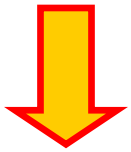
Ionization and Transport

FLUKA Beginner's Course

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

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

All share the same approach!

… but some extra features are needed for Heavy Ions

Charged particle dE/dx: Bethe-Bloch

Spin 0
(spin1 is similar):

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

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

- I : mean excitation energy , material-dependent;
- δ : density correction;
- C : is the shell correction, important at low energies
- T_{max} : maximum energy transfer to an electron (from kinematics);

Higher order corrections implemented in FLUKA

- L_1 : Barkas correction (z^3) responsible for the difference in stopping power for particles-antiparticles;
- L_2 : Bloch (z^4) correction
- G : Mott corrections

Valid for **m>>m_e**, However, the formulation for electron/positrons is similar, except for the "energetic" collisions with atomic electrons.

Discrete ionization events

Above a pre-set threshold, ionization is modeled as δ ray production (free electrons). The threshold refers to the kinetic energy of the emitted δ ray.

- Spin 0 or 1/2 δ-ray production (charged hadrons, muons)
- Mott for heavy ions
- Bhabha scattering (e^+)
- Møller scattering (e^-)

How to set this threshold?

- Electrons set by EMFCUT card through the PROD-CUT sdum;
- Charged hadrons/muons set by DELTARAY card:

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

where:

δThresh	production threshold, (from materials Mat1 to Mat2)
Ntab, Wtab	control the accuracy of dp/dx tabulations (advanced user)
PRINT	if is set (not def.) dp/dx tabulations are printed on stdout

Continuous energy losses

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

- Fluctuations of energy loss are simulated with a FLUKA-specific algorithm
- The energy dependence of cross sections and dE/dx is taken into account exactly (see later)
- The latest recommended values of ionization potential and density effect parameters implemented for each element (Sternheimer, Berger & Seltzer), but can be overridden by the user with (set yourself for compounds!)

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

Ionization fluctuations -I

The **Landau** distribution is limited in several respects:

- Maximal energy of δ ray is assumed to be infinite, therefore cannot be applied for long steps or low velocities;
- Cross section for close collisions is assumed to be equal for all particles;
- Fluctuations connected with distant collision are neglected, therefore they cannot be applied for small steps;
- Incompatible with explicit δ ray production.

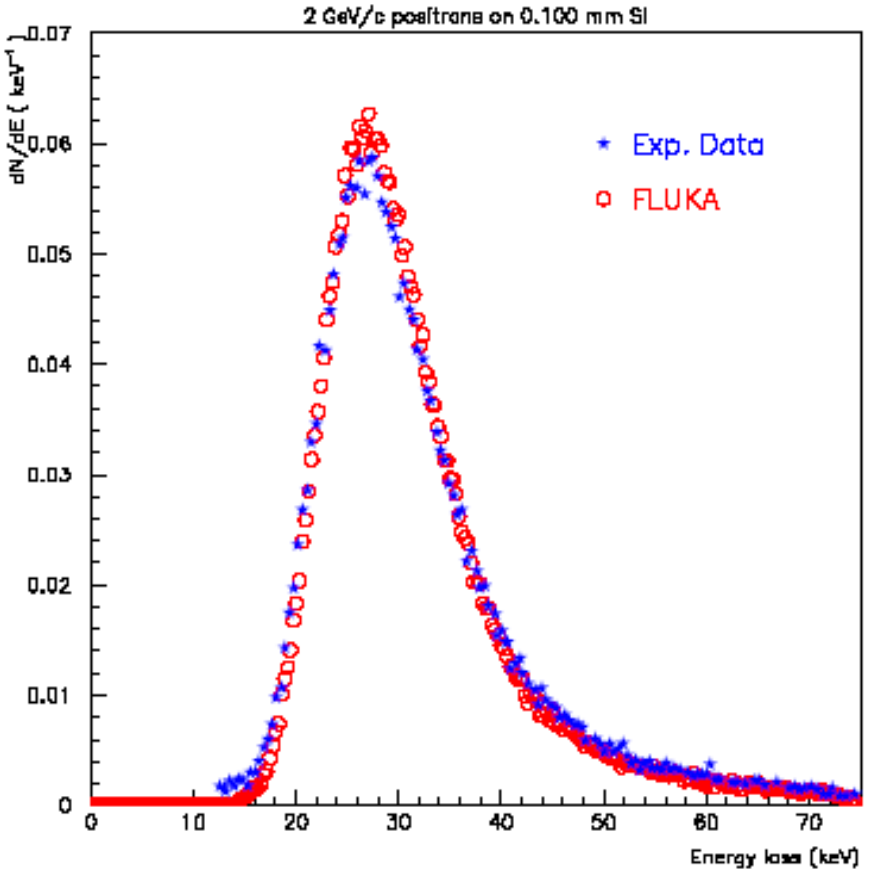
The **Vavilov** distribution overcomes some of the landau limitations, but is difficult to compute if the step length or the energy are not known a priori.

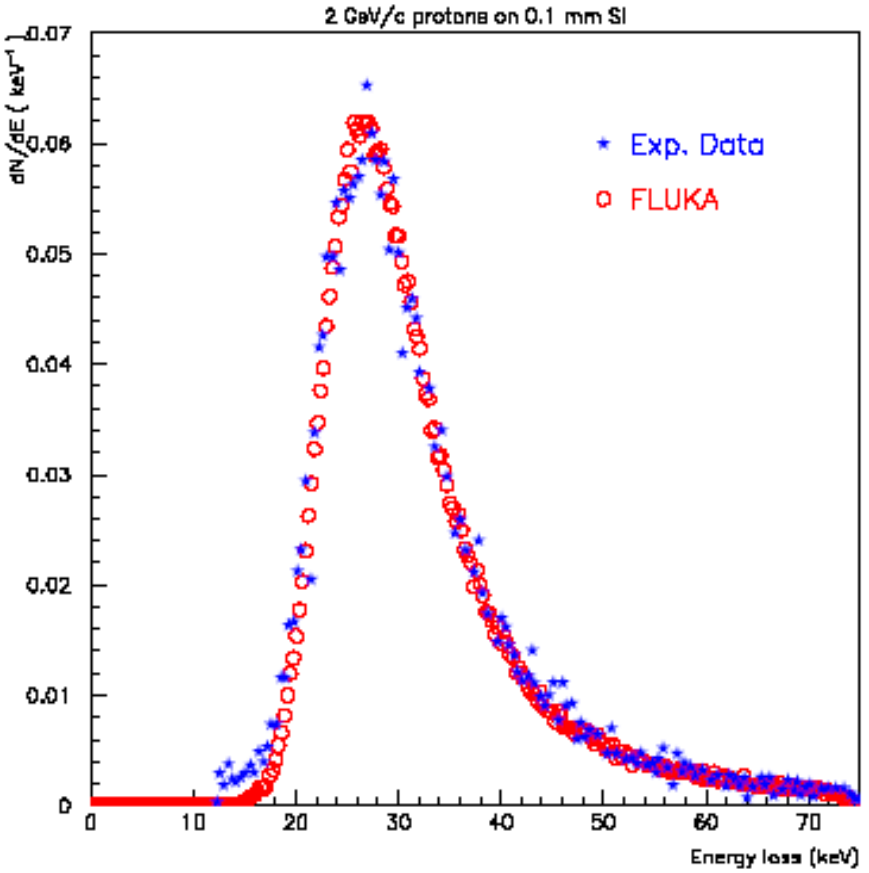
Ionization fluctuations -II

The FLUKA approach:

- Based on general statistical properties of the cumulants of a distribution (in this case a Poisson distribution convoluted with dσ/dE);
- Integrals can be calculated analytically and exactly *a priori* (min. CPU time);
- Applicable to any kind of charged particle, taking into account the proper spin dependent cross section for δ ray production;
- The first 6-moments of the energy loss distribution are reproduced: $k_n = \left\langle (x - \langle x \rangle)^n \right\rangle$

Ionization fluctuations -III





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

J.Bak et al. NPB288, 681 (1987)

Nuclear stopping power (NEW)

- Besides Coulomb scattering with atomic electrons, particles undergo Coulomb scattering also 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 (NIEL, DPA)

dpa: Displacements Per Atom

- FLUKA generalized particle name: DPA-SCO
- Is a measure of the amount of radiation damage in irradiated materials
  For example, means each atom in the material has been displaced from its 3 dpa 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

Damage to Electronics

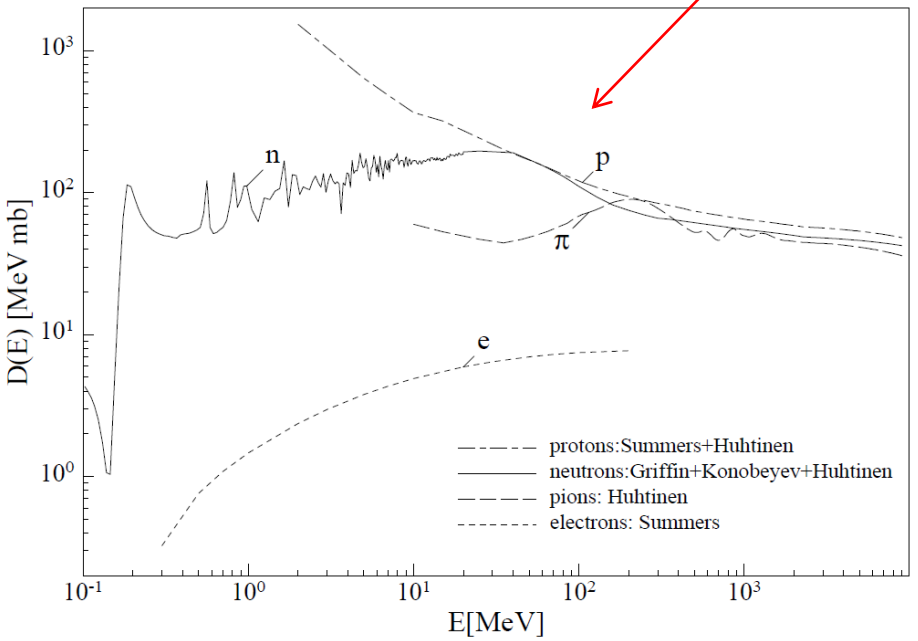
Generalized particle

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

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 ration 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 ant its maximum value between the two end point energies.

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
```

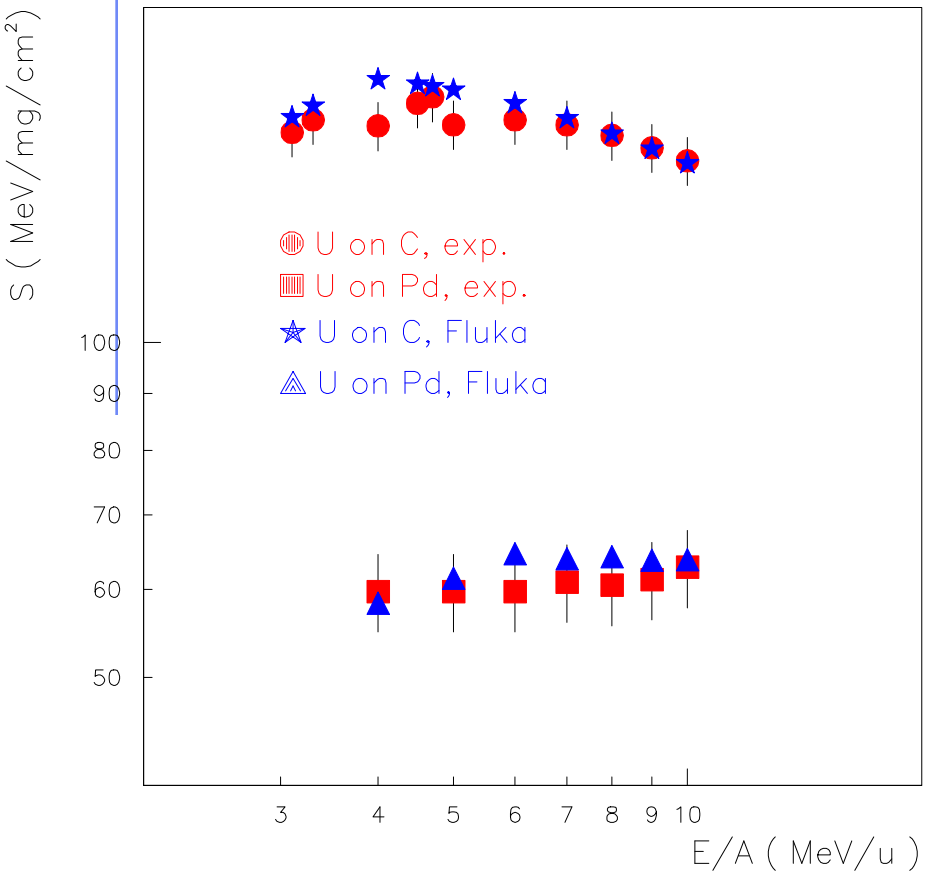
Remember always that δ-ray production is controlled independently and cannot be switched off for e^+/e^- (it would be physically meaningless)

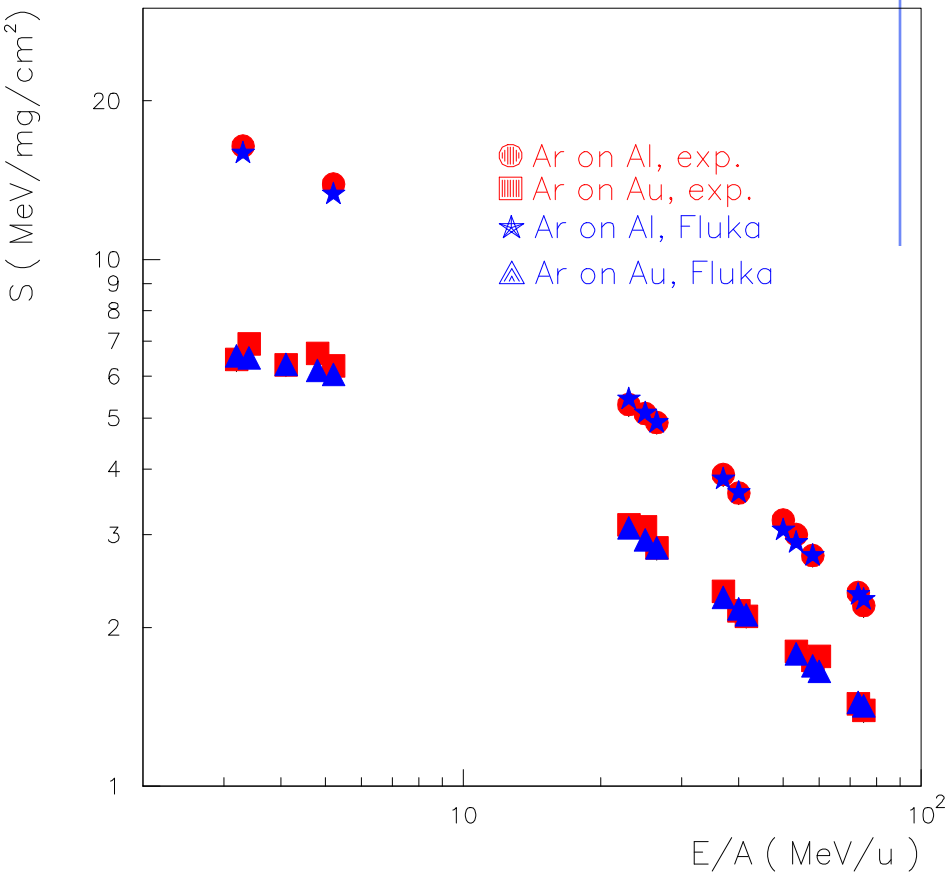
Heavy ions

Ionization energy losses

- Up-to-date effective charge parameterizations
- Energy loss straggling according to:
  - "normal" first Born approximation
  - Charge exchange effects (dominant at low energies, ad-hoc model developed for FLUKA)
  - Mott cross section
  - Nuclear form factors (high energies)
  - Direct e+/e- production

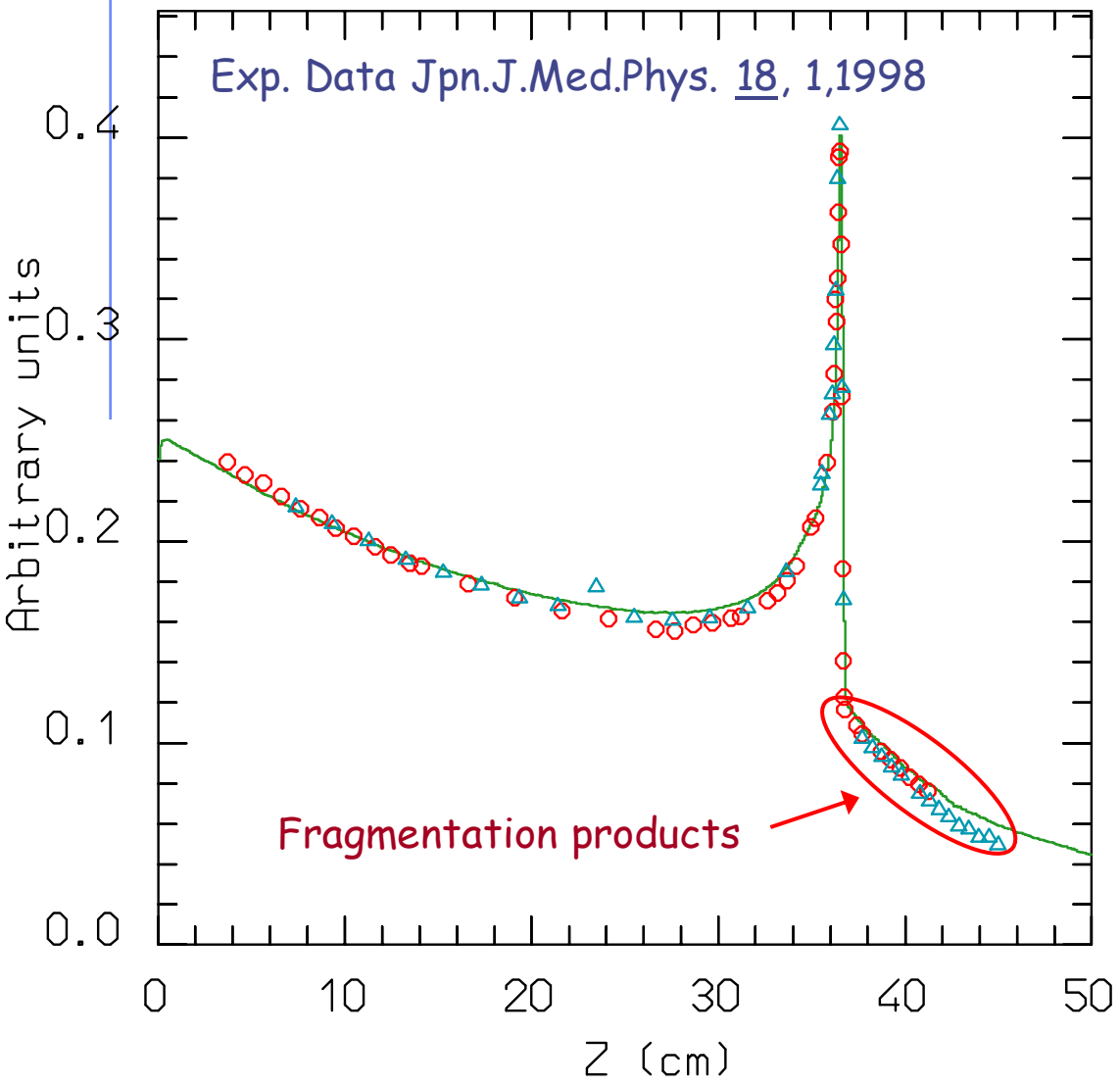
Heavy ions dE/dx





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.

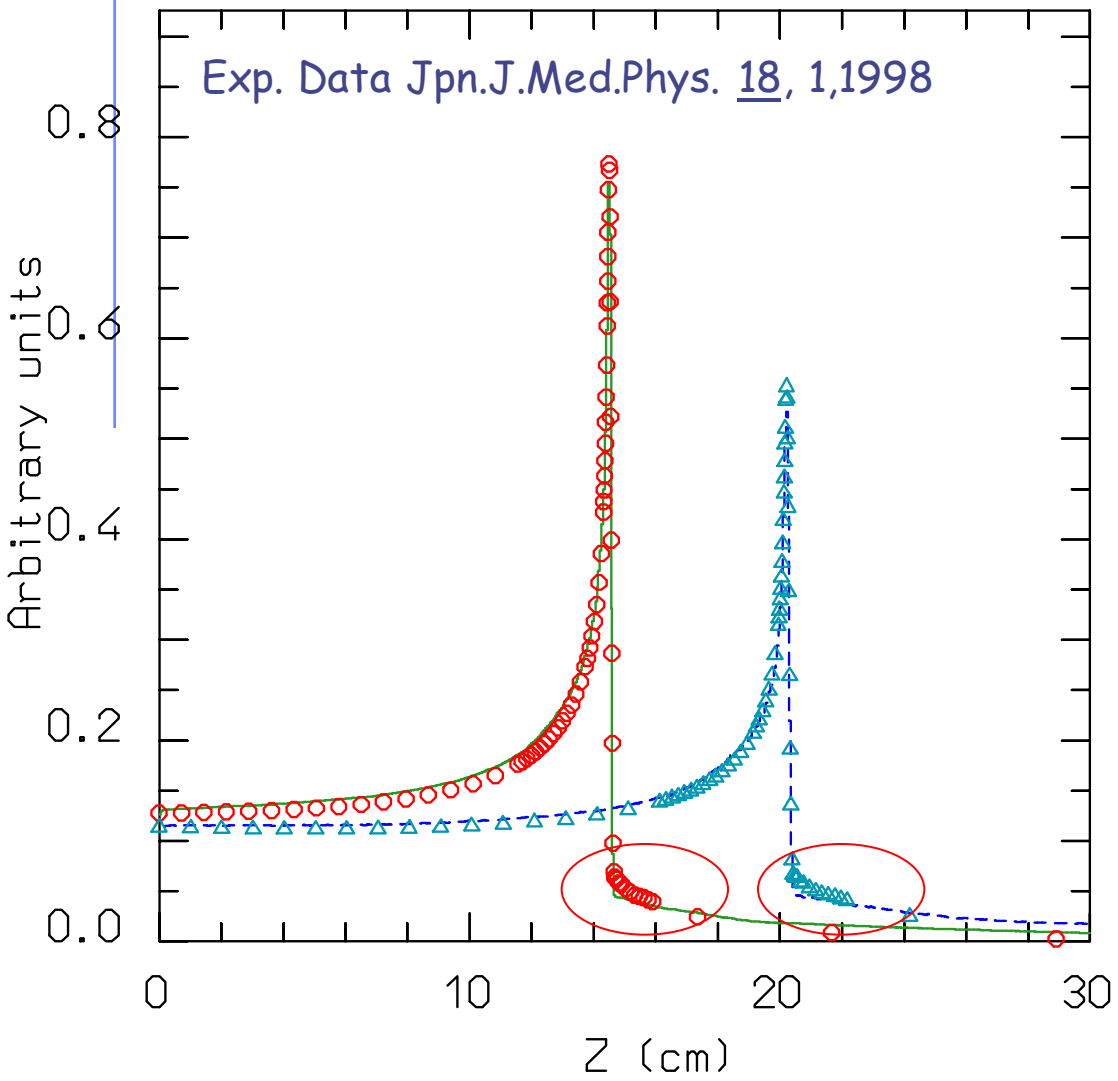
Bragg peaks vs exp. data: ^{20}Ne @ 670 MeV/n



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

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

Bragg peaks vs exp. data: ^{12}C @ 270 & 330 MeV/n

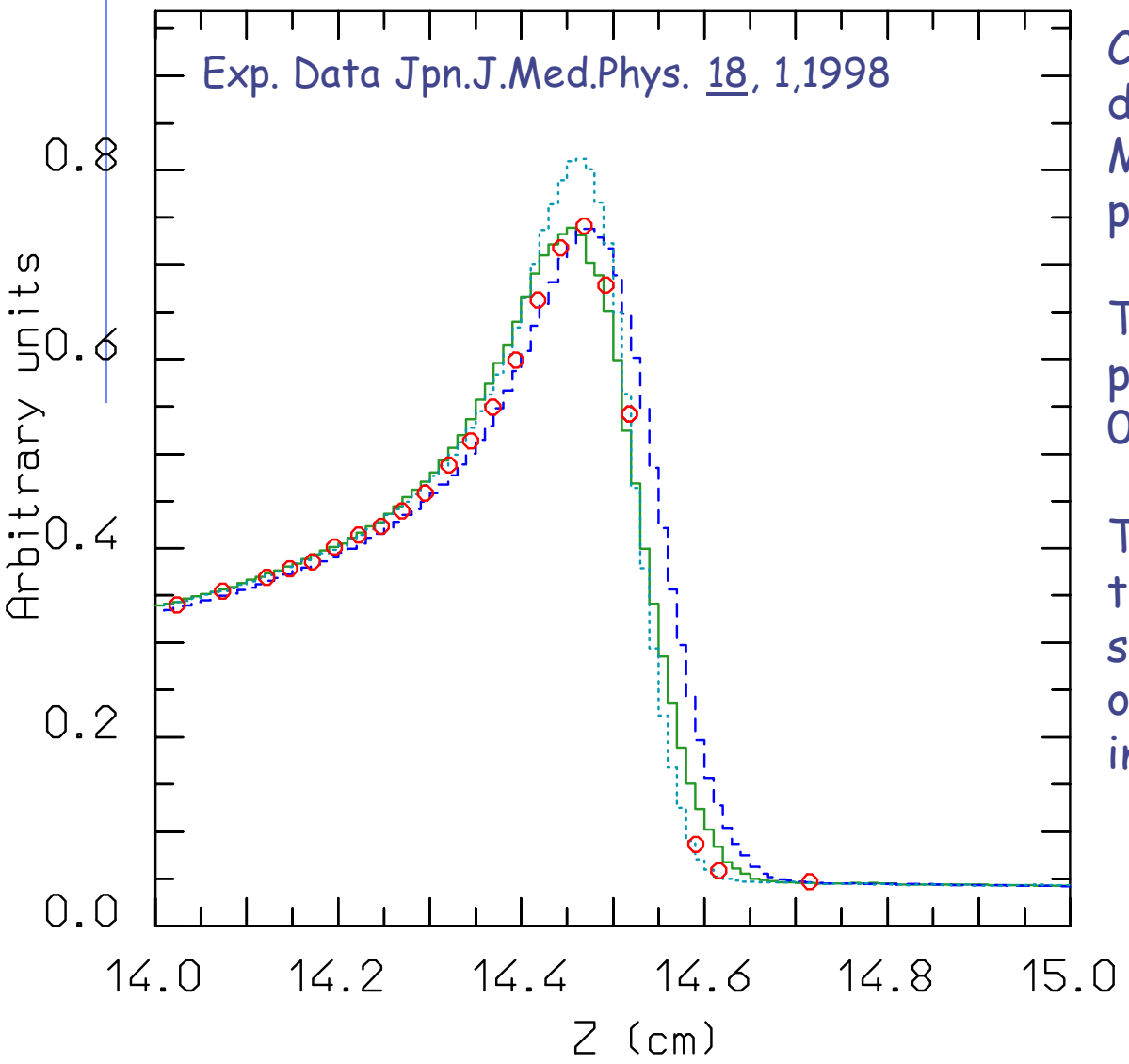


Dose vs depth distribution for 270 and 330 MeV/n ^{12}C ions on a water phantom.

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

The symbols are exp data from GSI.

Bragg peaks vs exp. data: ^{12}C @ 270 MeV/n



Close-up of the dose vs depth distribution for 270 MeV/n ^{12}C ions on a water phantom.

The green line is the FLUKA prediction with the nominal 0.15% energy spread.

The dotted light blue line is the prediction for no spread, and the dashed blue one the prediction for I increased by 1 eV.

Charged particle transport

Setting particle transport threshold

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

- Hadron and muon transport thresholds are set with this card (see the manual for details);
- The neutron threshold has a special meaning (as shown in the low energy neutron lecture), leave at the default value (1 x 10^{-5} eV);

Warning: the behavior of PART-THR for neutrons has changed with the 2008 release!!

- The threshold for nbar's and neutral kaons should always be zero.

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.
- Moliere 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

Electron Backscattering

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

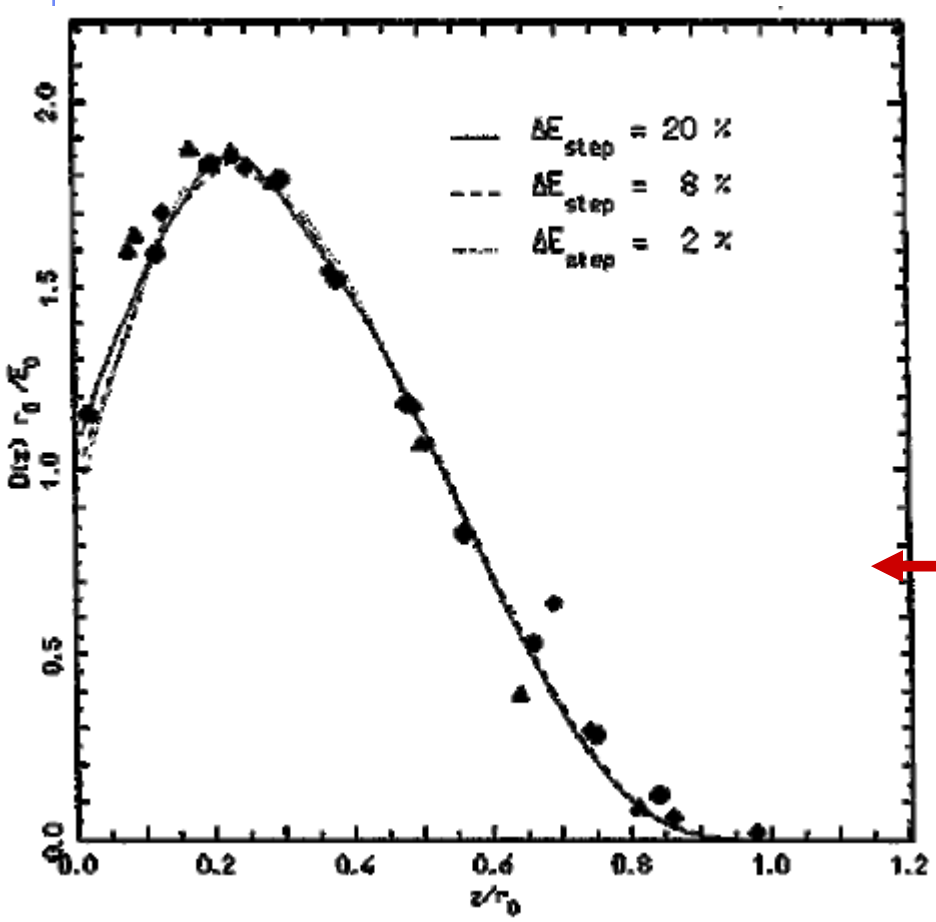
Fraction of normally incident electrons backscattered out of a surface. All statistical errors are less than 1%.

User control of MCS

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

- Allows to optimize the treatment of multiple Coulomb scattering;
- Not needed in shielding problems, but important for backscattering and precision dosimetry;
- Can be tuned by material;
- Special feature: possibility to suppress multiple scattering (applications: gas Bremsstrahlung, proton beam interactions with residual gas);
- Also very important: used to request transport with single scattering (CPU demanding, but affordable and very accurate at low electron energies, ***can be tuned x material!)***

Control of step size



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

Thanks to FLUKA mcs and boundary treatment, results are stable vs. (reasonable) step size

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

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)

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 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)
- 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

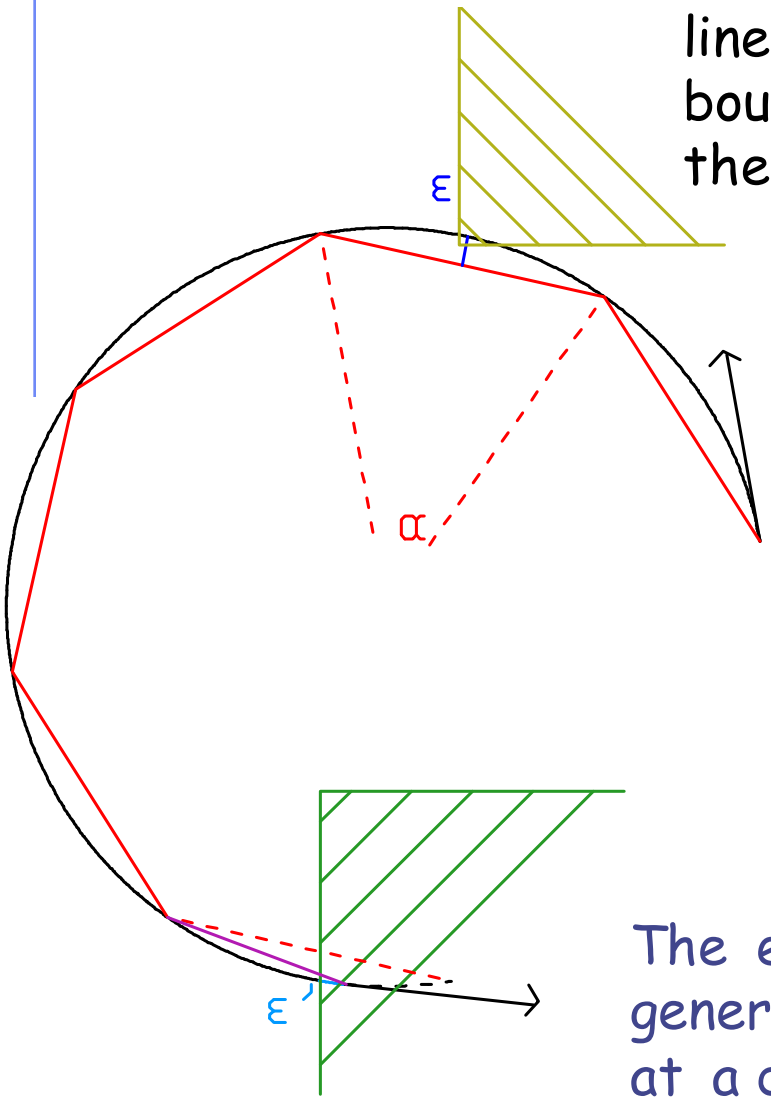
How to define a magnetic field

- 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 MGNFLD (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

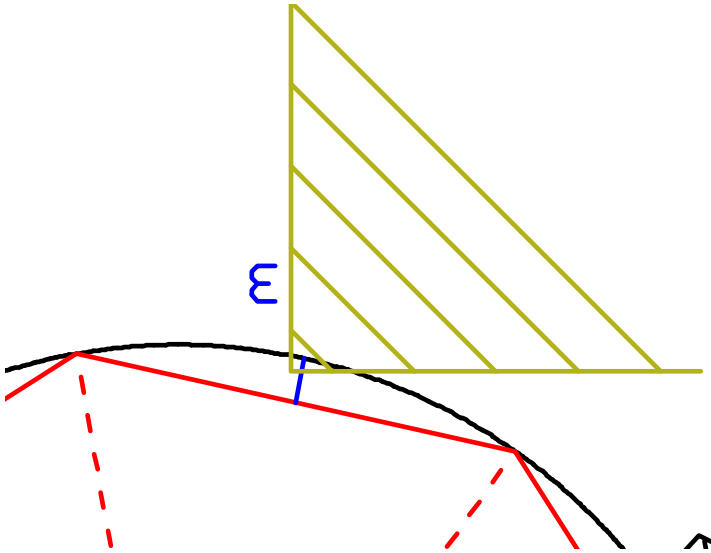
- α= max. tracking angle (MGNFIELD)
- ε = max. tracking/missing error (MGNFIELD or STEPSIZE)
- ε' = max. bdrx error (MGNFIELD or STEPSIZE)

The end point is ALWAYS on the true path, generally NOT exactly on the boundary, but at a distance < 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

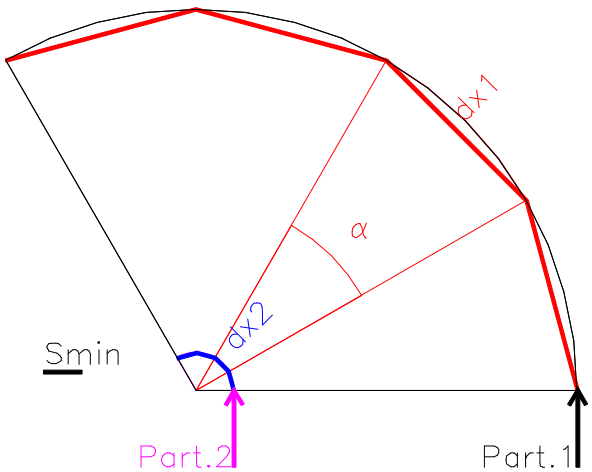


IF α and/or ε are too large, boundaries may be missed (as in the plot);
IF they are too small, CPU time explodes....
Both α and ε conditions are fulfilled during tracking.
→ Set them according to your problem
→ Tune ε by region with the STEPSIZE card
→ Be careful when very small regions exists in your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

Setting the tracking precision II

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

- Smin minimum sub-step length. If the radius of curvature is so small that the maximum sub-step compatible with α is smaller than Smin, 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 > Smin -> accept
Particle 2: the sub-step corresponding to α is < Smin -> increase α

Smin can be set by region with the STEPSIZE card

Setting precision by region

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

- Smin: (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.
- Smax: max step size in cm. Default: 100000. cm for a region without magnetic field, 10 cm without;
  - Smax 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

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:

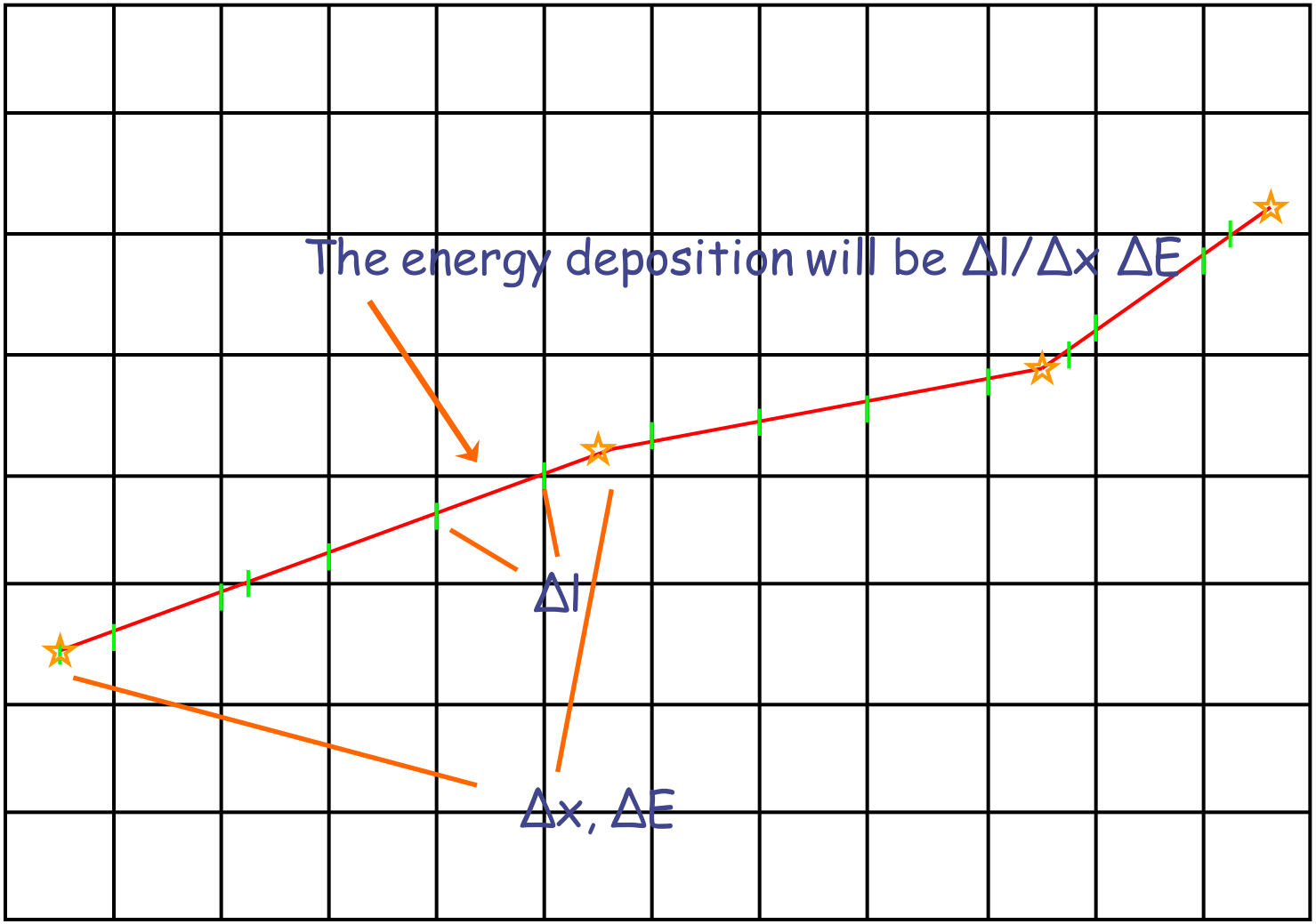
btx,bty,btz	=	cosines of the magn. field vector
B	=	magnetic field intensity (Tesla)
idisc	=	set to 1 if the particle has to be discarded

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

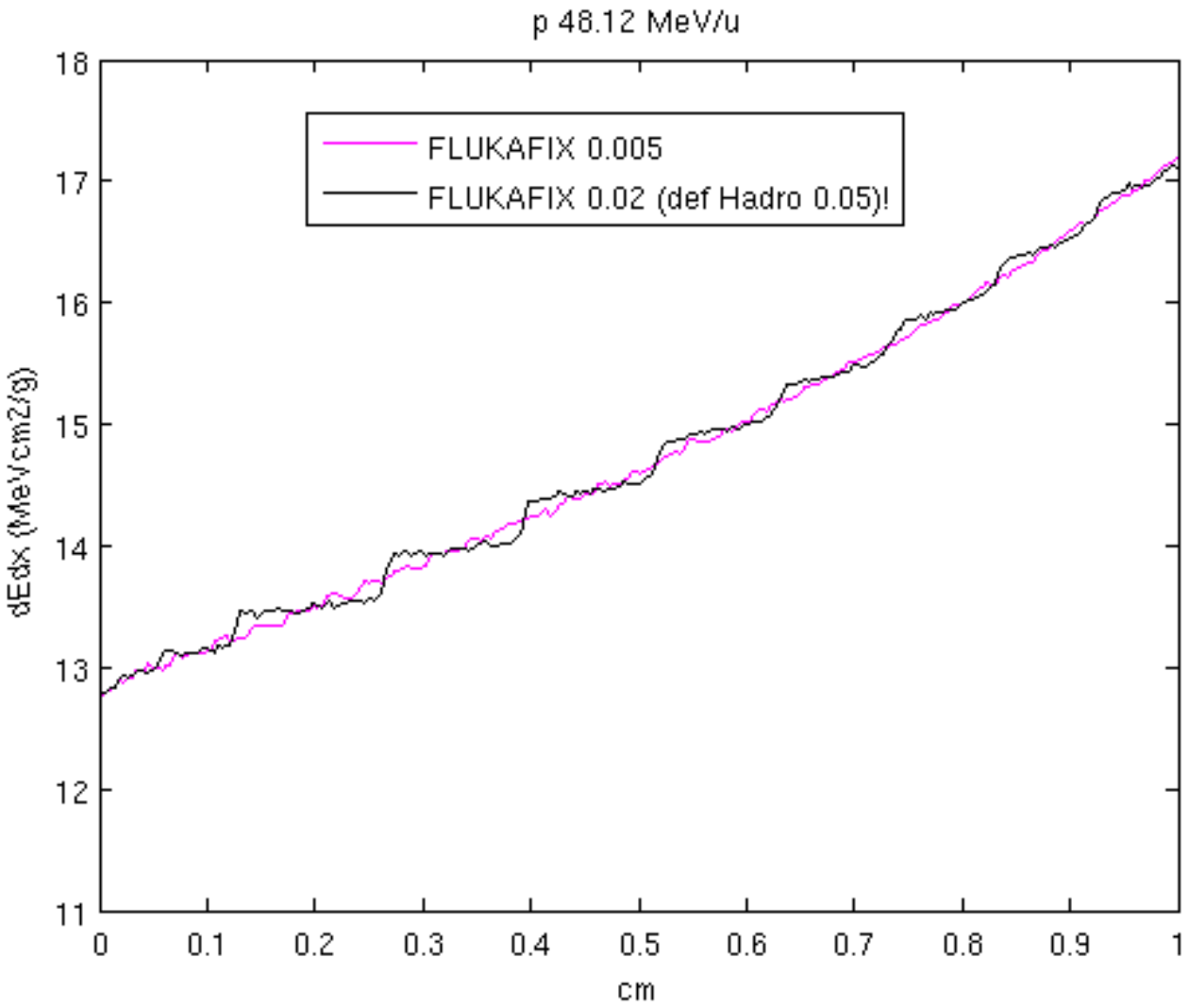
Some warnings about scoring:

- 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)

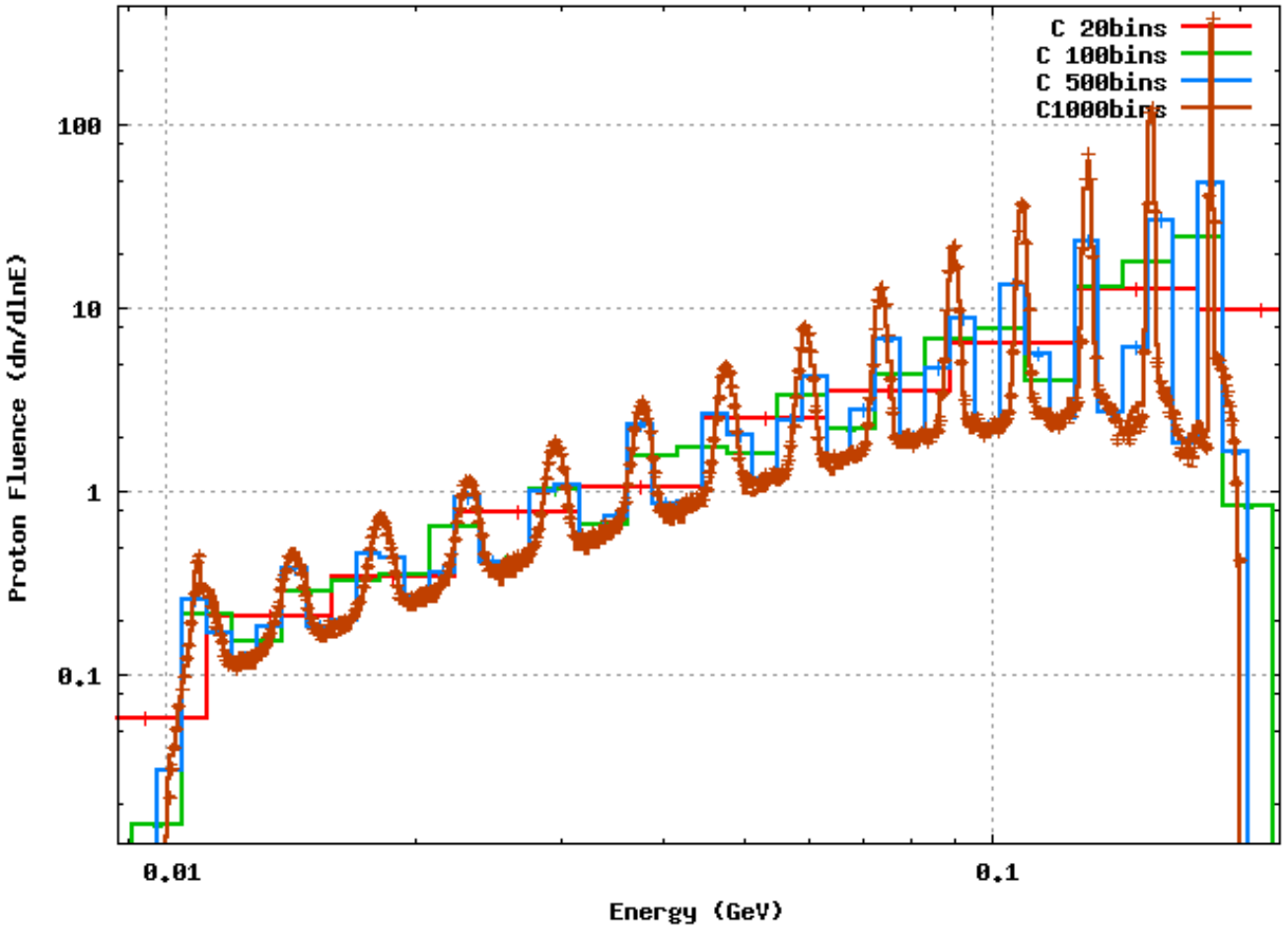
USRBIN track apportioning scoring



USRBIN track apportioning scoring



USRTRACK scoring: 200 MeV p on C



Default settings, ≈ 20% energy loss per step

Ionization Transport Cheat Sheet

DELTARAY - Modify Delta-ray effect parameters

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

IONFLUCT - Set Ionization fluctuation options
PART-THR - Set particle transport threshold

EMFFIX - Set Step Size control for EM
FLUKAFIX - Set Step Size control for Hadrons/Muons

MGNFIELD - Set magnetic field precision
STEPSIZE - Set stepsize in magnetic field