



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):

$\sim \ln \beta^4 \gamma^4$
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 $m \gg m_e$, 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       $\delta$ Thresh      Ntab      Wtab      Mat1      Mat2      Step PRINT
```

where:

- δ Thresh 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	δ_0 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.

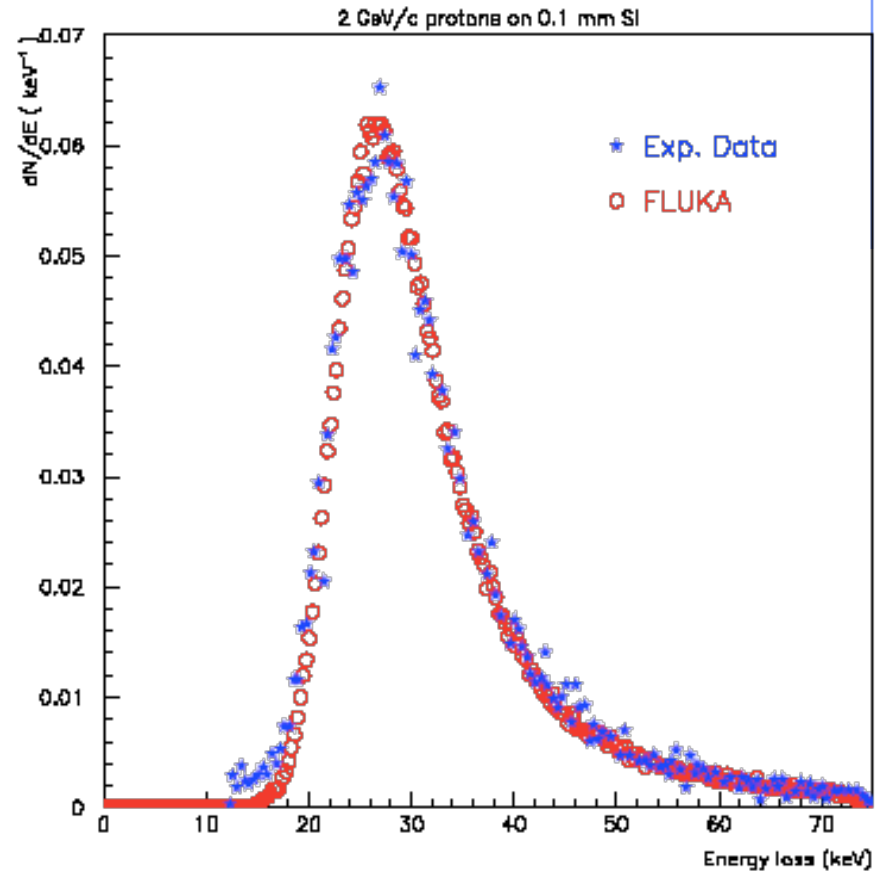
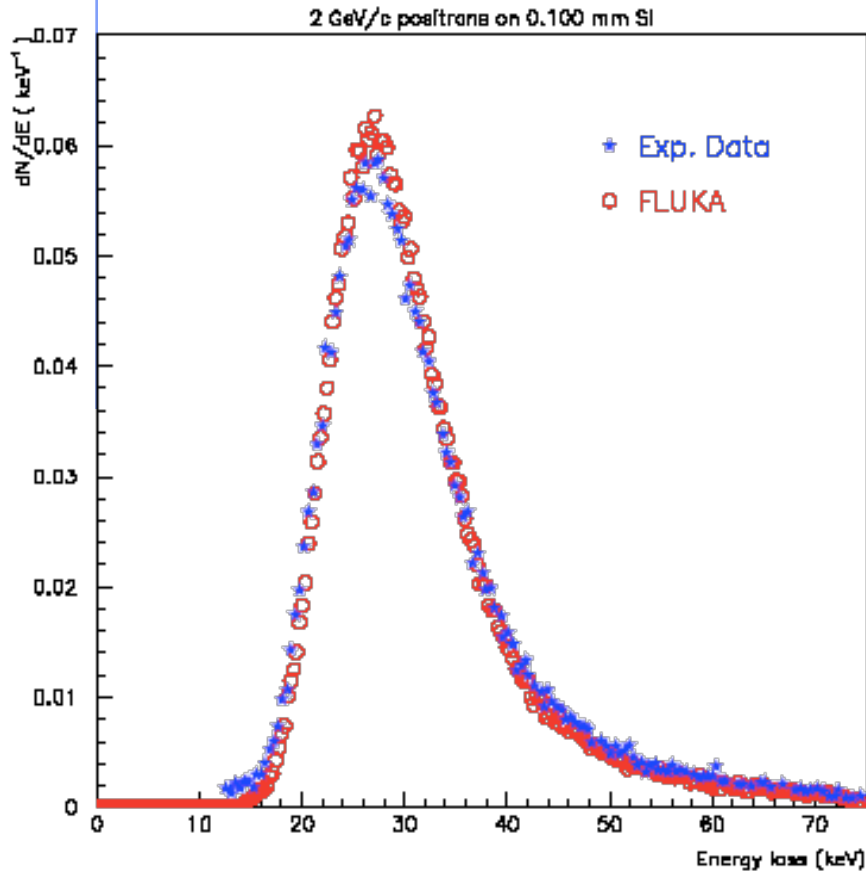
The Vavilov distribution overcomes some of the Landau limitations, but is difficult to compute if the step length or the energy are not known a priori.

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 $d\sigma/dE$);
- 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: $k_n = \left\langle \left(x - \langle x \rangle \right)^n \right\rangle$

Ionization fluctuations -III



Experimental¹ and calculated energy loss distributions for 2 GeV/c positrons (left) and protons (right) traversing 100 μm 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/cm³

N_i particles per interaction channel i

N_f^i Frenkel pairs per channel

Damage to Electronics

Generalized
particle

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

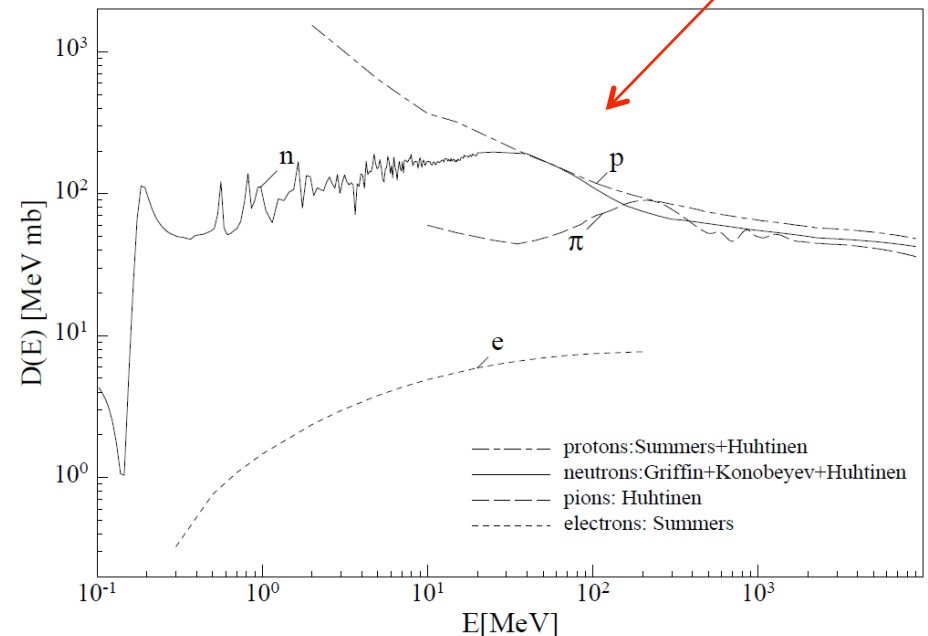
HADGT20M

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 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

Biassing the rejection technique on the ratio between the cross section value at the second endpoint and 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

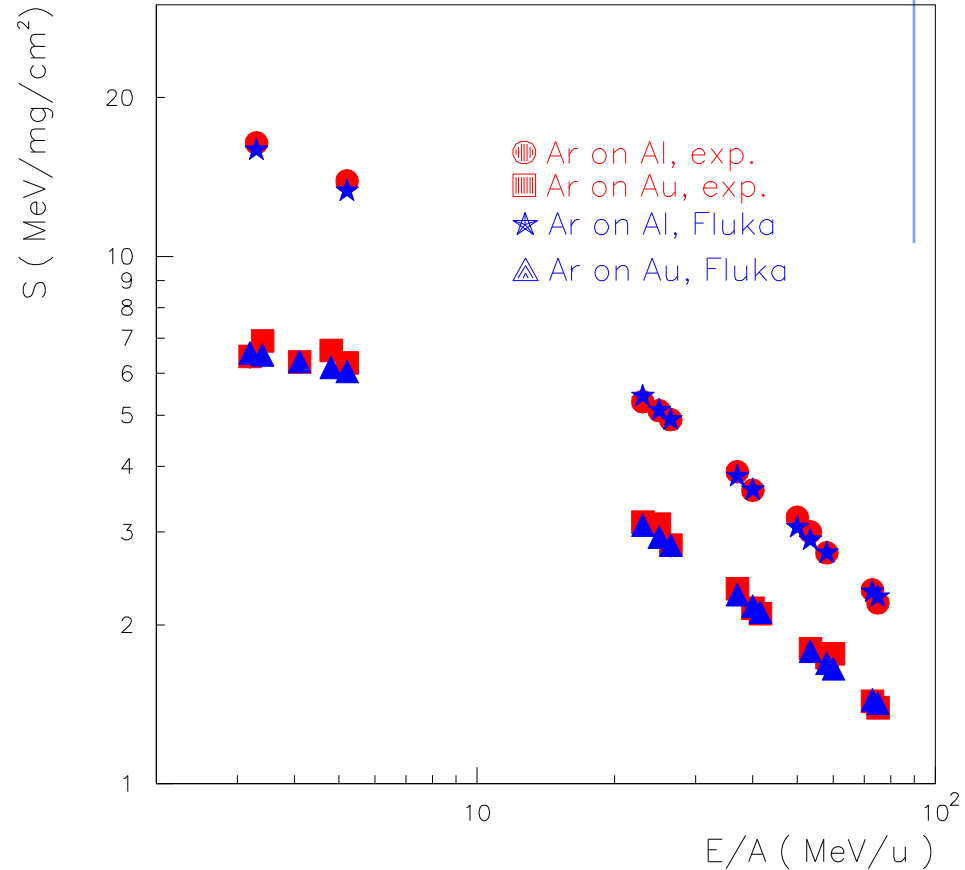
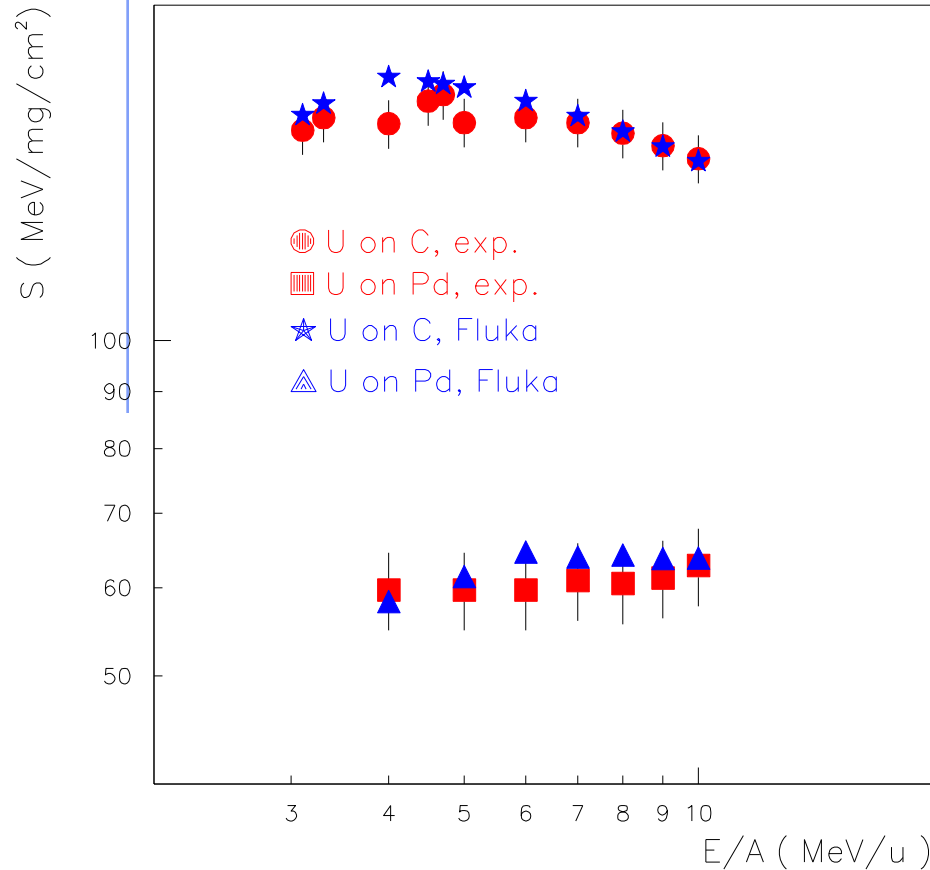
Remember always that δ -ray production is controlled independently and cannot be switched off for e^+/e^- (it would be physically meaningless)

Heavy ions

Ionization energy losses

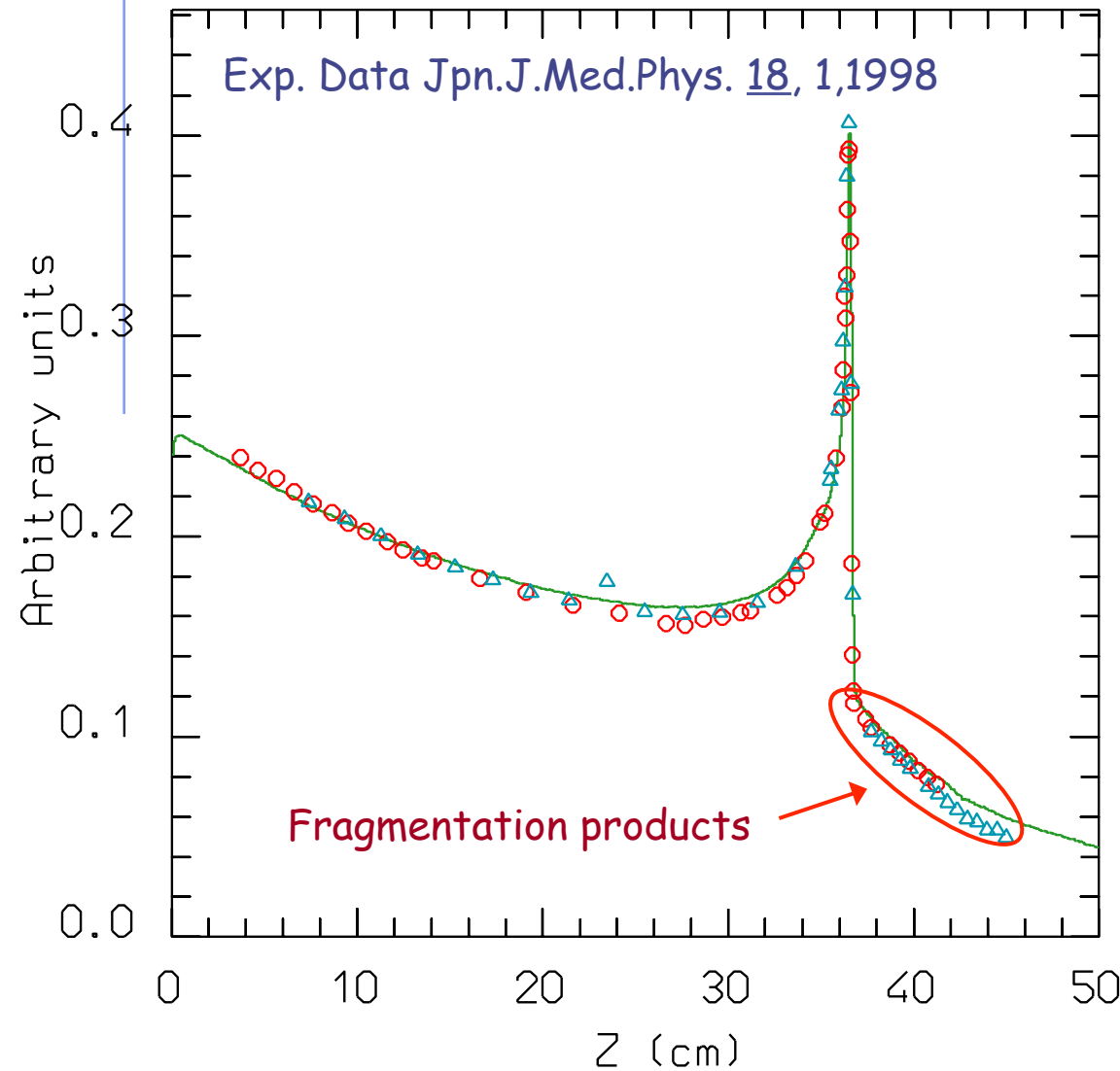
- Up-to-date effective charge parameterizations
- Energy loss straggling according to:
 - “normal” first Born approximation
 - Charge exchange effects (dominant at low energies, ad-hoc model developed for FLUKA)
 - Mott cross section
 - Nuclear form factors (high energies)
 - Direct e^+/e^- production

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.

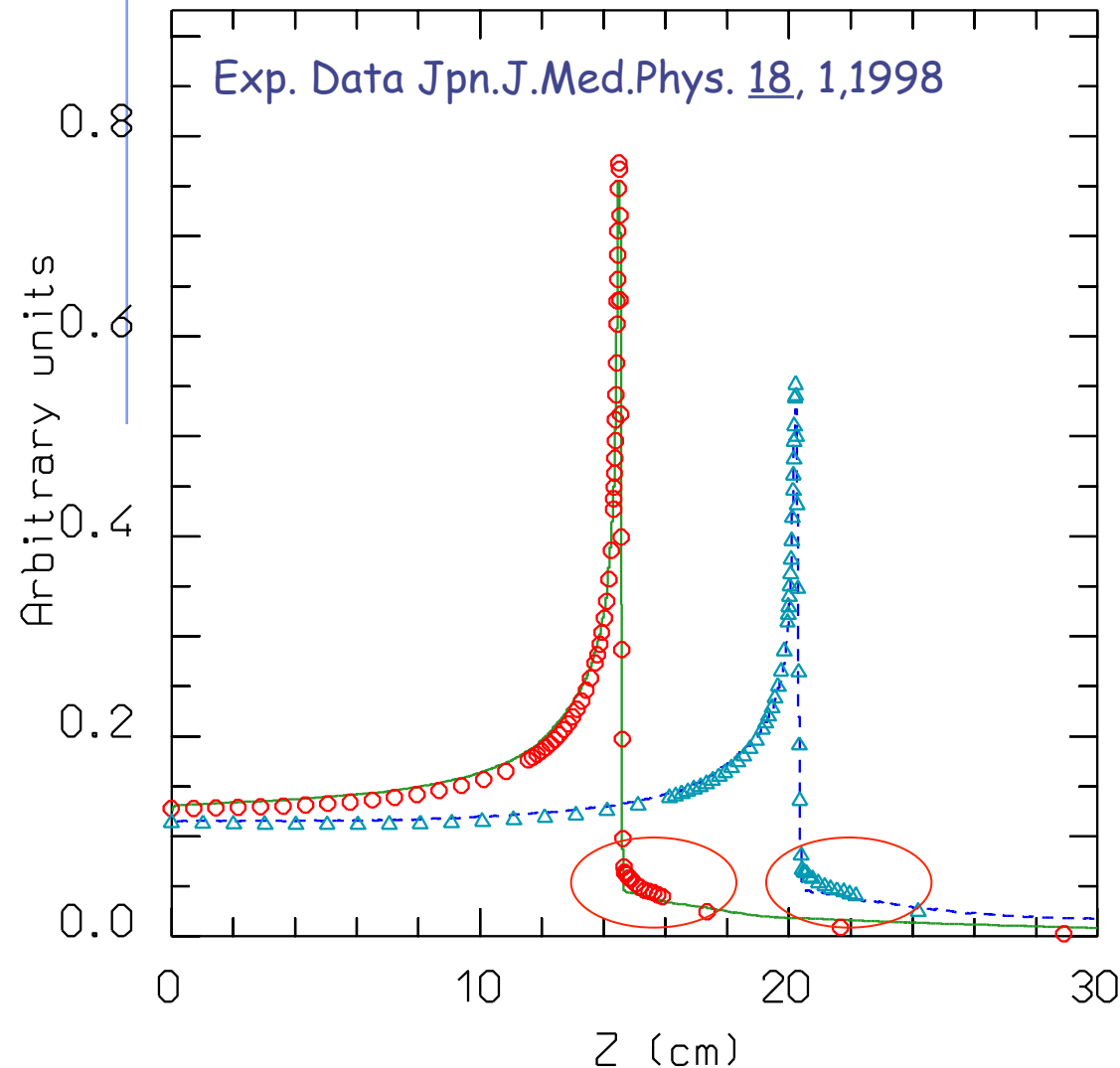
Bragg peaks vs exp. data: ^{20}Ne @ 670 MeV/n



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

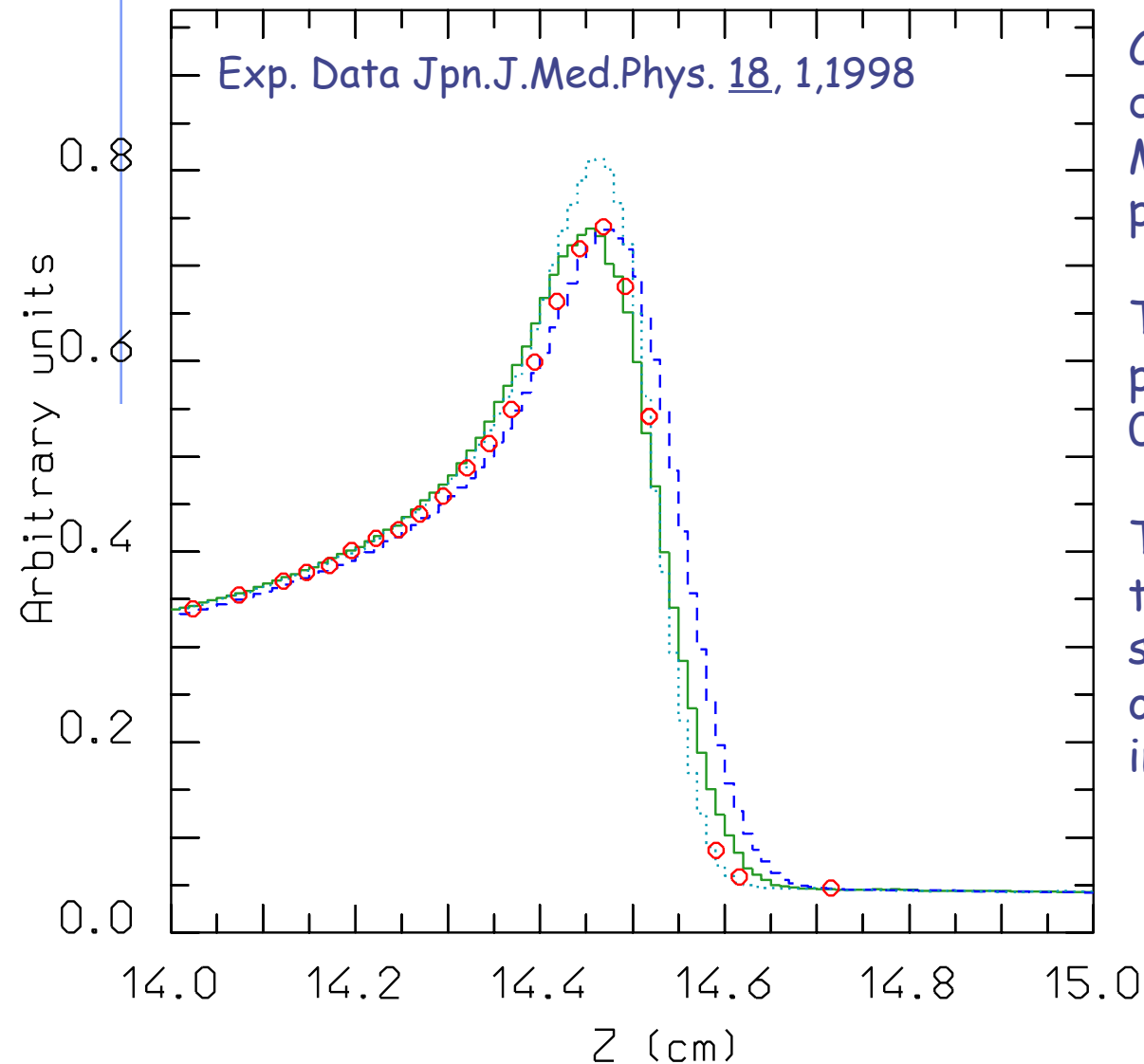


Dose vs depth distribution for 270 and 330 MeV/n ^{12}C ions on a water phantom.

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 (1×10^{-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 “wiggleness” 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%.

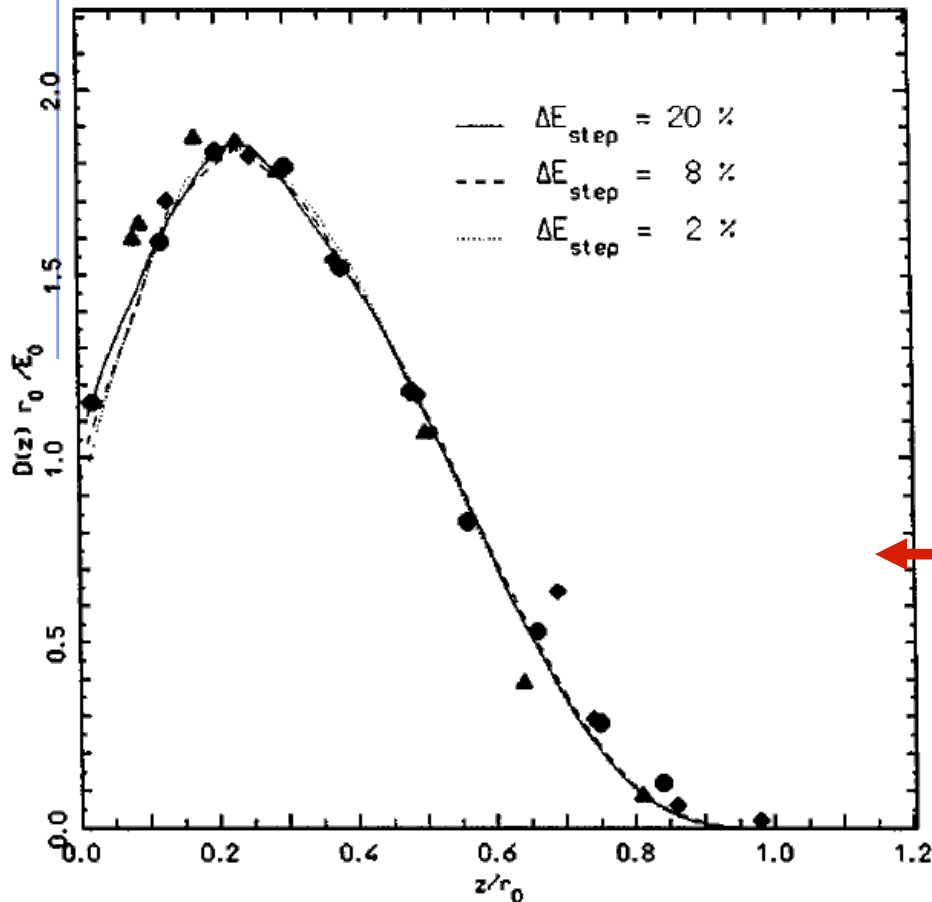
User control of MCS

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

SDUM

- 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 csa 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)
- $\alpha, \varepsilon, \mathbf{Smin}$ control the precision of the tracking, (see next slides) . They can be overridden/complemented by the STEPSIZE card

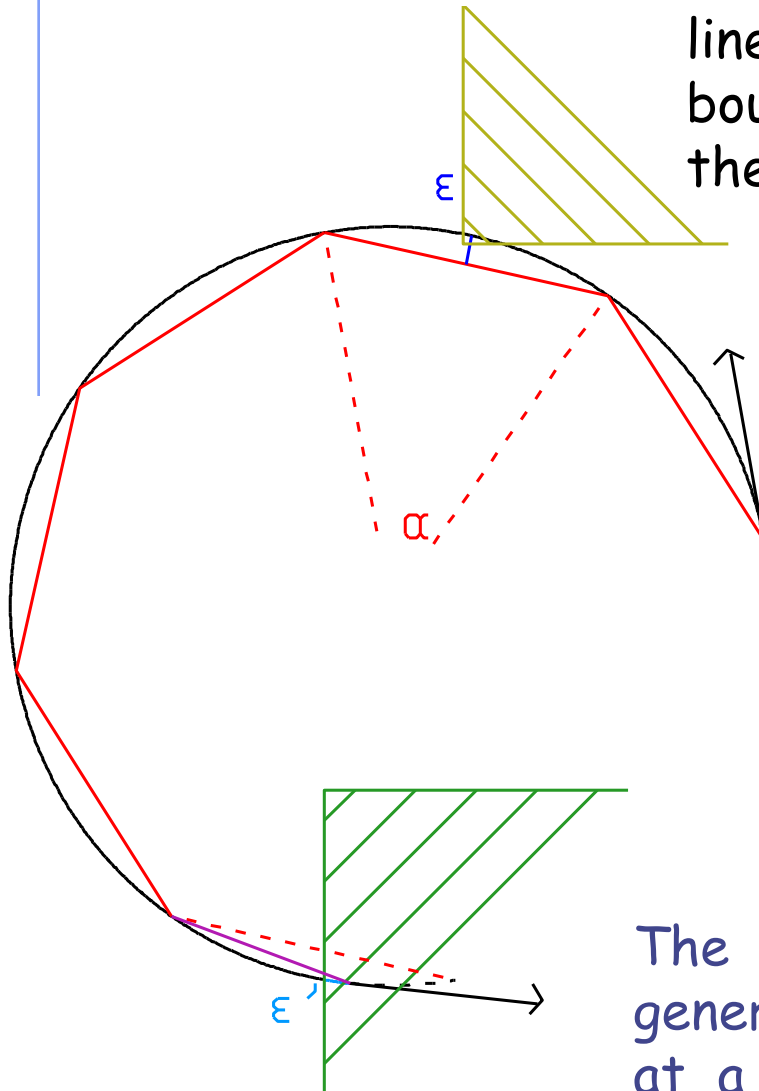
Magnetic field tracking in FLUKA

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)

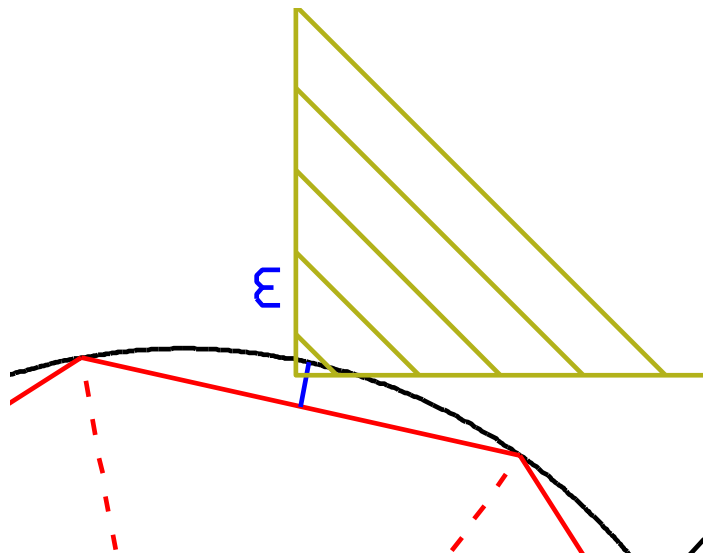
The end point is ALWAYS on the true path, generally NOT exactly on the boundary, but at a distance $< \epsilon'$ from the true boundary crossing (light blue arc)



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



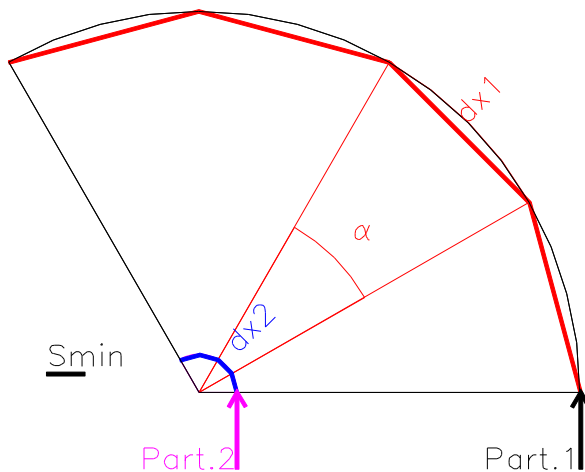
IF α and/or ϵ are too large, boundaries may be missed (as in the plot);
 IF they are too small, CPU time explodes....
 Both α and ϵ conditions are fulfilled during tracking.

- 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 $> S_{min}$ -> 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

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:

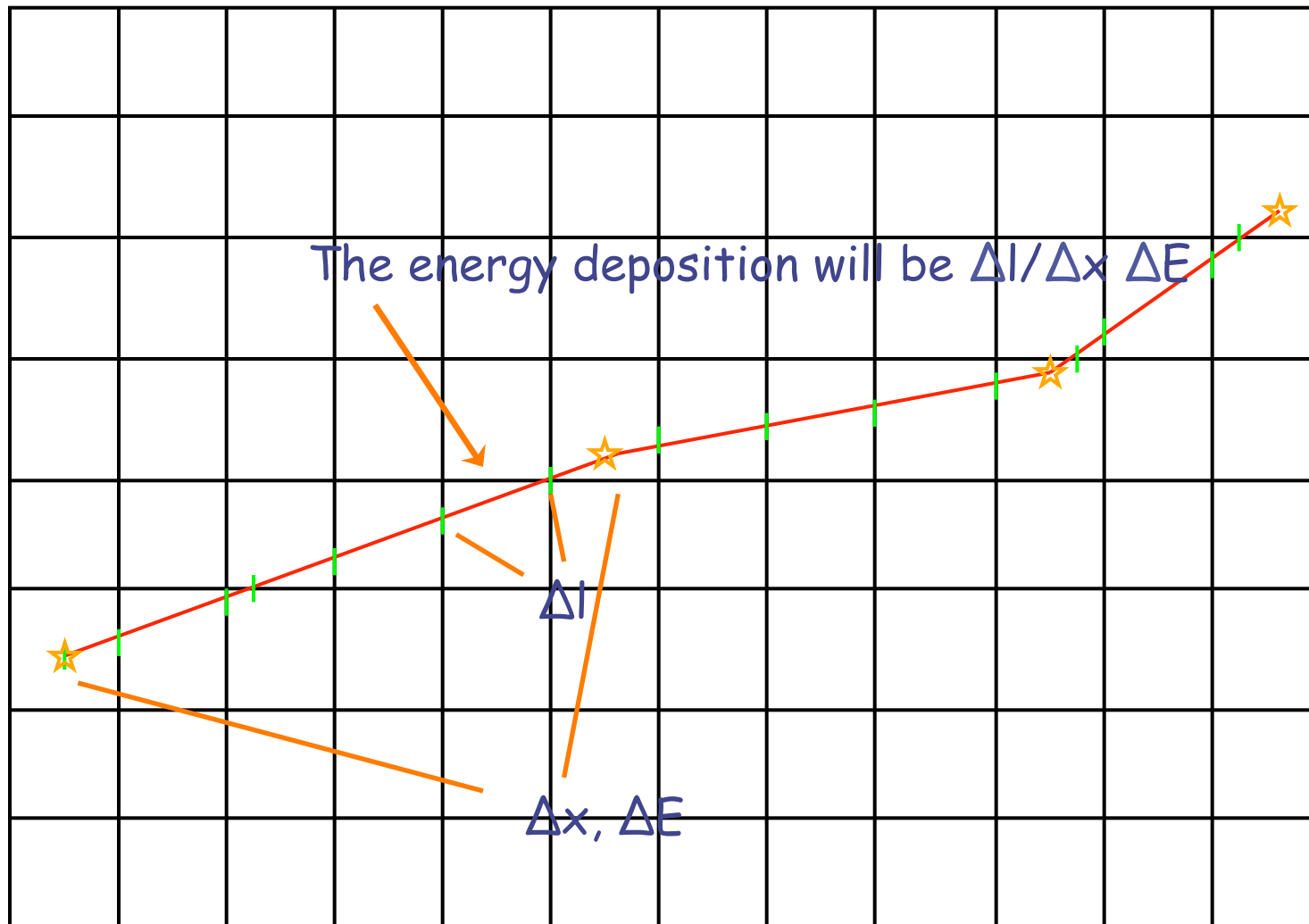
btx,bty,btz = cosines of the magn. field vector
B = magnetic field intensity (Tesla)
idisc = set to 1 if the particle has to be discarded

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

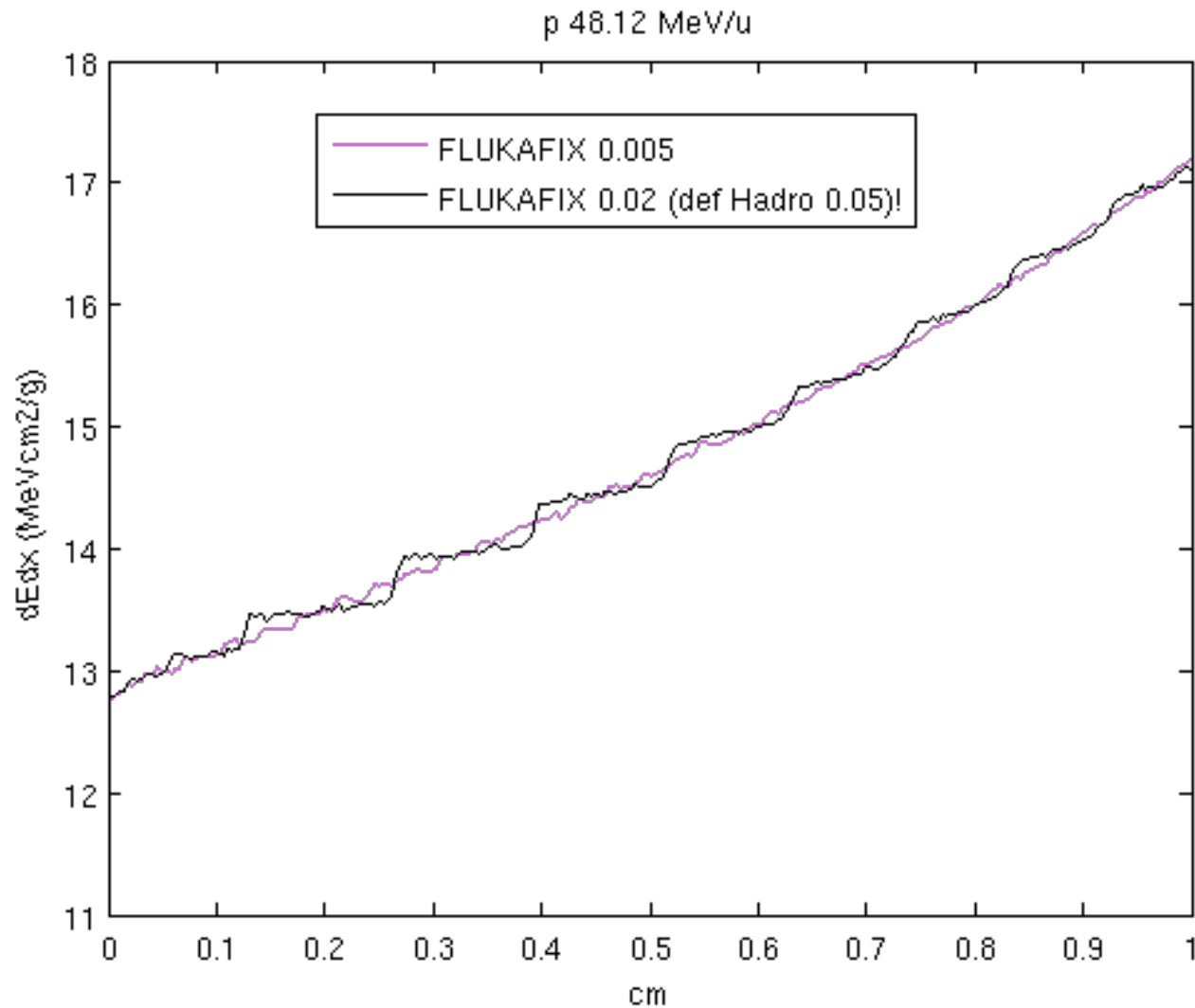
Some warnings about scoring:

- 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 \rightarrow a final ΔE is computed and used for scoring \rightarrow resulting in a scored *average effective $\Delta E/\Delta x$* uniform along that step
- The particle energy used for track-length estimators is the average one along the step ($E_0 - \Delta E/2$)

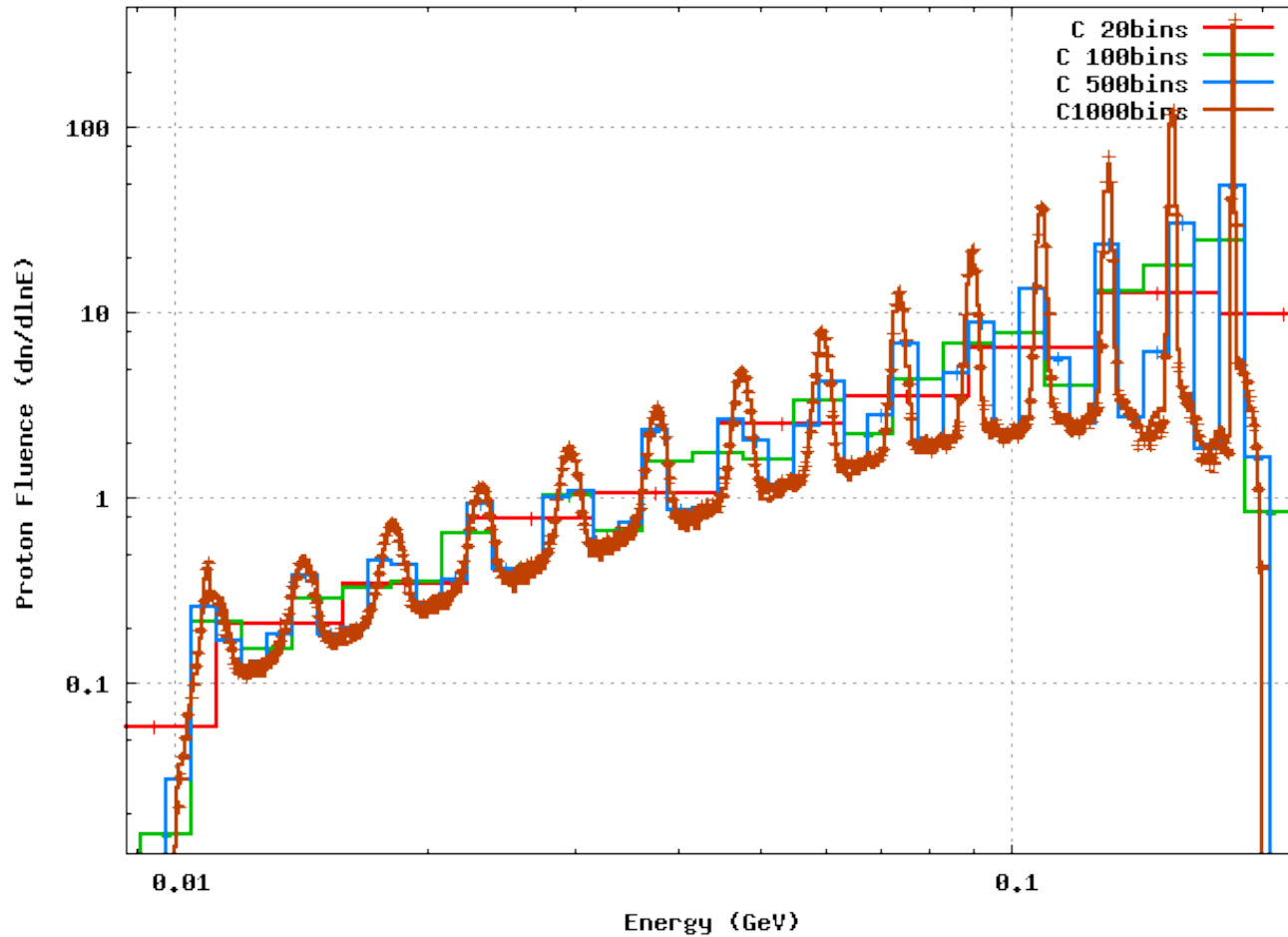
USRBIN track apportioning scoring



USRBIN track apportioning scoring



USRTRACK scoring: 200 MeV p on C



Default settings, $\approx 20\%$ 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