



Advanced settings

1st Fluka advanced course

Preliminary considerations:

FLUKA is NOT a toolkit!!!!

The development team strives to provide the best possible physics it can develop, rather than a choice among several possible alternative models

Hence there are not many "physics" knobs to play with (ideally there should be no one)

The user has mostly to set threshold,/cuts, and switch on/off a few processes which for various reasons are not on/off by default

The DEFAULT card

- The **DEFAULT** card is there to help you : choose the one nearest to your problem
- The "default" **NEW-DEFA** is the "crudest" one: maybe it is not suited for your problem, check with care, don't use it blindly..
- Check all settings: *look in the output*, at least the 1st time you setup a new problem!
- Always *set production and transport thresholds.*

Summary: ionization and tracking

- Charged particles tracking : according to *Molière* multiple Coulomb scattering (MCS), i.e., it computes deflection, displacement and step shortening as a cumulative effect of all Coulomb scatterings along a charged particle step.
- Ionization energy losses: divided in
 - Discrete, above a pre-set threshold (“ δ -ray” emission)
 - Continuous, below this threshold: energy is deposited uniformly along a step, according to the **average** and **fluctuation** of the specific energy loss.
- Tracking termination : particle below the transport threshold (or interaction, decay, escape...)

Reminder: discrete δ -ray events

Above a pre-set threshold, secondary electron production is modeled as *δ ray* production (free electrons)

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

The threshold refers to the kinetic energy of the emitted *δ ray*

- ✓ For Electrons: set by **EMFCUT** with `sdum= PROD-CUT`
- ✓ For charged hadrons/muons: **DELTARAY**

Both cards set (production) thresholds *by material*

- It can be complemented by (and *consistent*) with transport thresholds (**EMFCUT** with no `sdum`) if more granularity is required
- Tabulations are built at initialization time based on production thresholds: important for *precision*
- If very different settings are needed for the same material in different regions -> may be wise to define instead *different materials* with different production thresholds

Summary: particle transport thresholds

- Hadron and muon transport thresholds are set with the **PART-THRes** card for the *whole simulated setup*
- The total momentum/energy cut-off's of *heavy ions* are scaled from that of a 4-He ion (**4-HELIUM**) according to the ratios of the atomic weights
- The total momentum/energy cut-offs for light ions (4-He, 3-He, 3-H, 2-H) can be defined by **PART-THRes**. If this is not done, they are scaled from that of a proton according to the ratios of the atomic weights
- Electron and photon transport thresholds are set with the **EMFCUT** card by *region*
- Neutron thresholds through **PART-THR** or **LOW-BIAS**

What happens after?

- Electrons and photons are stopped, their energy is deposited "on spot"
- Charged hadrons/muons are ranged out to rest with approximate tracking if the threshold is lower than 100 MeV, and particles are decayed, or annihilated on a nucleus, or captured if applicable. For thresholds *higher than 100 MeV* hadrons are dumped *on spot* without further treatment.
- Low-E neutrons: when stopped, the *kinetic energy* is deposited on spot: *not realistic* for calculation of energy deposition and activation → **track them down to thermal unless you don't care!**

How to set thresholds ?

It depends on

- the **"granularity"** of the *geometry*
- the **granularity** of the *scoring mesh*
- the **"interest"** in a given region.
- **Electron equilibrium** at boundaries
- CPU time..

In practice : compare the dimensions of the "problem" with the range of particles at the threshold energy. Energy/range tables are very useful (see for instance <http://physics.nist.gov>)

Warning : to reproduce correctly electronic equilibrium, neighboring regions should have the same electron **energy** (**NOT range in cm**) threshold. To be kept in mind for sampling calorimeters

Warning: photons travel much more than electrons.

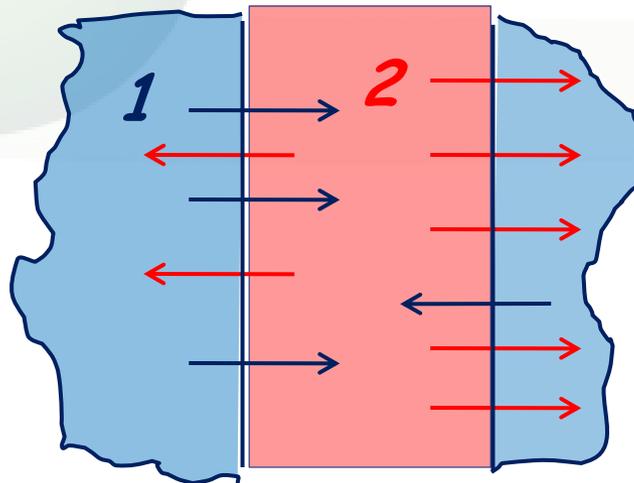
Warning: Threshold for antineutrons and neutral kaons should always be set=0.

Neutrons: see later

Electronic equilibrium, considerations:

The average stopping power, dE/dx , depends on the material only (weakly) for I (average ionization potential), and for $\langle Z/A \rangle$. The I dependence concerns only with distant collisions and it is not a source of disequilibrium at interfaces.

However electrons (δ -rays) emitted in close collisions can travel further and at an interface between 1 and 2 . This effect can reduce (increase) the stopping power experienced in 2 if $\langle Z/A \rangle_1$ is smaller (larger) than $\langle Z/A \rangle_2$



Electronic equilibrium, considerations II:

- For a precise measurement of dE/dx in medium 2 it is essential that $\langle Z/A \rangle_1 = \langle Z/A \rangle_2$ before and after the sensitive volume, so that electronic equilibrium is achieved
- The *thickness* of the layer of "equivalent" material should be comparable or larger of the *range of the most energetic secondary electrons* → impossible for incident electrons and relativistic particles
- *Density differences do not matter*, and they are automatically corrected for when results are expressed in deposited energy per unit mass (\equiv *dose*)
- The special case when medium 1 is *vacuum* produces the *buildup* region, which extends up to the range of the most energetic electrons
- Thresholds should be set according to these considerations, so that
 - They are equal on both sides of the interface
 - They are low enough to assure electronic equilibrium unless for a negligible region

Electronic equilibrium, considerations III:

When *photons* are involved or the energy of the incident particles is large enough to make bremsstrahlung significant:

- For a precise measurement of *dose* in medium 2 it is essential that $\langle Z/A \rangle_1 = \langle Z/A \rangle_2$ before and after the sensitive volume, so that electronic equilibrium is achieved for charged particles
- It is also essential that $\langle Z^2/A \rangle_1 = \langle Z^2/A \rangle_2$ before and after the sensitive volume for pair production and bremsstrahlung
- ... and also $\langle Z^n/A \rangle_1 = \langle Z^n/A \rangle_2$, $n \sim 5$, before and after the sensitive volume for photoelectric
- The *thickness* of the layer of "equivalent" material should be comparable or larger of the *range of the most energetic secondary electrons* produced by the photons → often impossible to achieve
- Threshold should be equal, and low enough to assure minimal disequilibrium

Electronic equilibrium, considerations IV:

When *neutrons* are involved or the energy of the incident hadron is large enough to make nuclear reactions significant:

- For a precise measurement of *dose* in medium *2* it is essential that the *chemical composition* before and after the sensitive volume is the same
- When this is not possible, at least the hydrogen (fractional) content should be made the same
- The *thickness* of the layer of "equivalent" material should be comparable or larger of the *range of the most energetic secondary charges particles (recoil protons for neutrons)* produced
- Unless you are sure, track neutrons down to thermal energies!

A practical example

Water- Lead-Aluminum layers

50 microns each

$25\mu\text{ Pb} = 2.8 \cdot 10^{-2} \text{ g/cm}^2$

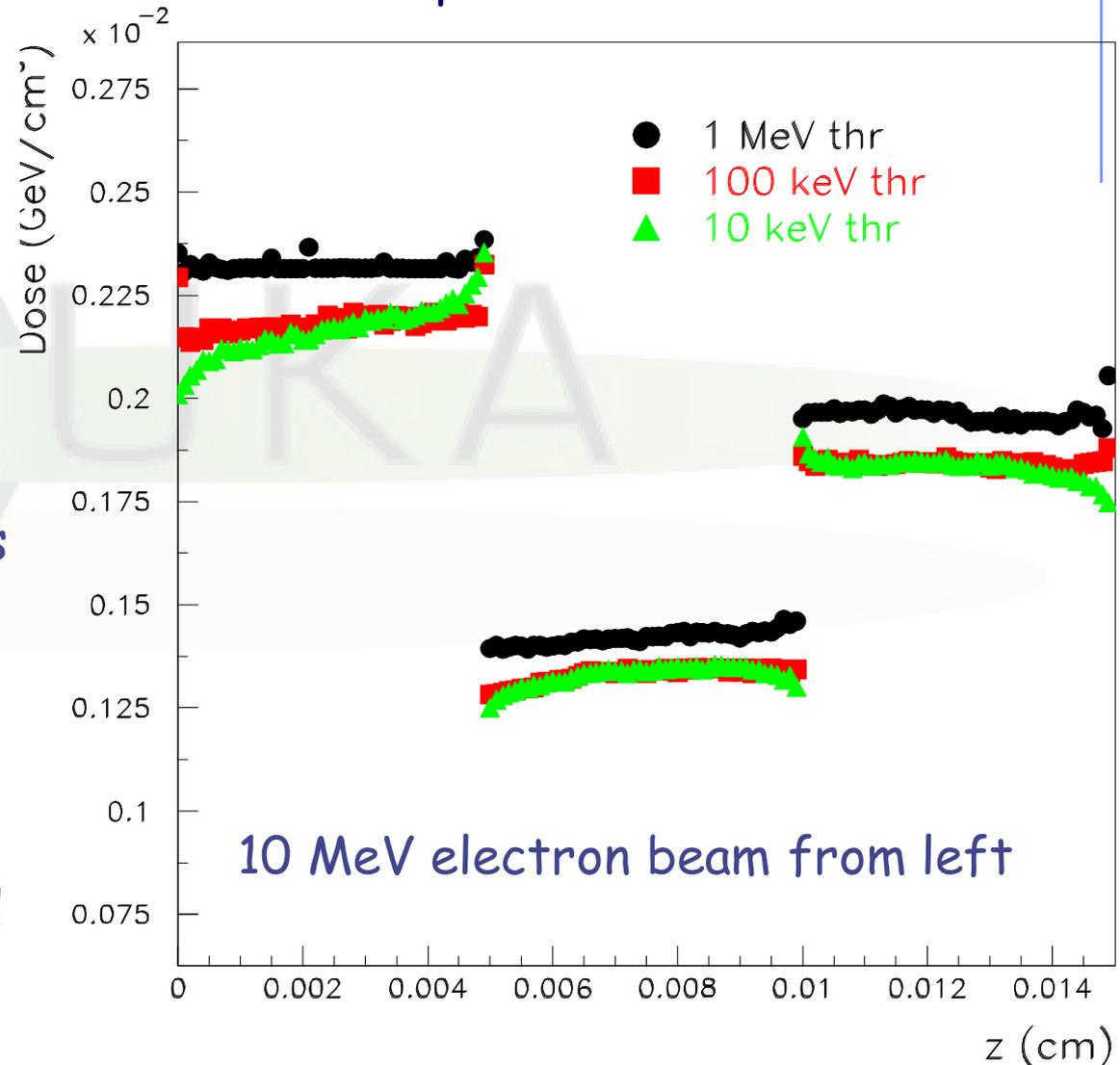
→ 100 keV

$1\mu\text{ Pb} = 1.1 \cdot 10^{-3} \text{ g/cm}^2$

→ 12keV

- High threshold gives overestimated results because electrons cannot escape
- Medium threshold is reasonable for average value in layer
- Low threshold needed if scoring grid is fine

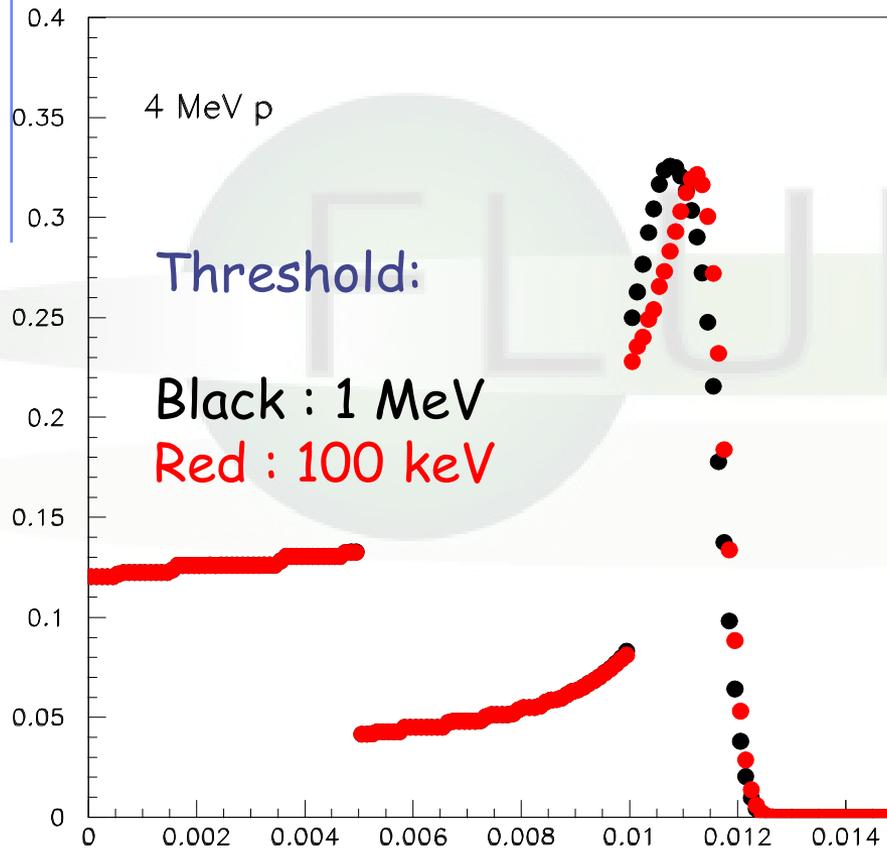
Deposited dose



The same with protons

4 MeV protons

run with the proton threshold at 1MeV and 100 keV



Neutron thresholds

Neutrons can interact at any energy, down to thermal, with exothermic or endothermic reactions. The simple assumption of kinetic energy deposition used below threshold is a gross approximation, therefore:

- For all problems involving energy deposition, residual nuclei production, and of course neutron propagation: *leave the default* (last thermal group, $1 \cdot 10^{-5} \text{eV}$)
- A threshold can be set (**PART-THR** if above 20 MeV, **PART-THR** or **LOW-BIAS** below) only if the problem treated is intrinsically not sensitive to low energy particles (detectors with a threshold, neutrino beams..)

Neutron setting for full analogue runs

- ***non-analogue absorption***: biasing technique used to increase/decrease the absorption probability in low-energy neutron transport. Used to save CPU since it minimizes bouncing of neutrons in materials with low absorption probability (or enhance survival in high absorption ones). In FLUKA, with many **DEFAULTs** options, ***non-analogue absorption is applied to all thermal groups***. This is ***not*** suited for ***fully analogue*** calculations, like for instance ***event-by-event detector response***, or for problems with very low absorption probability
- To inhibit it, use the **LOW-BIAS** card with **WHAT(2)=261** (last neutron group+1).
- **WHAT(3)** sets the level of non-analogue absorption through the value of its complement, the ***non-analogue survival probability***: physical value is $1 - \sigma_{\text{abs}} / \sigma_{\text{tot}}$, default value for thermal groups is 0.95 (**PRECISION** and **CALORIMETER** defaults excluded)

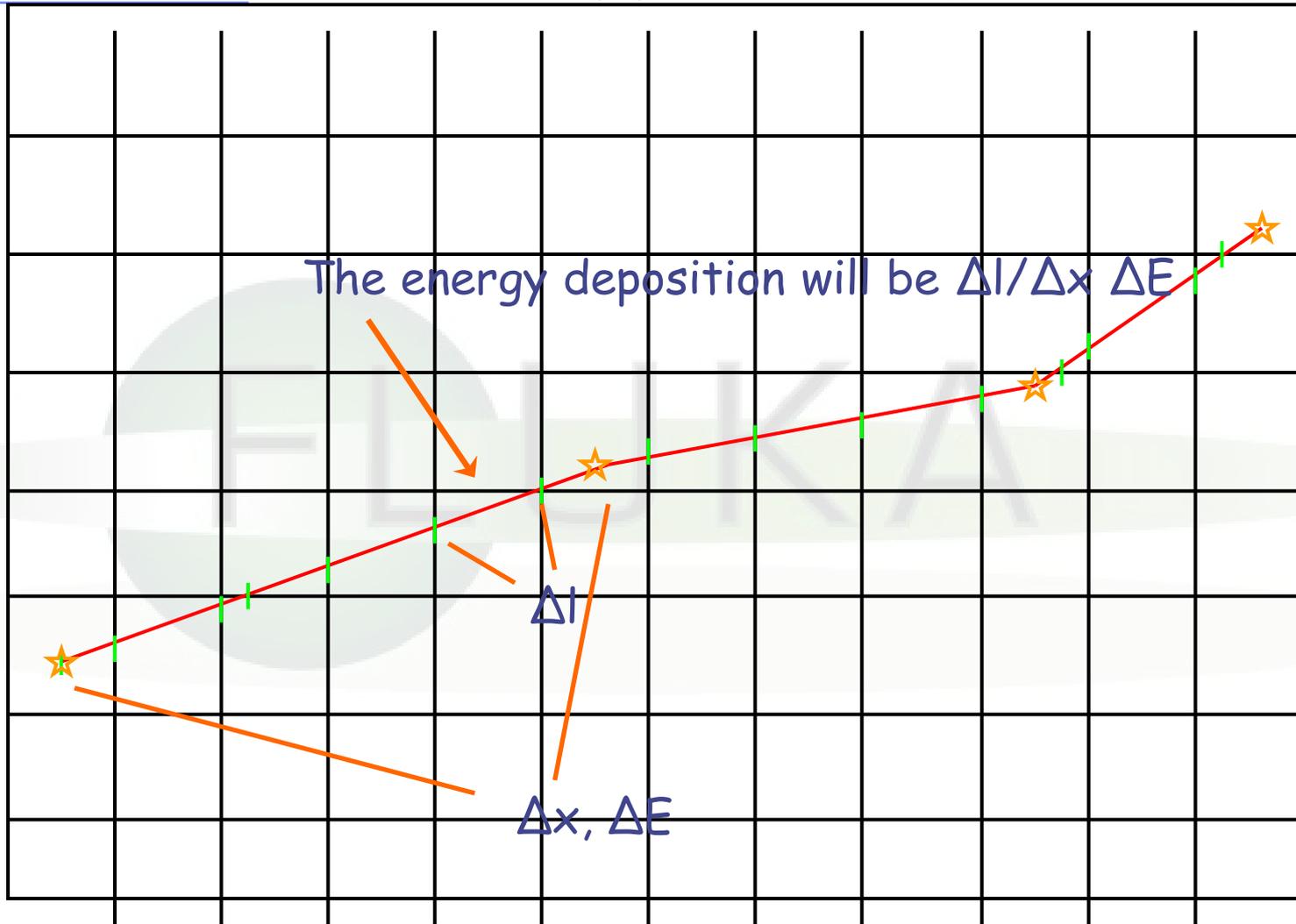
Neutron setting for full analogue runs -II

- *Pointwise neutron transport* is available for ^1H (above 10 eV if bound H requested, down to 10^{-5} eV otherwise) and ^6Li
- *Detailed correlated reaction products* are available for ^1H , ^6Li , ^{10}B (only for the reaction $^{10}\text{B}(n,\alpha)^7\text{Li}$), and the $^{14}\text{N}(n,p)$ reaction. All reaction products are then transported explicitly according to transport setting (**PHYSICS**).
- Recoil proton production is ON by default for H and $^{14}\text{N}(n,p)$
- while for the others and for pointwise treatment it depends on the **DEFAULT** set chosen
- Both are important for precision studies, detector response (exp. scintillators), borated materials...
- To require *pointwise neutron transport and reaction products* (where available), use the **LOW-NEUT** card with **WHAT(6)=1**.

Some warnings about scoring:

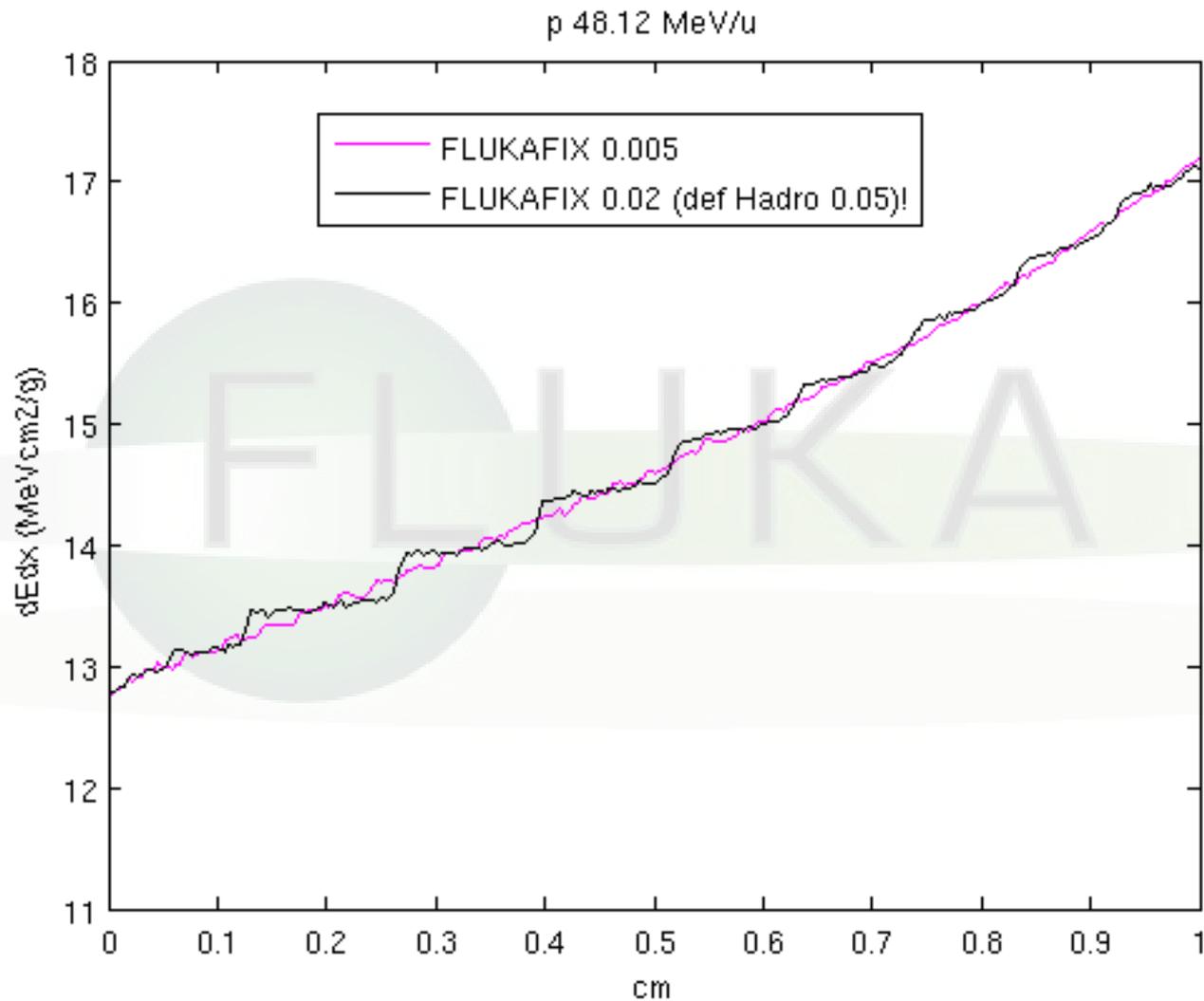
- Every charged particle step Δx has its length constrained by:
 - Maximum fractional energy loss (see **FLUKAFIX**)
 - Maximum step size for that region (see **STEPSIZE**)
 - **MCS** (or other) physical constraints
 - Distance to next interaction (nuclear, δ ray etc)
- The *average* energy loss is computed 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* utilized for track-length estimators (**USRTRACK**) is the *average one* along the step ($E_0 - \Delta E/2$)
- **Artifacts** can show up if the scoring meshes are inconsistent with the tracking parameters :

USRBIN track apportioning scoring



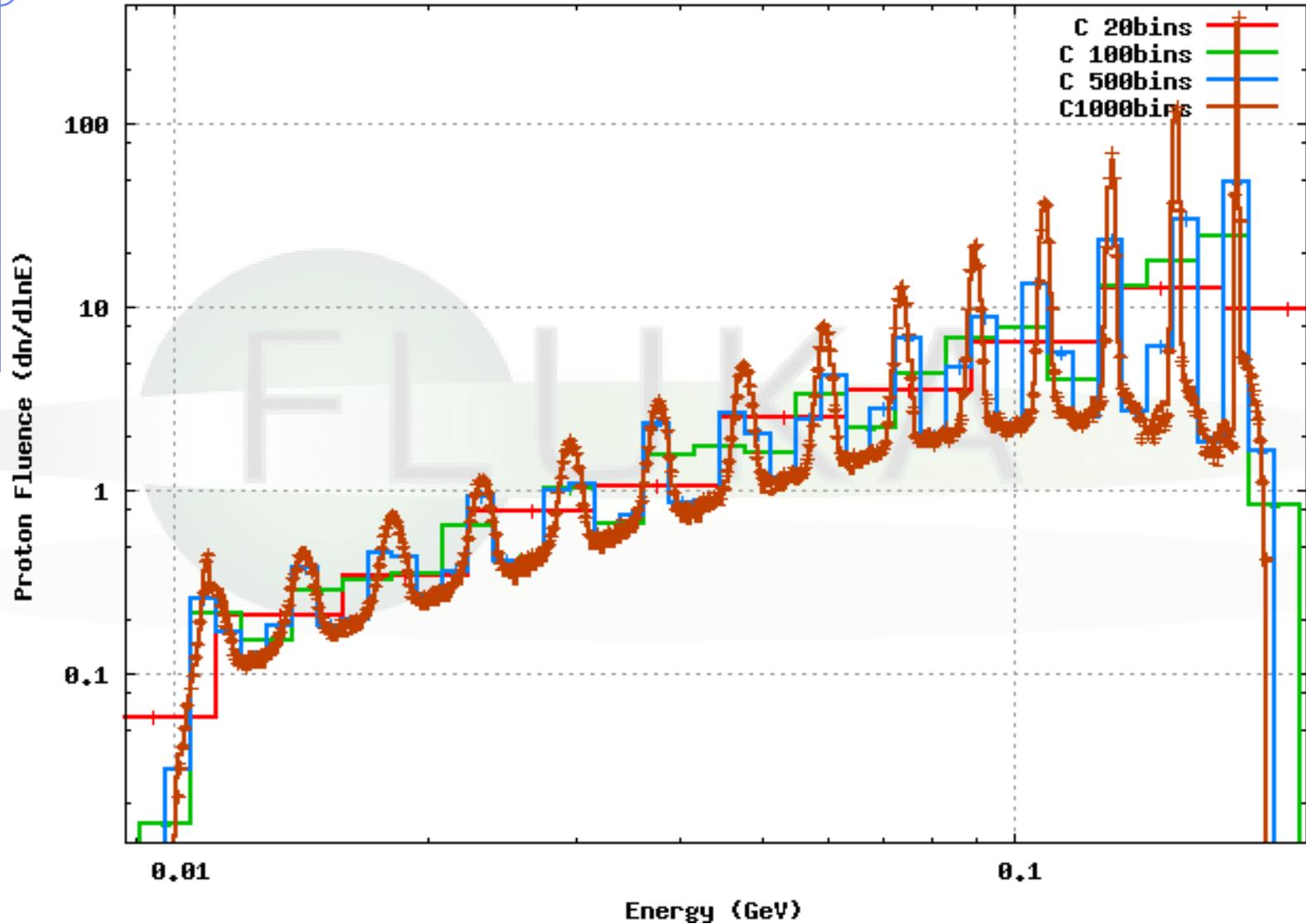
The energy deposited in a single physical step is EQUALLY distributed in the crossed cells (proportionally to dx)

USRBIN track apportioning scoring



Steps can appear in the scored results

USRTRACK scoring: 200 MeV p on C



Default settings, $\approx 20\%$ energy loss per step

Single Scattering

- In very *thin layers, wires, or gases*, the Molière theory of multiple scattering does not apply.
- In FLUKA, it is possible to replace the standard multiple scattering algorithm by *single scattering* in defined *materials* (option **MULSOPT**).
- CPU demanding, but affordable and very accurate at low electron energies, *can be tuned x material!*
- Can be activated separately for electrons and hadrons and muons
- Can be activated partially, i.e.
 - only near boundaries,
 - near boundaries and for short steps
 - near boundaries and for short steps and for too low energies
- Can be activated globally, always replacing MCS in the selected material(s). (Setting WHAT(6) > 1000.0 with SDUM = GLOBAL, GLOBHAD or GLOBEMF).

More control on multiple scattering

Further control of the multiple scattering algorithm can be done with the **MULSOPT** card:

- Require *optimisation* of MCS: in this case the program always makes the minimum step for which the Molière theory of multiple scattering is applicable. Very CPU consuming, discouraged, better use single scattering at boundaries or for very short steps
- Set the maximum step length near boundaries
- Activate all or part of the *corrections* to the Molière cross section (spin-relativistic, form factors)
- All not needed in shielding problems, but sometimes 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*, debugging)

Control of step size II

dE/dx 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 (= default) 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** (Mgn. Field lecture)

More control on ionization

Ionization fluctuations are simulated or not depending on the DEFAULTS used. Can be controlled by **IONFLUCT**. *Leave on unless for testing*

(Crude) primary ionization algorithm

For *gaseous detectors*, **FLUKA** can provide the list of *primary ionization events*, their location and energy according to (a very simplified) model. In order to activate it a few user-provided parameters are required

IONFLUCT	1stIon	np_mip	model	Mat1	Mat2	MatStep	PRIM-ION
----------	--------	--------	-------	------	------	---------	----------

- 1stion: effective 1st ionization potential of the gas (eV)
- np_mip: number of primary ionizations per cm for a minimum ionizing particle
- model: 1-4 (there are 4, all very approximate, models available)
- From material Mat1 to material Mat2, in steps of MatStep

The primary ionization events for each (charged) particle step will be recorded in common **(ALLDLT)** (*look at it for details!*)

Reminder : The FLUKA hadronic Models

Hadron-nucleus: PEANUT

Elastic, exchange
Phase shifts
data, eikonal

$P < 3-5 \text{ GeV}/c$
Resonance
prod
and decay
hadron

hadron

hadron

low E
 π, K
Special

High Energy
DPM
hadronizati

Sophisticated
G-Intranuclear
Cascade

Gradual onset of
Glauber-Gribov
multiple interactions

Preequilibrium

Coalescence

Evaporation/^{on}Fission/Fermi break-
up

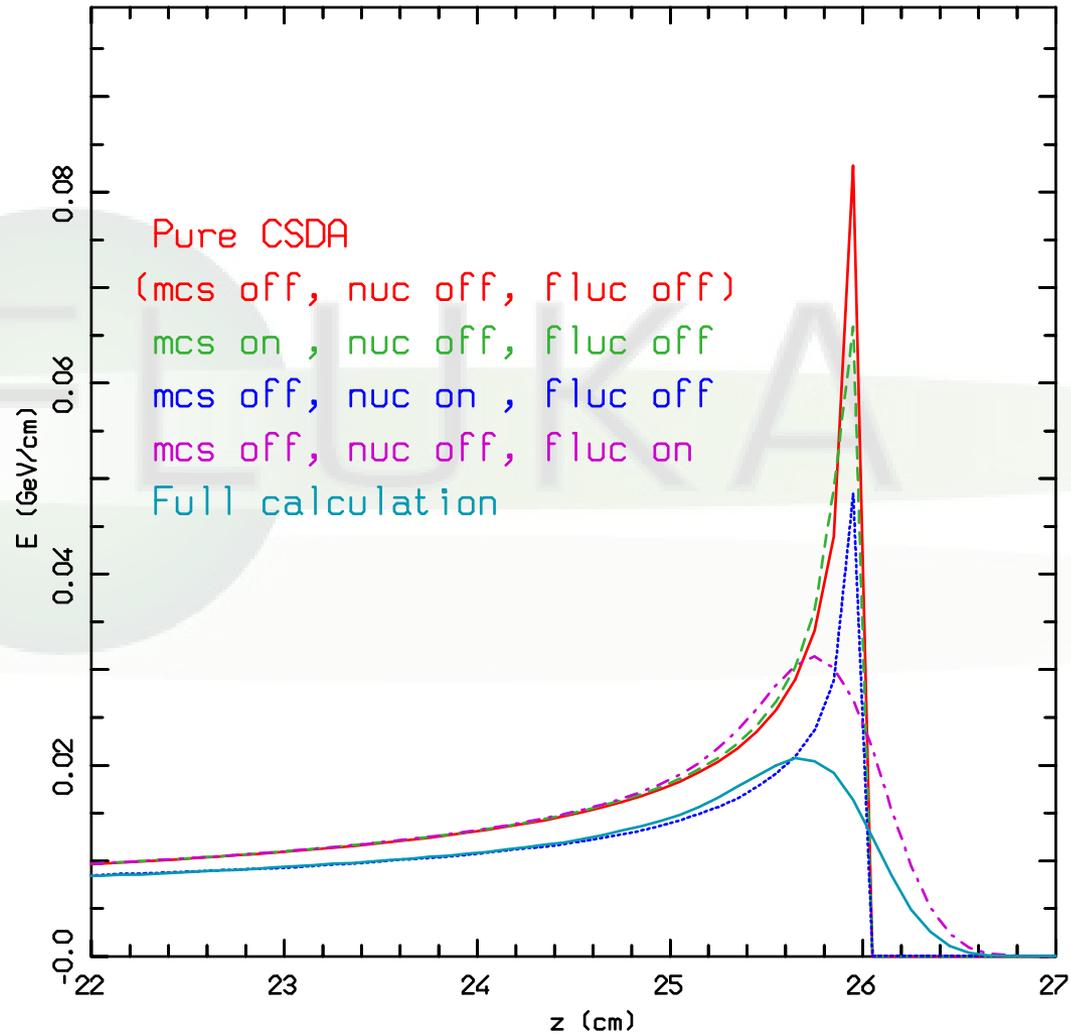
γ deexcitation

Hadronic interactions

- For activation, radiation damage, and similar studies: switch on *coalescence and heavy fragment emission* (**PHYSICS** card)
- Do not forget to enable ion transport and interactions (**EVENTYPE**) and link with *ldpmqmd(bme)* when heavy ions are of interested
- For "precision" hadron physics at high energies, or neutrino beam production: use the extended PEANUT model (**PEATHRESH**) [**reminder**: the default is to use the old, less refined intranuclear cascade model for projectile momenta $\gtrsim 5 \text{ GeV}/c$]
- For electron accelerators, muon transport and underground physics: remember that muon and photon nuclear interactions are *OFF by default*. Switch them on with **MUPHOTON** and **PHOTONUC**, and *bias them*
- ONLY for understanding the relative impact of different processes, hadron elastic and/or inelastic *interactions can be switched OFF* with the **THRESHOLD** card.

Bragg peaks: ideal proton case

200 MeV p on water (pencil beam)



Heavy ion transport and interactions

- The accuracy level of Heavy Ion transport can be set through the **EVENTYPE** card:
 - $WHAT(3) \leq -1.0$: no ion transport at all
 - $WHAT(3) = 1.0$: approximated transport of ions and recoils (dE/dx only)
 - $WHAT(3) = 2.0$: all heavy recoils and ions are transported with energy loss and multiple scattering,
 - ◆ without nuclear interactions if $SDUM = \text{blank}$ or $= \text{EVAP}$,
 - ◆ with nuclear interactions if $SDUM = \text{DPMJET}$ (and heavy ion generators linked)
 - $3.0 \leq WHAT(3) \leq 6.0$: heavy recoils up to $|particle\ id| = WHAT(3)$ are transported with energy loss and multiple scattering, but no nuclear interactions (3=d,4=t,5=3-He,6=4-He)
- With many **DEFAULTs**, there is ***no transport at all!***
- Remember to ***select ion transport and interactions*** for precision problems (i.e. precision dosimetry)
- Remember to select ion ***transport and interactions*** if coalescence and/or fragmentation are active

Summary of precision hadronic settings

Activate PEANUT at all energies

```
PHYSICS 1000. 1000. 1000. 1000. 1000. 1000. PEATHRESH
```

Activate Coalescence

```
PHYSICS 1. COALESCE
```

Activate heavy fragment evaporation

```
PHYSICS 3. EVAPORAT
```

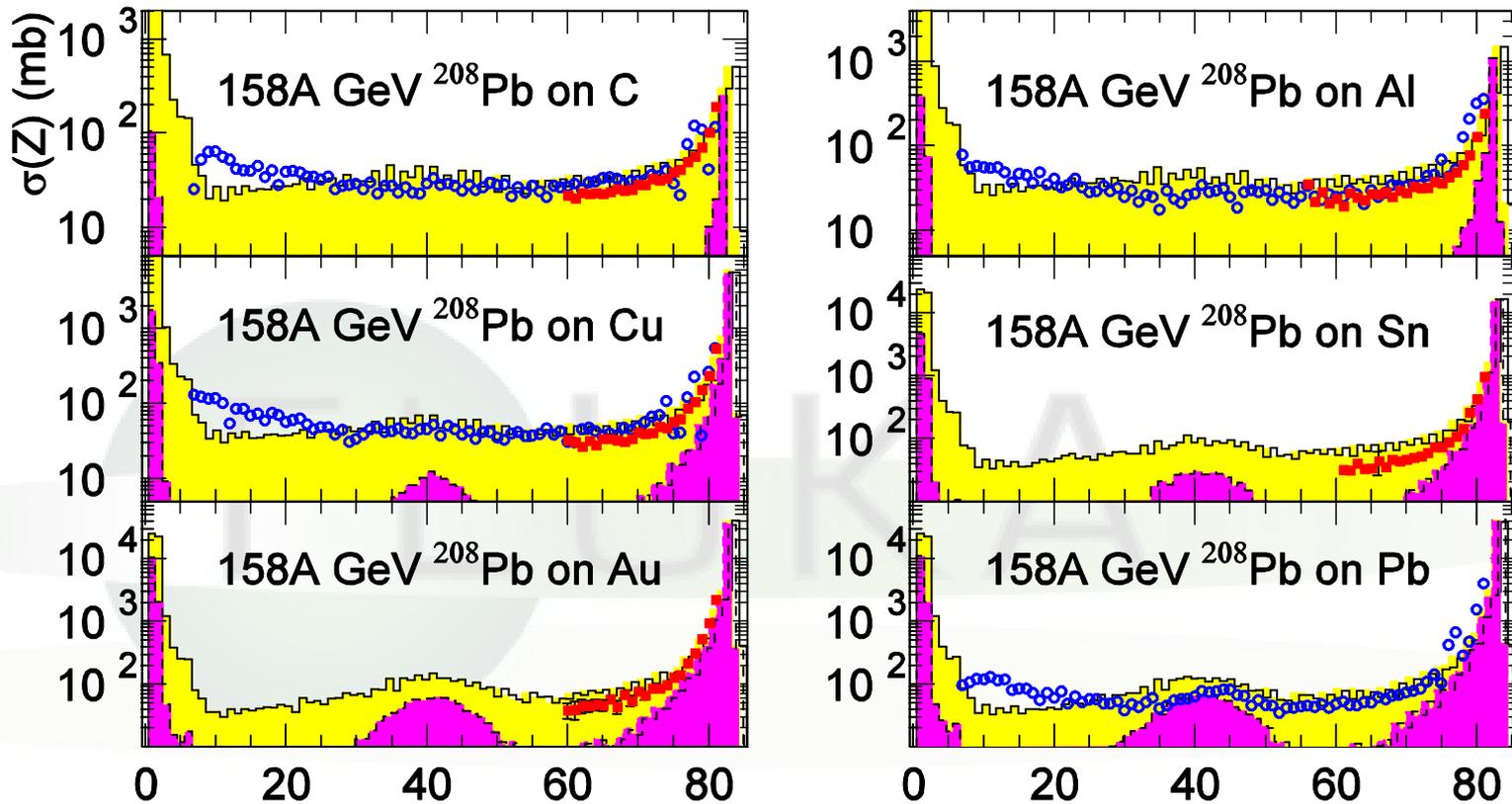
Activate ion transport and interactions

```
EVENTYPE 2.0 DPMJET
```

And for energetic heavy ions, activate electromagnetic dissociation

```
PHYSICS 2. EM-DISSO
```

EMD: 158 GeV/n Pb ion fragmentation

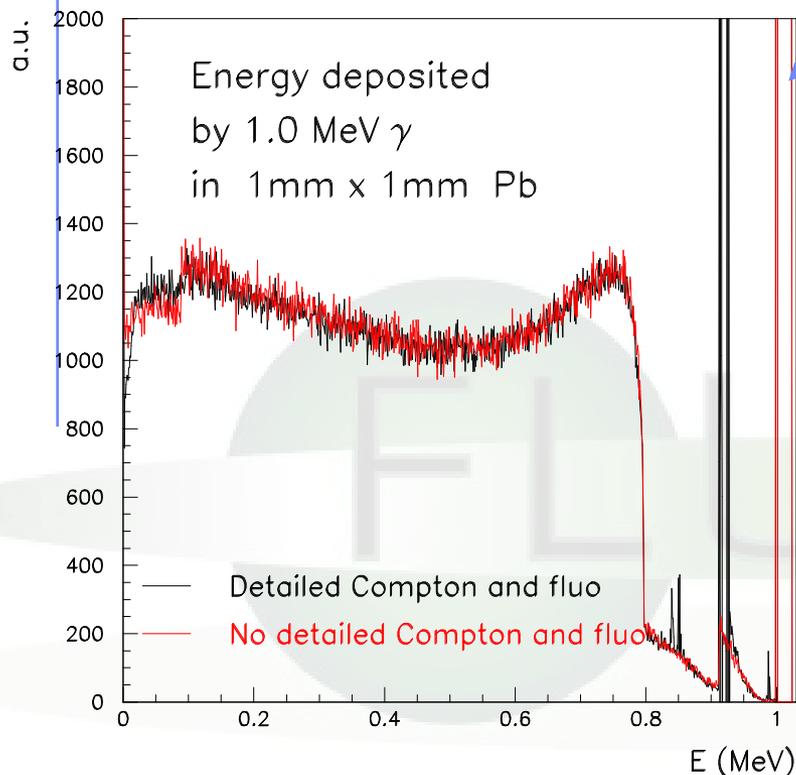


Fragment charge cross section for 158 AGeV Pb ions on various targets. Data (symbols) from NPA662, 207 (2000), NPA707, 513 (2002) (blue circles) and from C.Scheidenberger et al. PRC70, 014902 (2004), (red squares), yellow hists are FLUKA (with DPMJET-III) predictions: purple hists are the electromagnetic dissociation contribution

E-M interactions

- Cards are available to tailor the level of precision in the simulation of E-M processes. As usual, precision has a price in terms of CPU.
- Precision settings require consistent transport thresholds: it is useless to generate a fluorescence x-ray if it is immediately dumped.
- There is even the possibility to *switch off* (or increase the threshold) some of the E.M. interactions through the **EMFCUT** card with sdums **ELPO-THR, ANNH-THR, PHOT-THR, PHO2-THR**. *Use only for debugging purposes*
- Don't forget that *photon and muon photonuclear interactions are off* by default

Photoelectric effect



To activate/deactivate
fluorescence:

EMFFLUO card, works
by material

Fluorescence after photoelectric is
activated only with a subset of
DEFAULTs

If non-active, the energy equivalent
to the x-ray is dumped at the
interaction point

If active, an x-ray is emitted and
tracked. (or Auger electron)

CPU time vs. *precision in small
granularity.*

Important, for instance, in
dosimetry, or whenever the
granularity of the problem
compares with the range of
fluorescence x-rays.

Compton/ Rayleigh: EMFRAY card.

- Activates/ deactivates photon Rayleigh scattering. Little effect on energy deposition and transport, useful only for specific photon transport problems
- Controls the treatment of Compton scattering.

green = free electron

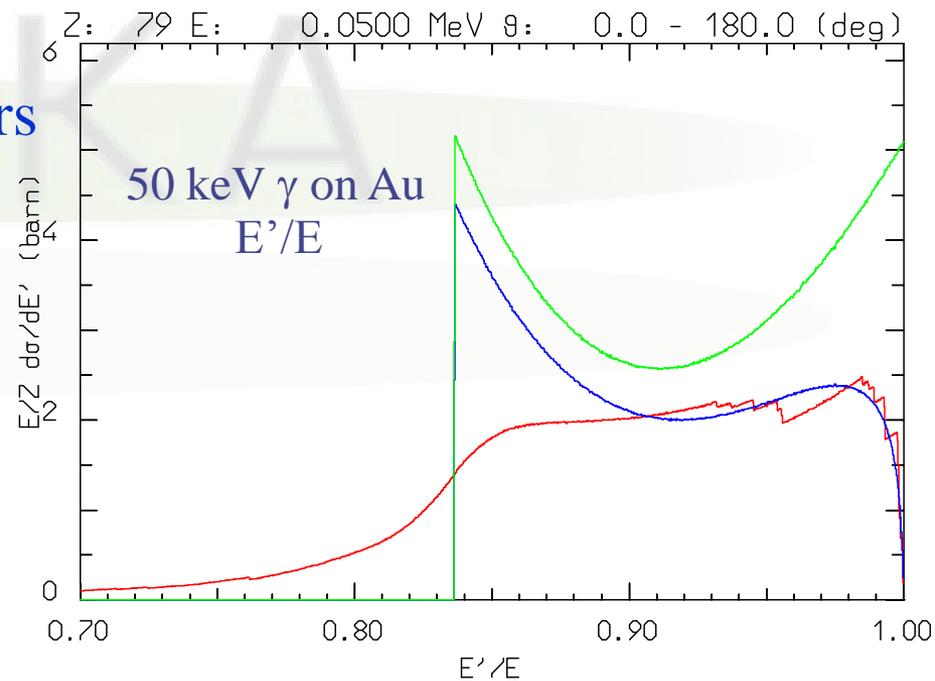
blue = binding with form factors

red = binding with shells and orbital motion

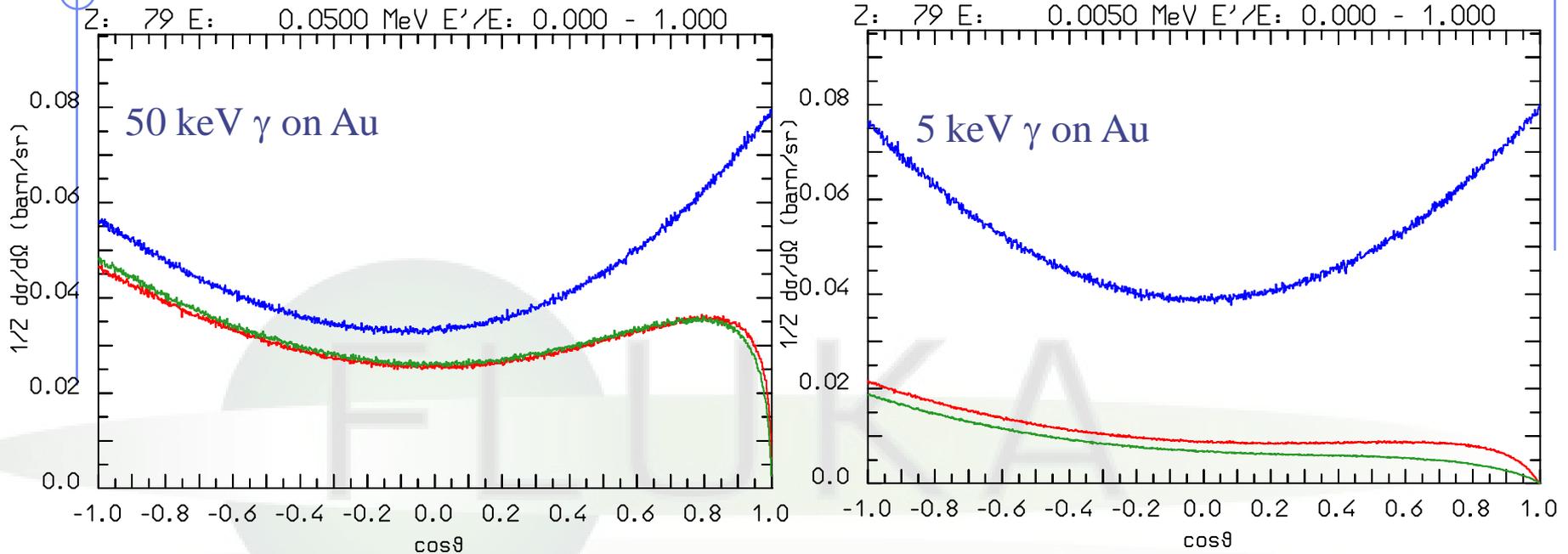
Larger effects at low energy , High-Z materials.

blue curve (old default) ok for most applications

Use the most refined (what(1)=4) for specific low-energy photon transport (default for "precision" defaults....)



Compton ang. distr.: examples II



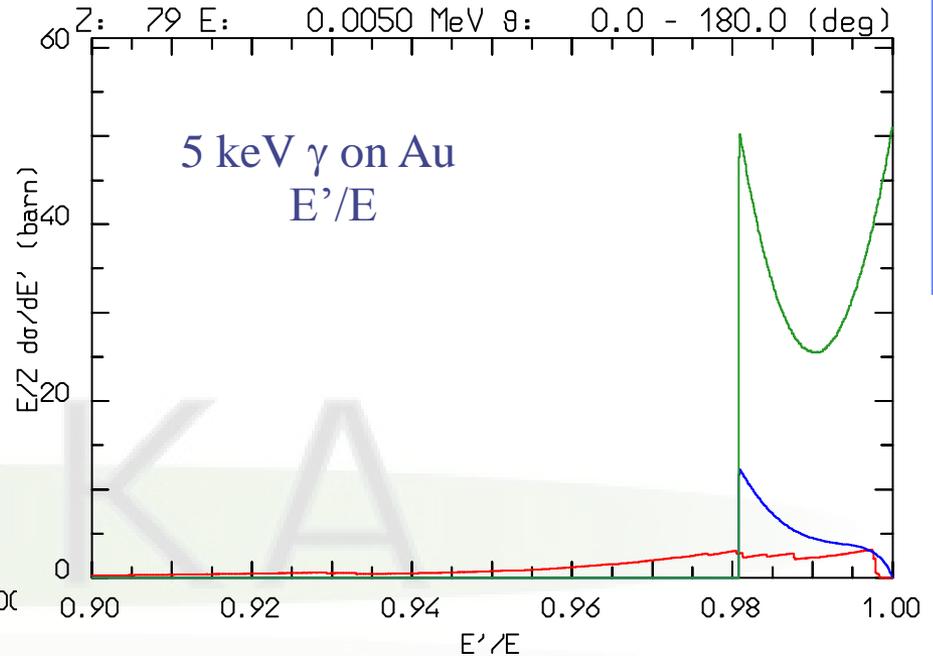
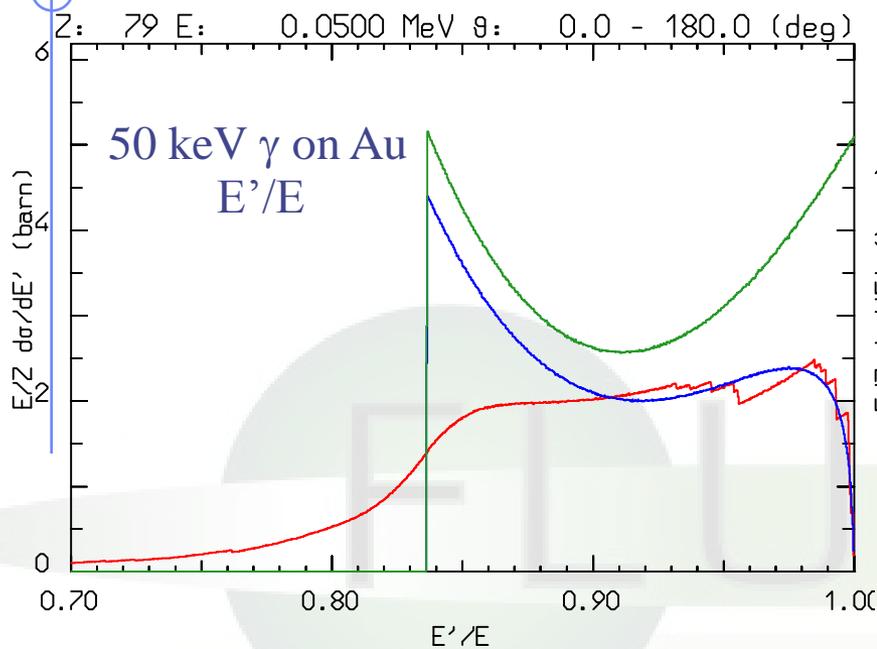
blue = free electron

green = binding with form factors

red = binding with shells and orbital motion

Effects visible only at $\cos\theta$ close to 1. The $S(q, Z)$ approximation is still very good at 50 keV,

Compton profile: examples II



green = free electron

blue = binding with form factors

red = binding with shells and orbital motion

Note the change of colours wrt the previous slide



Larger effect at very low energies, where, however, the dominant process is photoelectric. Please note that the actual cross section goes down again at low energies!!

Visible: shell structure near $E'=E$, smearing from motion at low E'

Bremsstrahlung and pair production by muons/hadrons

At high energies, *bremsstrahlung and pair production* are important also for *muons and charged hadrons*. For instance, in Lead the muon energy loss is dominated by these processes above 300 GeV.

Activation of these processes and thresholds of **EXPLICIT** γ and e^\pm production depend on the **DEFAULT**s chosen. They are controlled by the card **PAIRBREM** by material. Three choices are possible for each process :

- **Inhibited**: not simulated at all, energy loss NOT taken into account (what(1) < 0)
- **Inactive** : energy loss is treated as continuous (i.e., without generating secondaries and depositing their energy at the point of production). This reproduces correctly the average ranges but not the straggling and the dose distributions. (what(1) >0, what(2) or what(3) <0)
- **Active** : the process is fully simulated, with production of secondaries. A threshold for the production can be set, below which energy loss is accounted for in a continuous approximation

HINT : Activate only for high energy problems

Miscellaneous physics settings

Activate photonuclear interactions for all materials

```
PHOTONUC 1. 1. @LASTMAT
```

... maybe with biasing (x 50 in this case)

```
LAM-BIAS 0.02 PHOTON
```

Activate $\mu^+ \mu^-$ pair prod. by photons for all materials (biased x10)

```
PHOTONUC 1. -0.1 1. @LASTMAT MUMUPAIR
```

Activate muon/charged hadrons brems. (above 100 keV) and e^+e^- pair production for all materials (by default for some DEFAULTS)

```
PAIRBREM 3. 0.0 0.0001 1. @LASTMAT
```

Activate muon photonuclear interactions for all materials

```
MUPHOTON 1. 1. @LASTMAT
```

On top of pairbrem, in order to activate *heavy ion* direct e^+e^- pair production for all materials

```
PHYSICS 1. 1. @LASTMAT IONBRPAI
```