Charged particle transport

7th Fluka course

NEA Paris, Sept.29-Oct.3, 2008

Setting particle transport threshold

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PART-THR Thresh Part1  Part2   Step
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- 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 behaviour 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:

$$\text{PLC} \Leftrightarrow \text{lateral deflection}$$
$$\text{lateral displacement} \Leftrightarrow \text{longitudinal displacement}$$
$$\text{scattering angle} \Leftrightarrow \text{longitudinal displacement}$$

- 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

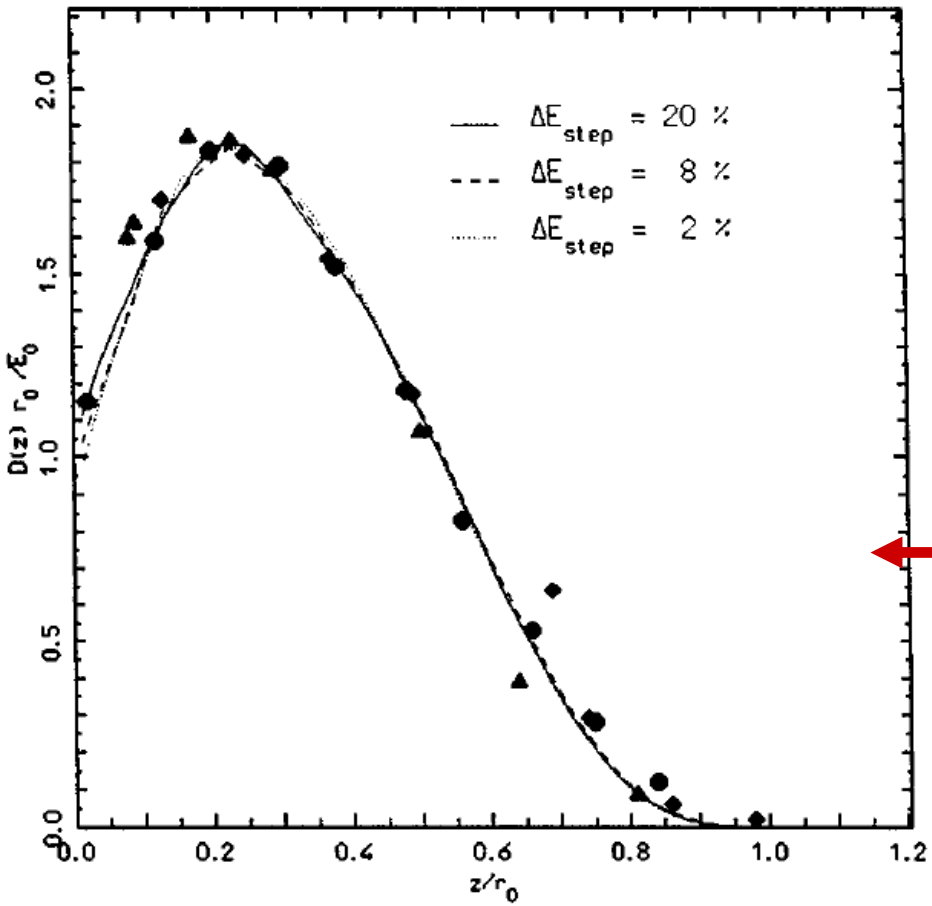
Fraction of normally incident electrons backscattered out of a surface.
All statistical errors are less than 1%.

User control of MCS

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 csda range

Control of step size II

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

```
EMFFIX  Mat1    DEstep1 Mat2    DEstep2 Mat3    DEstep3
```

EM

```
FLUKAFIX DEstep                 Mat1    Mat2    Step
```

Had
μ

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

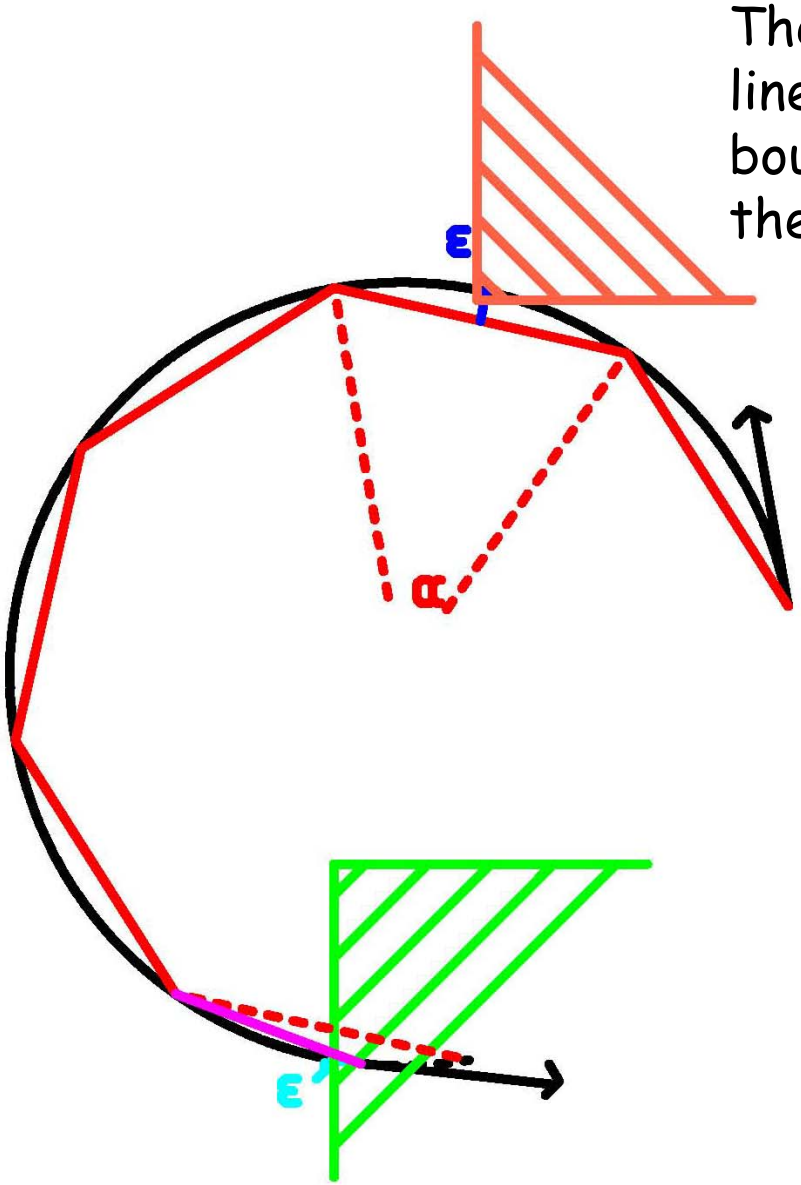
How to define a magnetic field

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

MGNFIELD	α	ε	Smin	B_x	B_y	B_z

- 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)

Setting the tracking precision

MGNFIELD	α	ε	Smin	B_x	B_y	B_z

- 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
- 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
- MGNFIELD sets the same parameter for all regions with magnetic field
- For region-by-region tuning, use STEPSIZE

Setting precision by region

```
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 mag field, 10 cm with mag field.
  - 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:

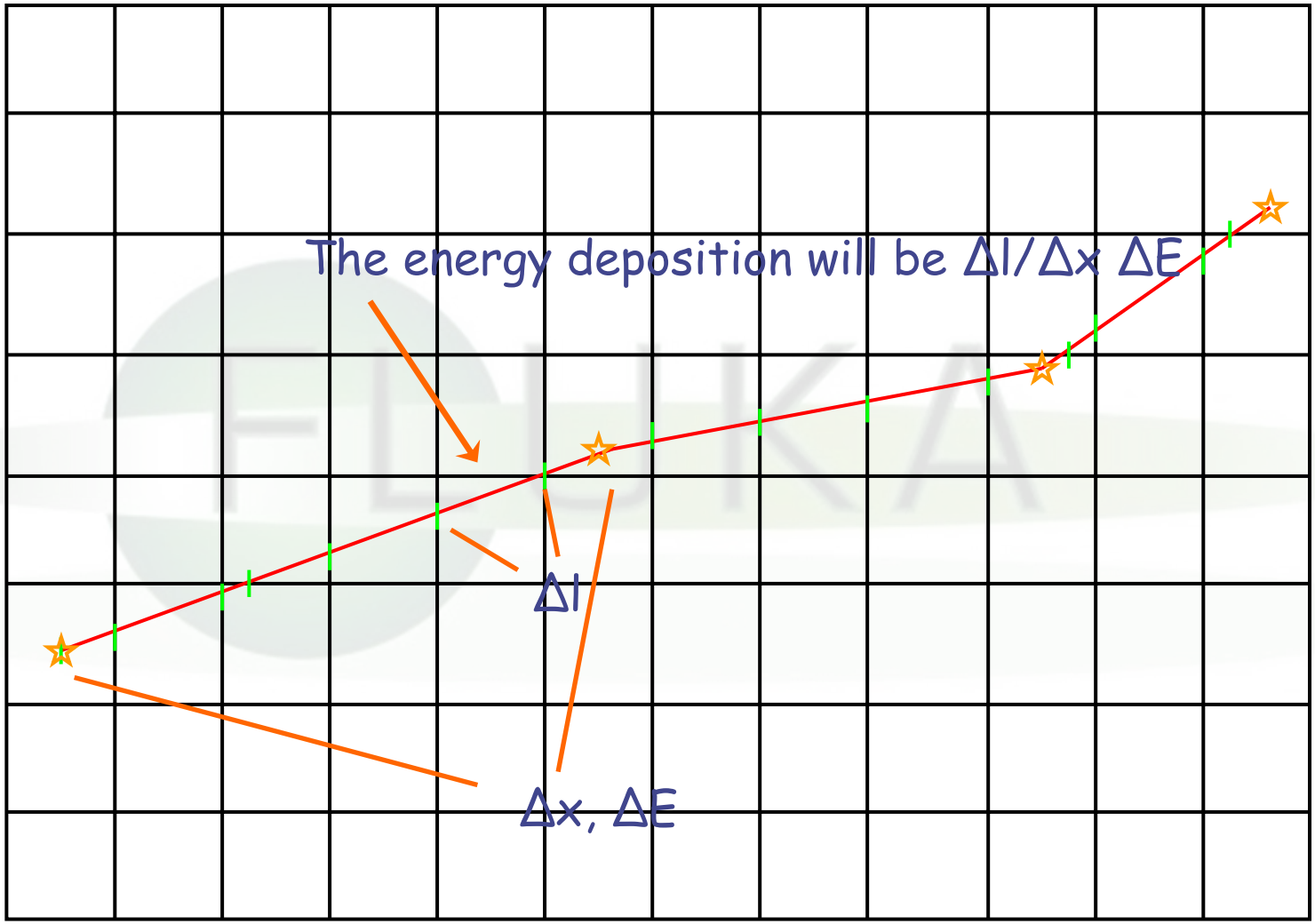
btx,bty,btz	=	cosines of the magn. field vector
B	=	magnetic field intensity (Tesla)
idisc	=	set to 1 if the particle has to be discarded

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

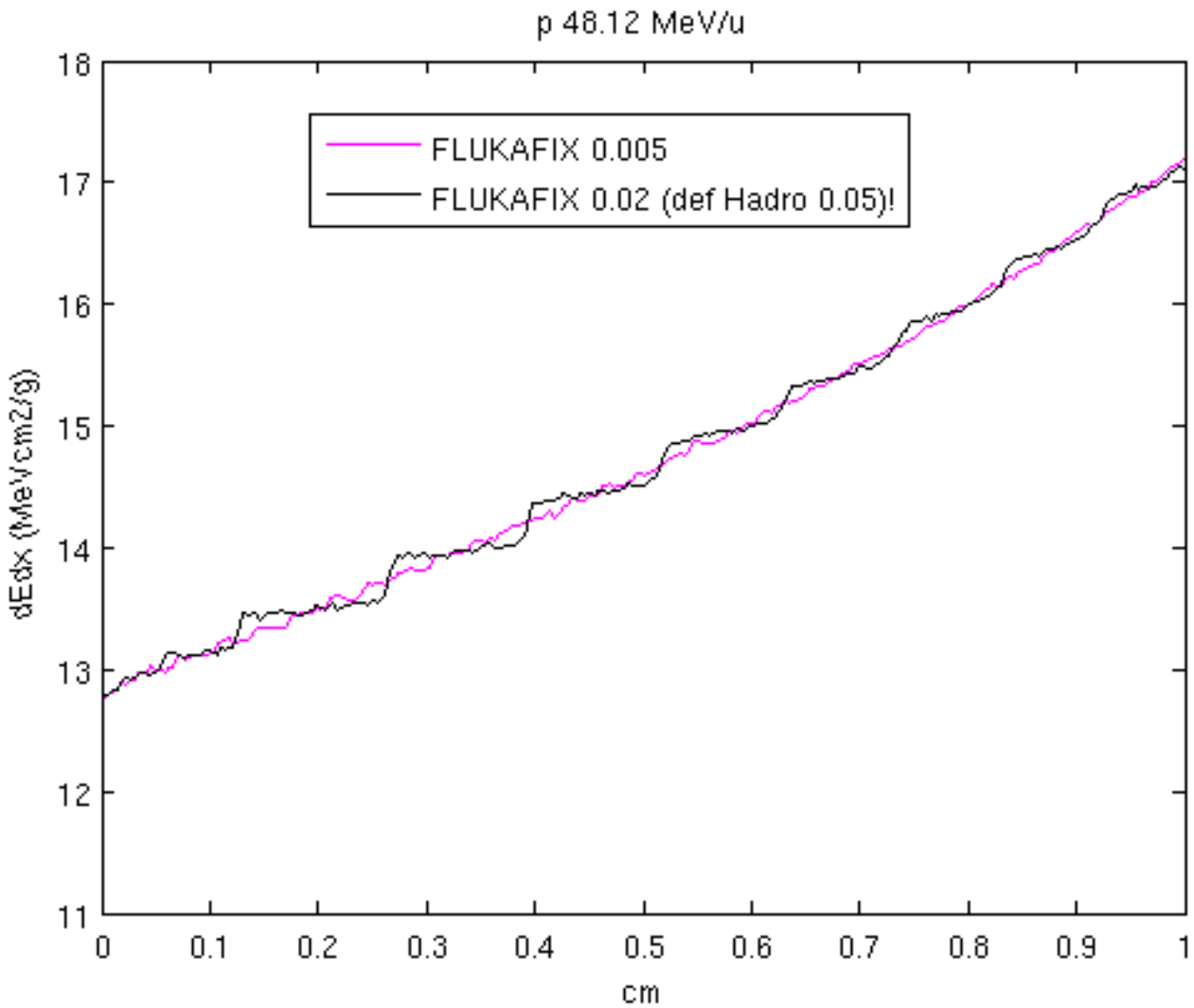
Some warnings about scoring:

- 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)

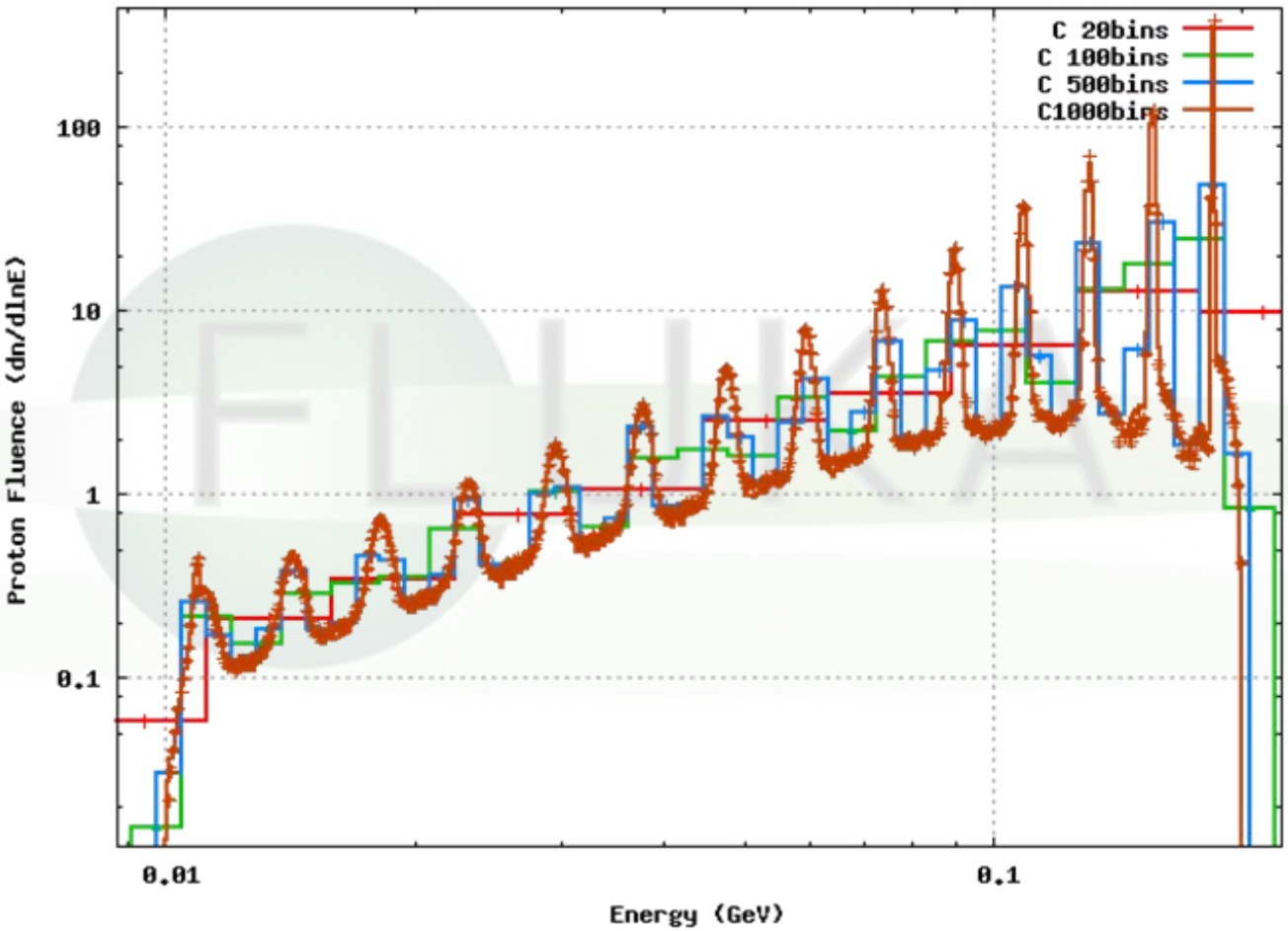
USRBIN track apportioning scoring



USRBIN track apportioning scoring



USRTRACK scoring: 200 MeV p on C



Default settings, ≈ 20% energy loss per step