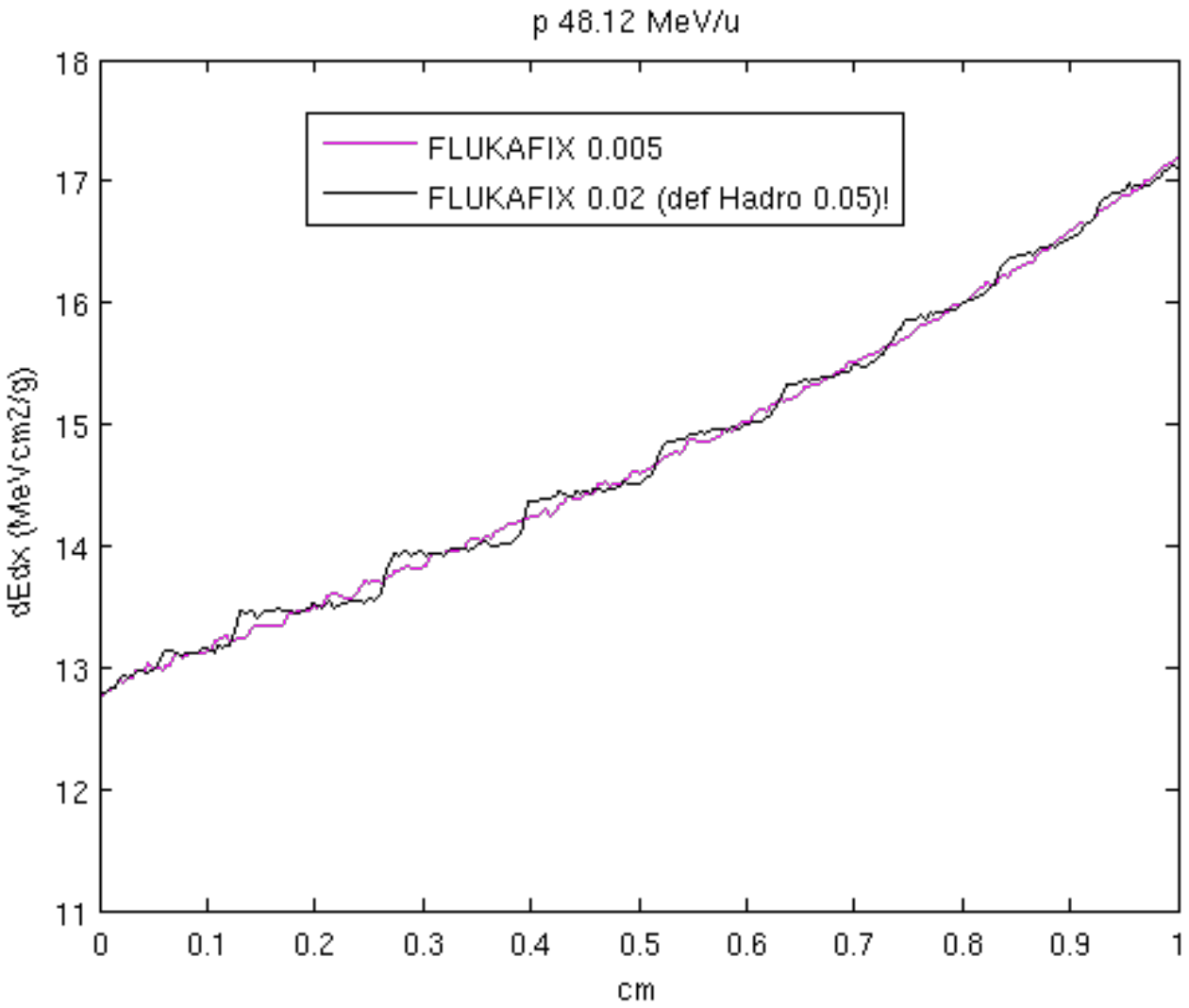
Some warnings about scoring:

- Every charged particle step ***Δx*** has its length constrained by:
  - Maximum fractional energy loss (see **FLUKAFIX**)
  - Maximum step size for that region (see **STEPSIZE**)
  - MCS (or other) physical constraints
  - Distance to next interaction (nuclear, δ ray etc)
- The ***average*** energy loss is computed as a ***careful integration*** over the dE/dx vs energy curve and ***then*** it is fluctuated → a final ***ΔE*** is computed and used for scoring → resulting in a scored ***average effective ΔE/Δx*** uniform along that step
- The particle energy used for track-length estimators is the average one along the step (E_0-ΔE/2)

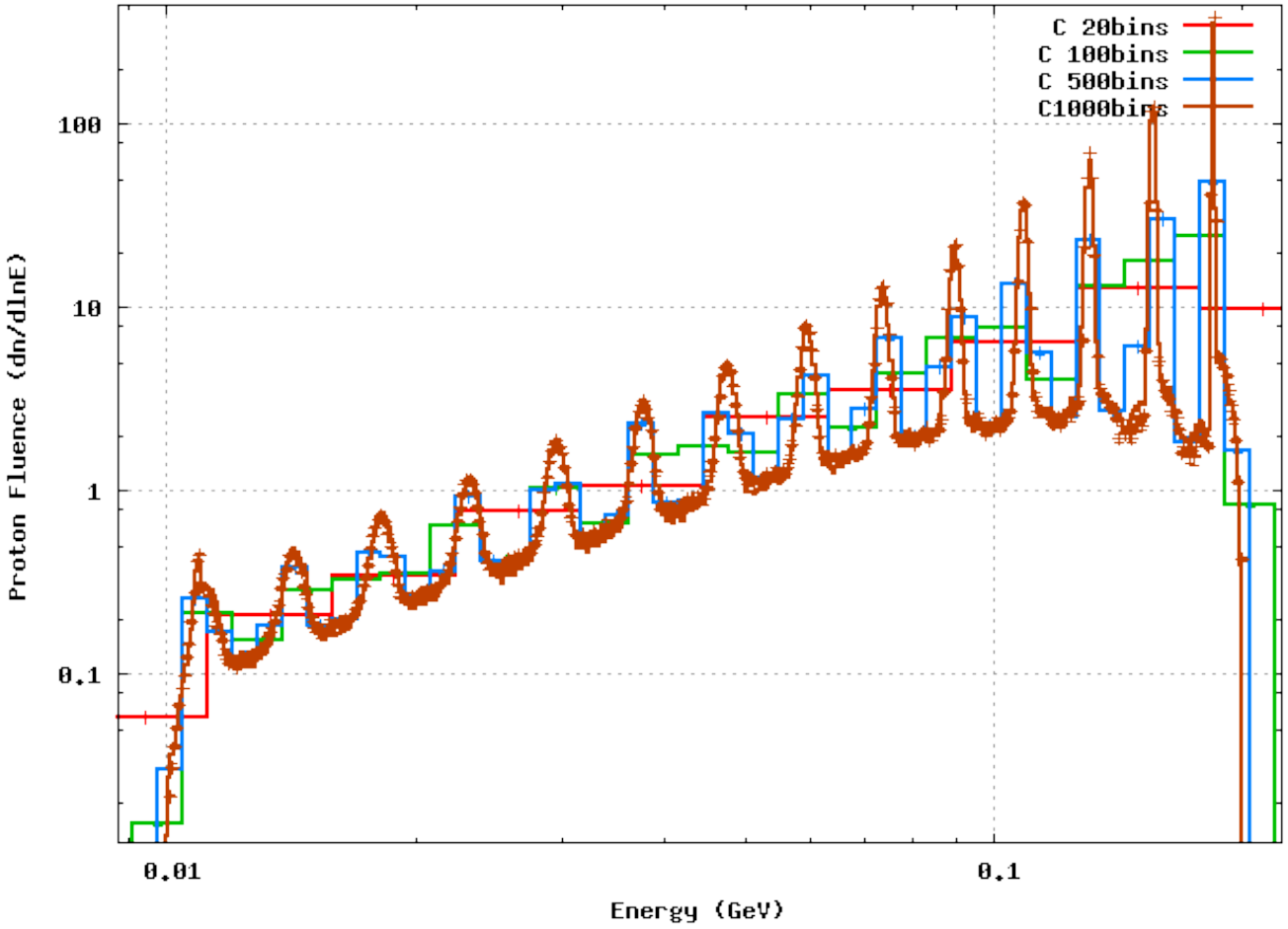
USRBIN track apportioning scoring



USRBIN track apportioning scoring



USRTRACK scoring: 200 MeV p on C



Default settings, ≈ 20% energy loss per step

Ionization Transport Cheat Sheet

DELTARAY – Modify δ-ray effect parameters (for charged hadrons, muons)

EMFCUT – Set δ-ray production and transport threshold (for electrons/positrons)

PART-THR - Set particle transport threshold (for hadron, muons)

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

IONFLUCT – Set ionization fluctuation options

EMFFIX - Set step size control for electrons/positrons

FLUKAFIX – Set step size control for hadrons/muons

MGNFIELD - Set magnetic field precision

STEPSIZE - Set stepsize in magnetic field

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?

Landau distribution

- Lev Landau (1944), assuming:
- No Bremsstrahlung, only ionization events.
- Short path lengths ↔ Δ << E, where Δ = total energy loss.
- Hard events via Thomson cross section:

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

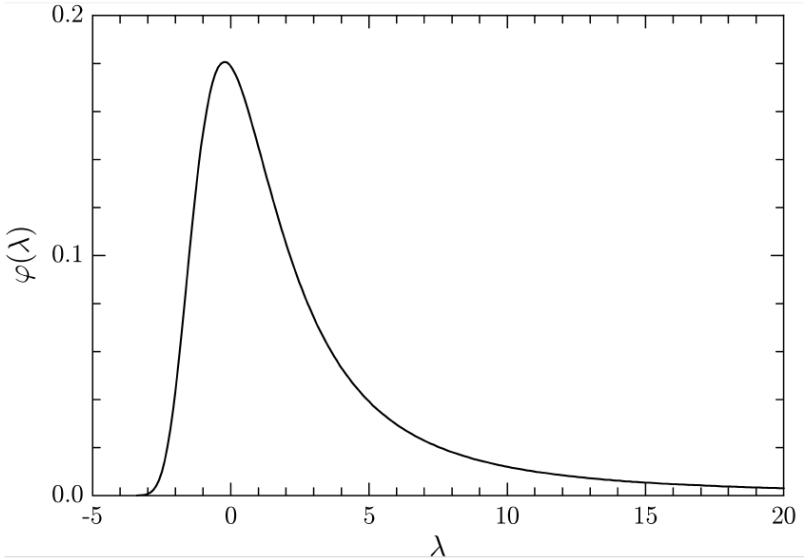
- Distant collisions (small losses): Bethe stopping formula, no fluctuations.
- $T_\delta \rightarrow$ infinity (Laplace transform involved)
- With all these approximations, he derived the distribution of energy losses after the projectile has traveled path length s

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

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

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

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



FLUKA's approach to loss fluctuations

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!

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:

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

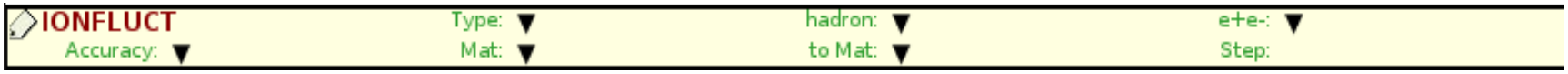
Advantages of FLUKA's approach

- As opposed to Landau distribution (see additional slides), it does not rely on a particular 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* (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.

Ionization fluctuation options

Ionization fluctuations are simulated or not depending on the DEFAULTS used. Can be controlled by the IONFLUCT card:

```
* ..+....1....+....2....+....3....+....4....+....5....+....6....+....7..
IONFLUCT        FlagH    FlagEM  Accuracy       Mat1       Mat2       STEP
```



Remember always that δ-ray production is controlled independently and cannot be switched off for e^+/e^- (it would be physically meaningless)

$T > T_\delta$: detailed sampling

Depending on projectile, discrete energy losses are 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^+)

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

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

T is sampled from these differential xs according to projectile type.
All moments reproduced: avg energy loss, fluctuations, etc

Energy dependent quantities I

- Most charged particle transport programs sample the next collision point by evaluating the cross-section at the beginning of the step, neglecting its energy dependence and the particle energy loss;
- The cross-section for δ ray production at low energies is roughly inversely proportional to the particle energy;

  a typical 20% fractional energy loss per step would correspond to a similar variation in the cross section
- Some codes use a rejection technique based on the ratio between the cross section values at the two step endpoints, but this approach is valid only for monotonically decreasing cross sections.

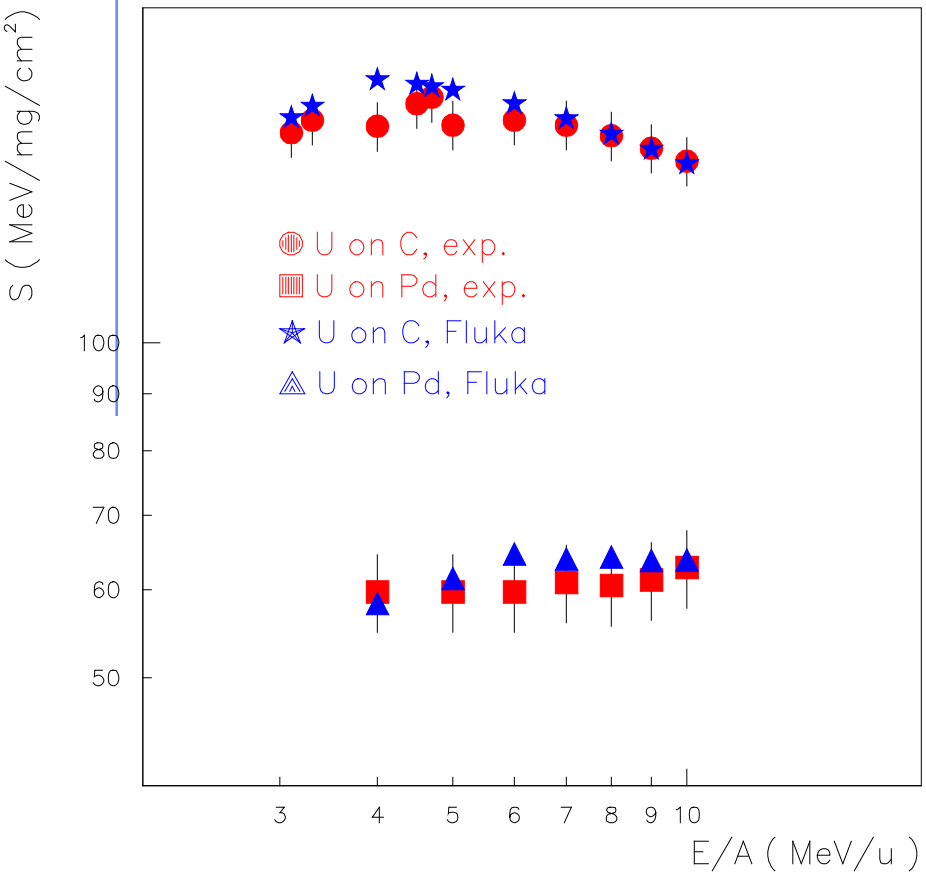
Energy dependent quantities II

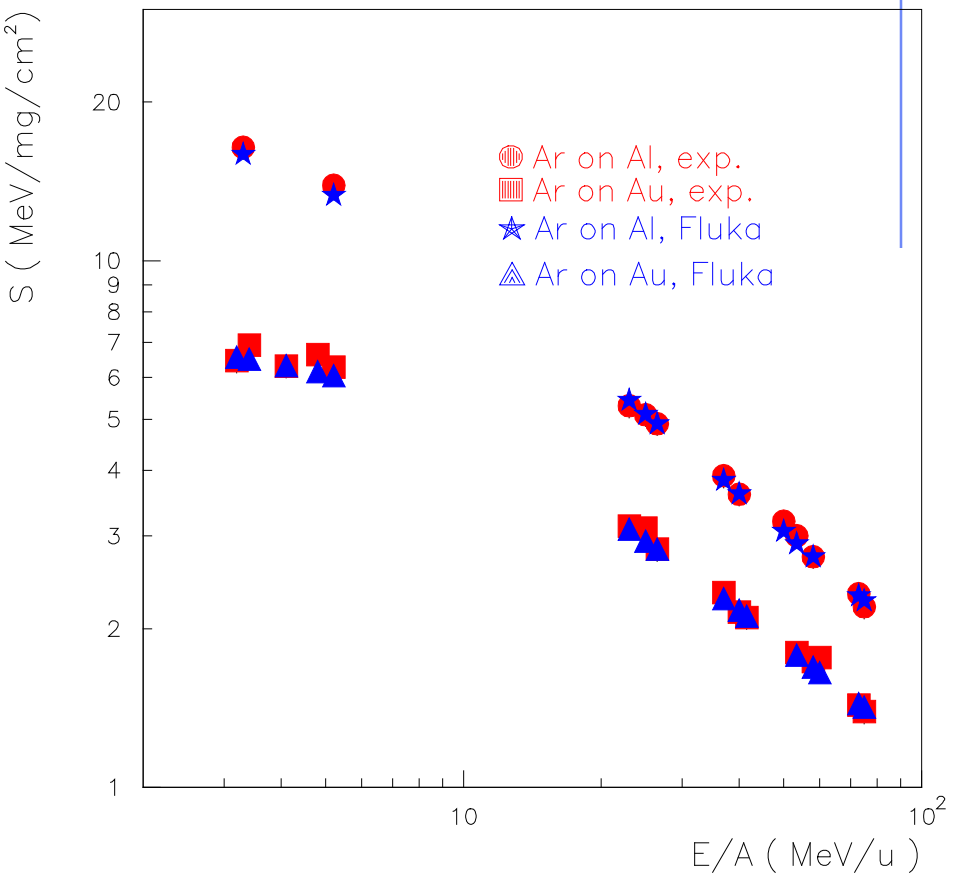
FLUKA takes in account exactly the continuous energy dependence of:

- Discrete event cross section
- Stopping power

Biasing the rejection technique on the ratio between the cross section value at the second endpoint and its maximum value between the two endpoint energies.

Heavy ions dE/dx





Comparison of experimental (R.Bimbot, NIMB69 (1992) 1) (red) and FLUKA (blue) stopping powers of Argon and Uranium ions in different materials and at different energies.

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
```

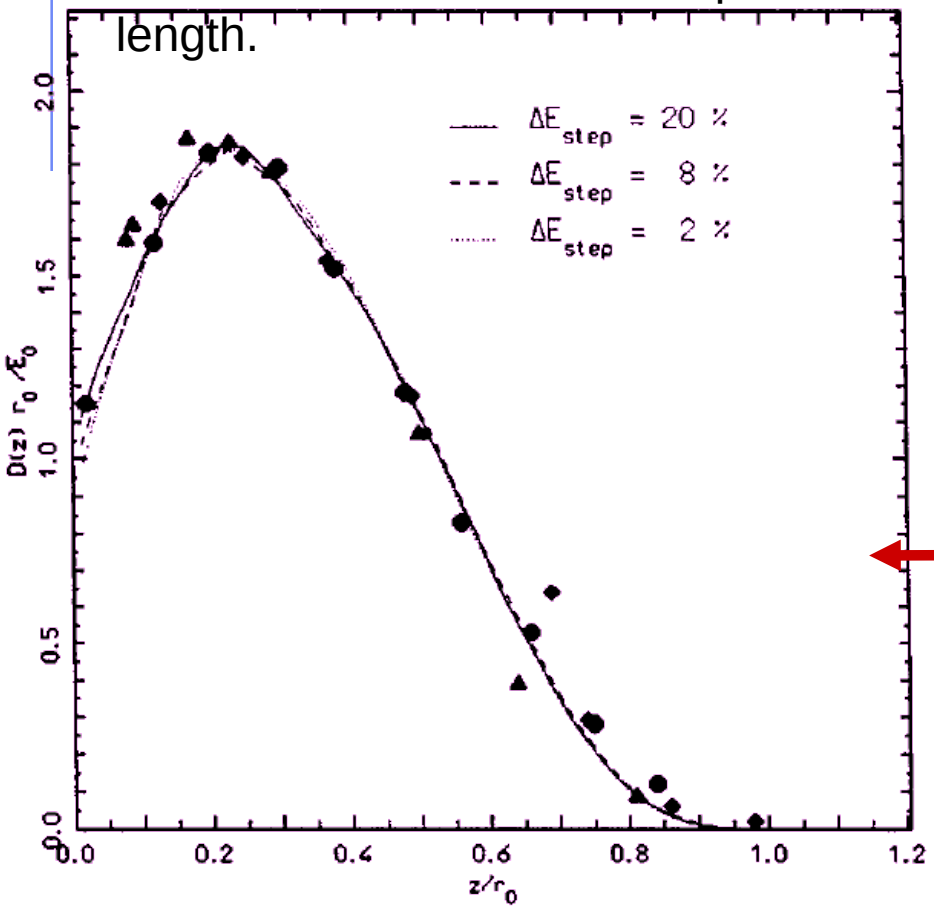
For Had/μ

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

Maximum step size

Moliere: assumes constant energy along the step (!)

One should not abuse of step length.



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

Electron Backscattering

Energy (keV)	Material	Experim. (Drescher et al 1970)	FLUKA Single scattering	FLUKA Multiple scattering	CPU time single/mul t 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%.

What about the delta-ray production threshold?

- EMFCUT with SDUM=PROD-CUT allows to control the threshold for secondary production in any e-/e+/γ interactions

EMFCUT	e±Thresh	γThresh	Fudgem	Mat1	Mat2	Step	PROD-CUT

Fudgem is related to multiple scattering. = 0 below ≈ 10 keV , = 1 above
MUST be set, if the field is empty ➔ 0

Warning 1: if prod-cut < transport cut, CPU is wasted in producing/dumping particles on spot. Sometimes it could be convenient to define several "equal" materials with different production thresholds (and different names)

Warning 2: if prod-cut > transport cut , the program automatically increases the transport threshold , because it cannot transport a particle that it is not supposed to handle.

Bremsstrahlung and pair production by muons and charged hadrons (1/2)

- PAIRBREM card allows to control the production threshold for bremsstrahlung and pair production by muons, light ions (up to alphas) and charged hadrons
- Depending on the DEFAULTS, the processes might be active without explicit production of secondaries (only continuous energy loss treated – see manual)

```
PAIRBREM Flag  e±Thresh γThresh Mat1  Mat2    Step
```

Bremsstrahlung and pair production by muons and charged hadrons (2/2)

- Evidently, the photon transport threshold requested by the EMF-CUT card should be lower than the Bremsstrahlung production threshold set via PAIRBREM
- On the other hand, it is generally recommended to set the e-/e+ pair production threshold to 0 (there is anyway a natural threshold for pair production)
- With high thresholds energy loss straggling and energy deposition is not correctly reproduced (but allows to correctly reproduce the average range of muons)

Charged particle transport

Besides energy losses, charged particles undergo scattering by atomic nuclei. The Molière multiple scattering (MCS) theory is commonly used to describe the cumulative effect of all scatterings along a charged particle step. However

- Final deflection wrt initial direction
- Lateral displacement during the step
- Shortening of the straight step with respect to the total trajectory due to "wiggliness" of the path (often referred to as PLC, path length correction)
- Truncation of the step on boundaries
- Interplay with magnetic field

MUST all be accounted for accurately, to avoid artifacts like unphysical distributions on boundary and step length dependence of the results

The FLUKA MCS

- Accurate PLC (not the average value but sampled from a distribution), giving a complete independence from step size
- Correct lateral displacement even near a boundary
- Correlations:

PLC	$\Leftrightarrow$	lateral deflection
lateral displacement	$\Leftrightarrow$	longitudinal displacement
scattering angle	$\Leftrightarrow$	longitudinal displacement

- Variation with energy of the Moliere screening correction
- Optionally, spin-relativistic corrections (1st or 2nd Born approximation) and effect of nucleus finite size (form factors)
- Special geometry tracking near boundaries, with automatic control of the step size
- On user request, single scattering automatically replaces multiple scattering for steps close to a boundary or too short to satisfy Moliere theory. A full Single Scattering option is also available.
- Molière theory used strictly within its limits of validity
- combined effect of MCS and magnetic fields

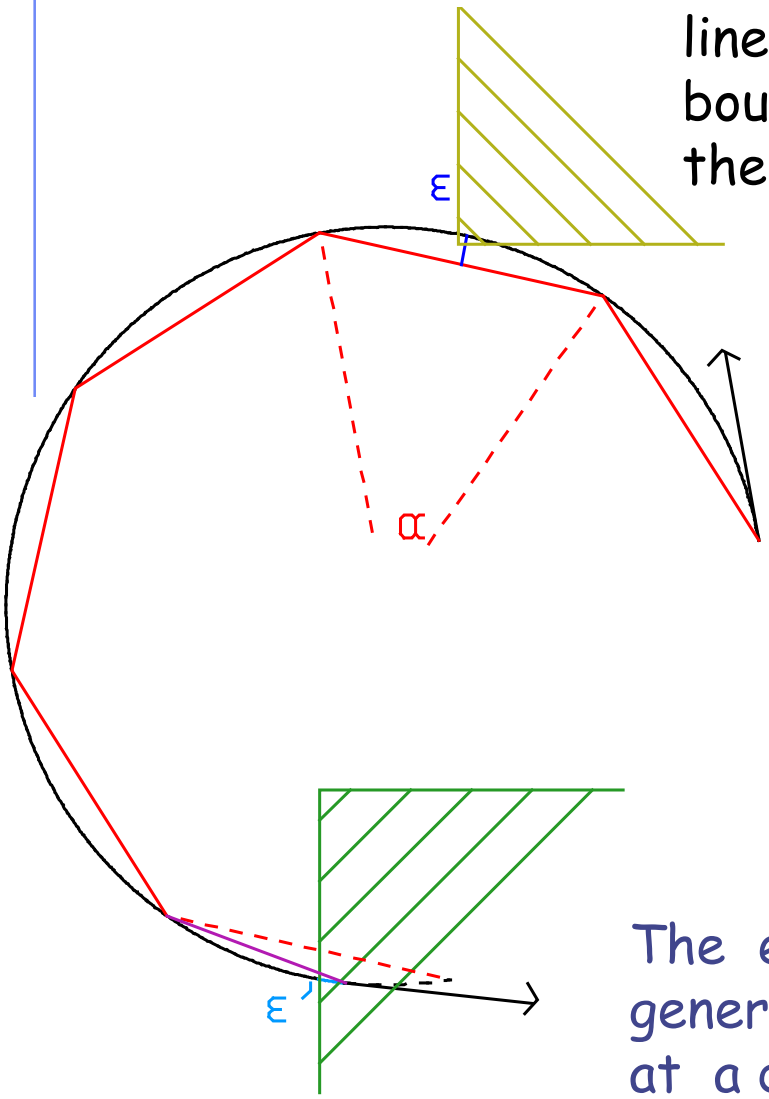
The FLUKA MCS - II

- 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.

Single Scattering

- In very thin layers, wires, or gases, Molière theory does not apply.
- In FLUKA, it is possible to replace the standard multiple scattering algorithm by single scattering in defined materials (option MULSOPT).
- Cross section as given by Molière (for consistency)
- Integrated analytically without approximations
- Nuclear and spin-relativistic corrections are applied in a straightforward way by a rejection technique

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

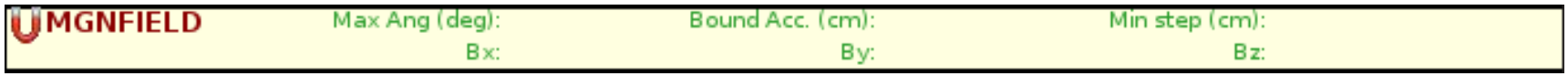
The red line is the path actually followed,
the magenta segment is the last substep, shortened because of a boundary crossing

- α= max. tracking angle (MGNFIELD)
- ε = max. tracking/missing error (MGNFIELD or STEPSIZE)
- ε' = max. bdrx error (MGNFIELD or STEPSIZE)

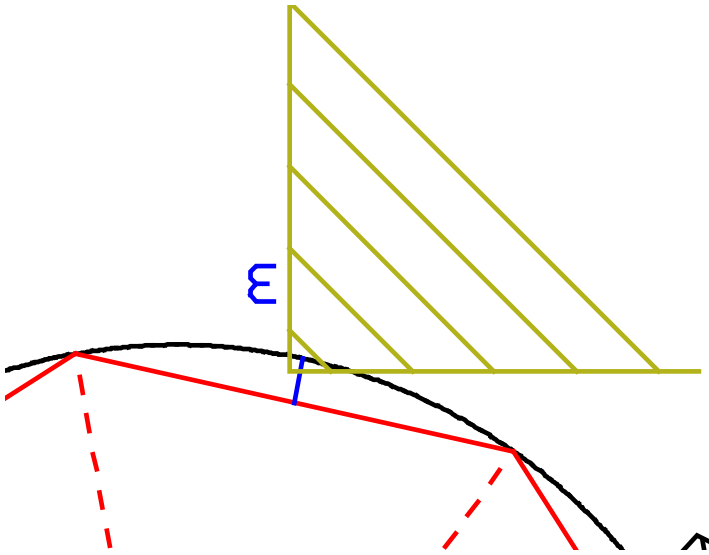
The end point is ALWAYS on the true path, generally NOT exactly on the boundary, but at a distance $< \varepsilon'$ from the true boundary crossing (light blue arc)

Setting the tracking precision I

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



- α largest angle in degrees that a charged particle is allowed to travel in a single sub-step. Default = 57.0 (but a maximum of 30.0 is recommended!)
- ε upper limit to error of the boundary iteration in cm (ε' in fig.). It also sets the tracking error ε. Default = 0.05 cm



IF α and/or ε are too large, boundaries may be missed (as in the plot);
IF they are too small, CPU time explodes....
Both α and ε conditions are fulfilled during tracking.
→ Set them according to your problem
→ Tune ε by region with the STEPSIZE card
→ Be careful when very small regions exists in your setting : ε must be smaller than the region dimensions!

Setting precision by region

```
* ..+....1....+....2....+....3....+....4....+....5....+....6....+....7..
STEPSIZE      Smin/ε       Smax       Reg1       Reg2       Step
```

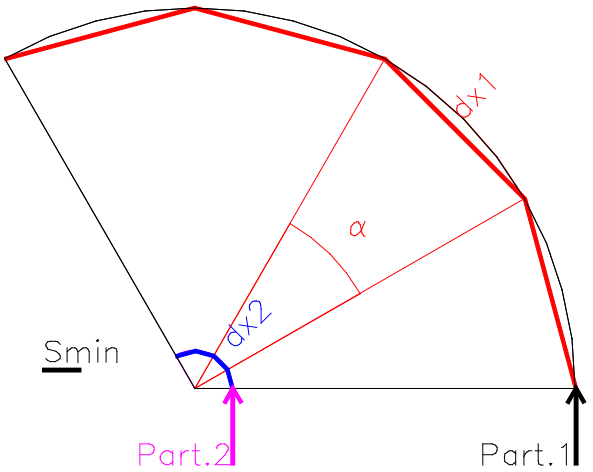
- S_{min}: (if what(1)>0) minimum step size in cm Overrides MGNFIELD if larger than its setting;
- ε (if what(1)<0) : max error on the location of intersection with boundary;
  - The possibility to have different “precision” in different regions allows to save CPU time.
- S_{max}: max step size in cm. Default:100000. cm for a region without magnetic field, 10 cm with field;
  - S_{max} can be useful for instance for large vacuum regions with relatively low magnetic field
  - It should not be used for general step control, use EMFFIX, FLUKAFIX if needed
- Settings apply to all charged particles.

Setting the tracking precision II

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

MGNFIELD | Max Ang (deg): | Bound Acc. (cm): | Min step (cm):
Bx: | By: | Bz:

- S_{min} minimum sub-step length. If the radius of curvature is so small that the maximum sub-step compatible with α is smaller than S_{min}, then the condition on α is overridden. It avoids endless tracking of spiraling low energy particles. Default = 0.1 cm



Particle 1: the sub-step corresponding to α is > S_{min} → accept
Particle 2: the sub-step corresponding to α is < S_{min} → increase α

S_{min} can be set by region with the STEPSIZE card

The magfld.f user routine

This routine allows to define arbitrarily complex magnetic fields:

SUBROUTINE MAGFLD (X, Y, Z, BTX, BTY, BTZ, B, NREG, IDISC)

Input variables:

x,y,z	=	current position
nreg	=	current region

Output variables:

btx,bty,btz	=	cosines of the magn. field vector
B	=	magnetic field intensity (Tesla)
idisc	=	set to 1 if the particle has to be discarded

- All floating point variables are double precision ones!
- BTX, BTY, BTZ must be normalized to 1 in double precision

Damage to Electronics

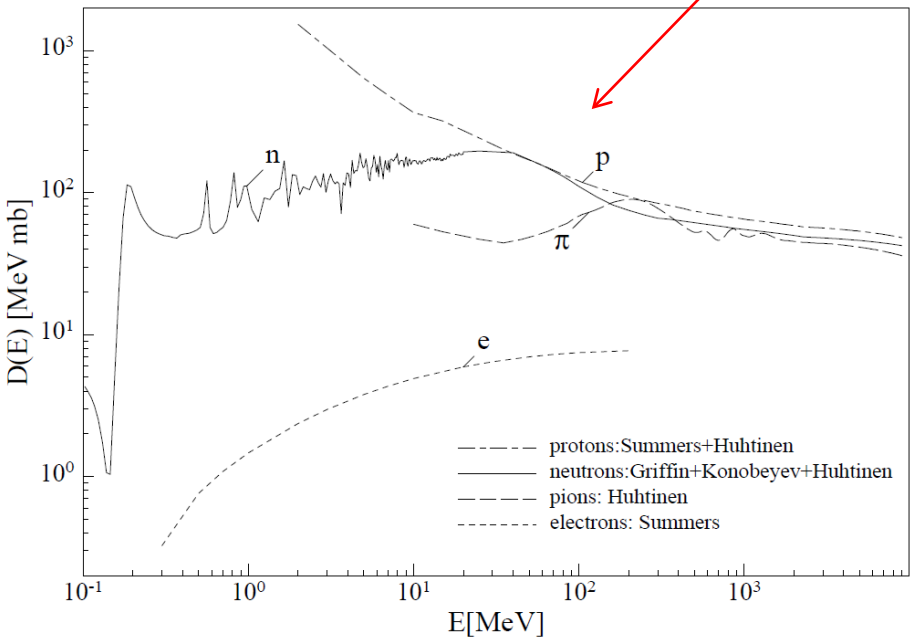
Generalized particle

Category		Scales with simulated/measured quantity
Single Event effects (Random in time)	***Single Event Upset (SEU)***	High-energy hadron fluence (>20 MeV)* [cm-2]
	Single Event Latchup (SEL)	High-energy hadron fluence (>20 MeV)** [cm-2]
Cumulative effects (Long term)	***Total Ionizing Dose (TID)***	Ionizing Dose [GeV/g]
	Displacement damage	1 MeV neutron equivalent [cm-2] {NIEL}

HADGT20M

DOSE

SI1MEVNE



* Reality is more complicated (*e.g.*, contribution of thermal neutrons)

** Energy threshold for inducing SEL is often higher than 20 MeV