Advanced settings

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 thresholds/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: often it will not be suited for your problem, check with care, don't use it blindly..
- The "default" **DEFAULT** proposed by **FLAIR** is **PRECISIO** while for the code is **NEW-DEFA**
- Check all settings: *look in the output*, at least the 1st time you setup a new problem!
- Always *set production and transport thresholds*.

Managing DEFAULTS with FLAIR

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…)

* Single scattering available on option

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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

* Remember : what(3) is related to multiple scattering.
MUST be set, if the field is empty➔0   set= 0 below ≈ 10 keV , = 1 above

Summary: particle transport thresholds

- Hadron and muon transport thresholds are set with the **PART-THR**es 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-THR**es. 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, no sdum, by *region,* *production* threshold again with the **EMFCUT** card, sdum=**PROD-CUT**, by *material*

- 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!

Setting Thresholds with FLAIR

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 **<Z/A>.** 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. At an interface between **1** and **2** this effect can reduce (increase) the stopping power experienced in **2** if **<Z/A>$_1$** is smaller (larger) than **<Z/A>$_2$**
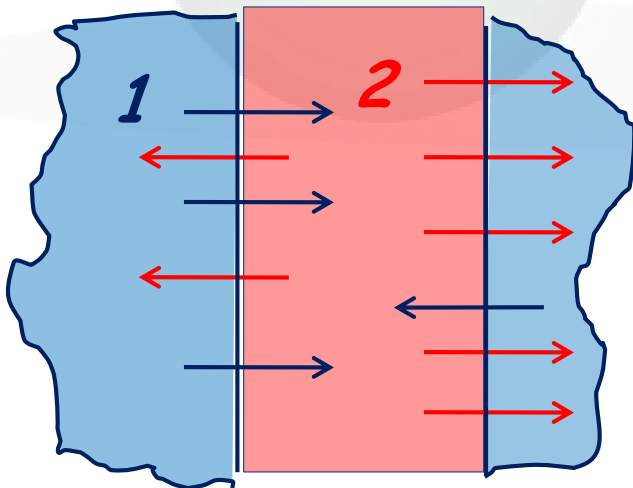
➢ For a correct measurement of stopping power in a given material, surrounding materials should be chosen with care

➢ For a correct evaluation of energy deposition in a given multilayer setup, thresholds must be accurately set in the interested regions and in the surrounding ones

Electronic equilibrium, considerations II:

➢ For a precise measurement of *dE/dx* in medium *2* it is essential that *<Z/A>₁=<Z/A>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 (≡**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 except 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~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 $\rightarrow$ 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!

Example 1: A huge geometry

- CERN LHC tunnel adjacent to ATLAS
- Interested in debris 200m downstream source point
- How to get 'better' statistics
  - Heavy biasing
  - High thresholds in areas not of interest
- BUT: then use of same setup to have a look on the dose profile along the beam-line

IR1 beamline (top view)
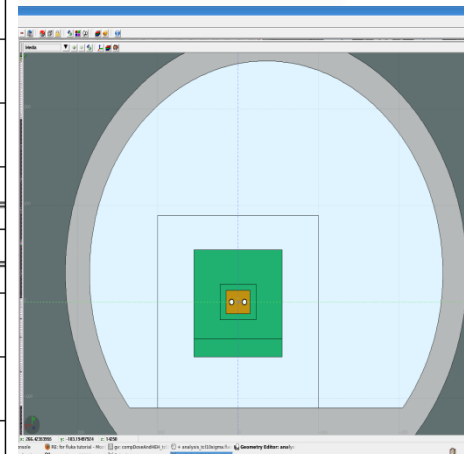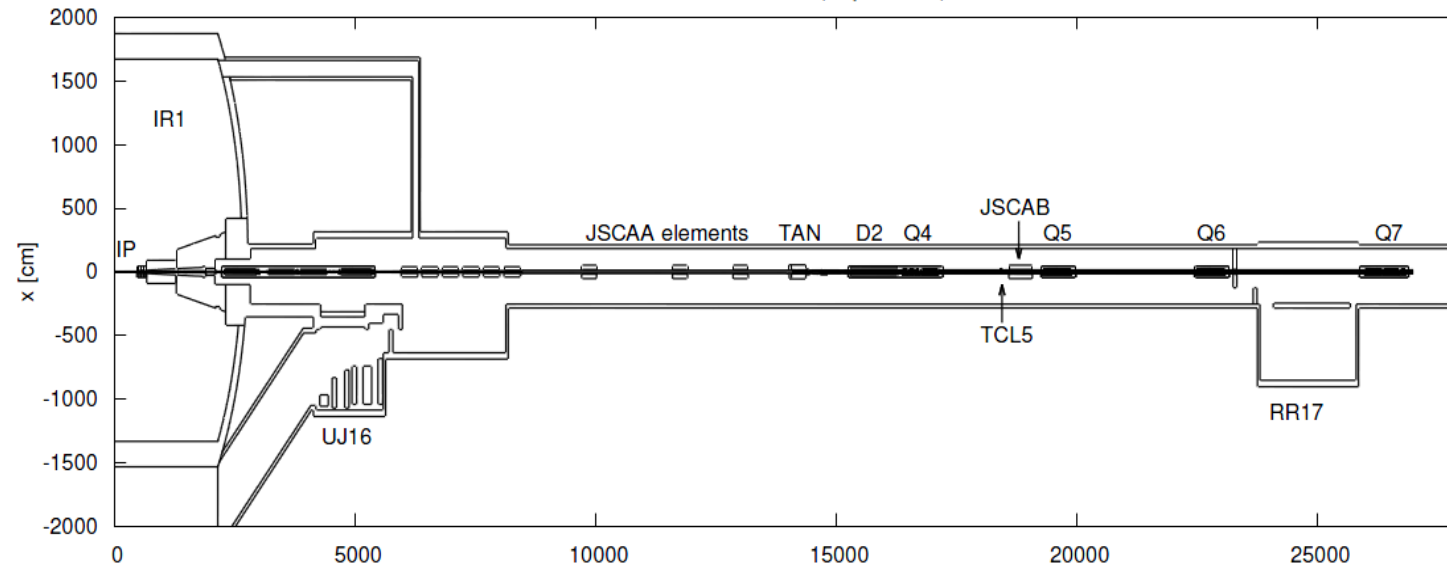
First Results look first 'possible'

option 3 and TCL closed: pp induced dose (normalised to 50 inv. fb at cme = 14 TeV)

2D cut shows peaks where there is no object!

option 3 and TCL closed: pp induced dose (normalised to 50 inv. fb at cme = 14 TeV)
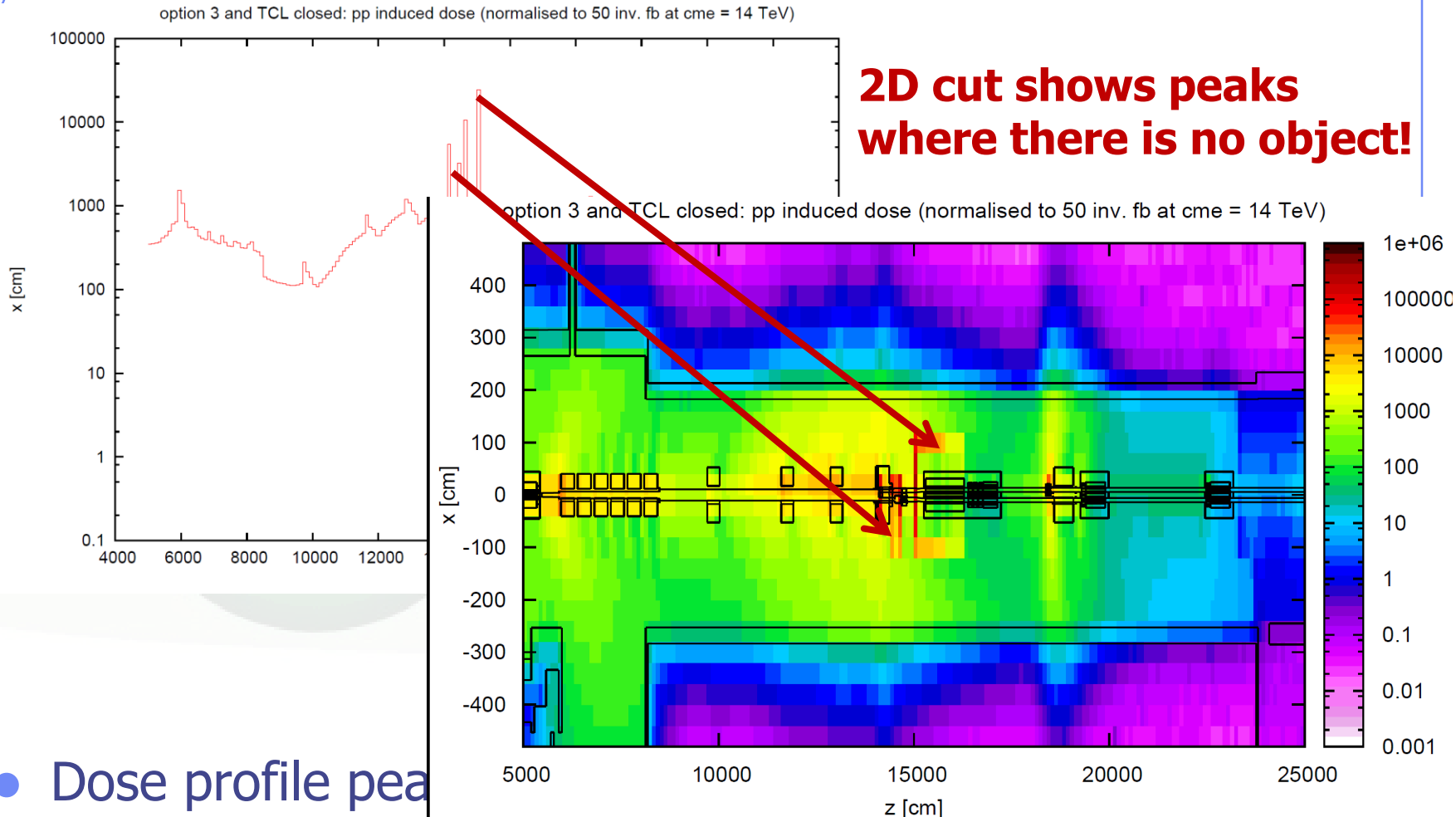
- Dose profile pea
- **BUT**: values are a factor of 10 higher than an 'over the thumb check' (fortunately) -> the reason?

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Reason & Correction

- High thresholds in tunnel air regions:

```
*...+....1....+....2....+....3....+....4....+....5....+....6....+....7..
EMFCUT       -0.050    0.0500       0.0 R208
EMFCUT       -0.050    0.0500       0.0 R204
EMFCUT       -0.050    0.0500       0.0 R206
```

- Lead to unnatural energy deposition on the spot
- Lowering the thresholds solves the issue
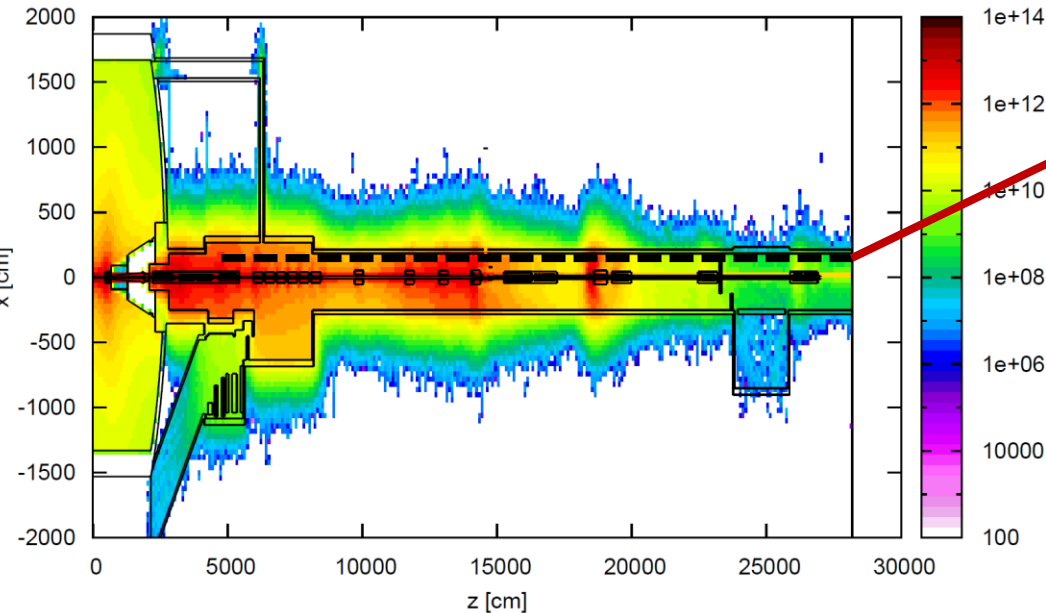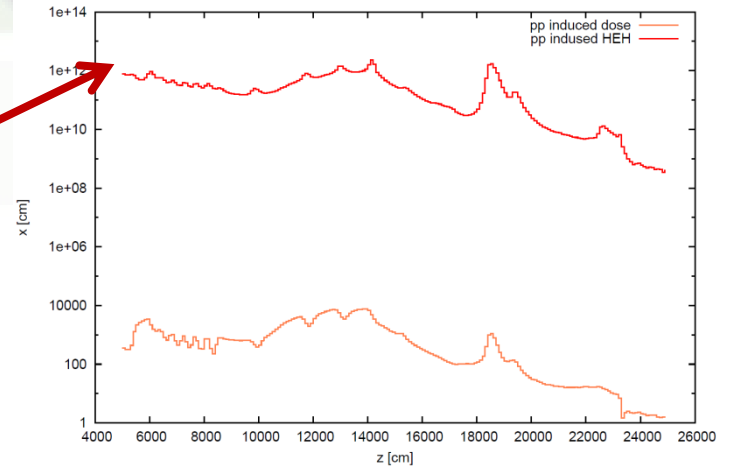
Example 2:

Water- Lead-Aluminum layers
50 microns each

25μ Pb = 2.8 10^{-2} g/cm^2
➔ 100 keV

1μ Pb = 1.1 10^{-3}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

10 MeV electron beam from left
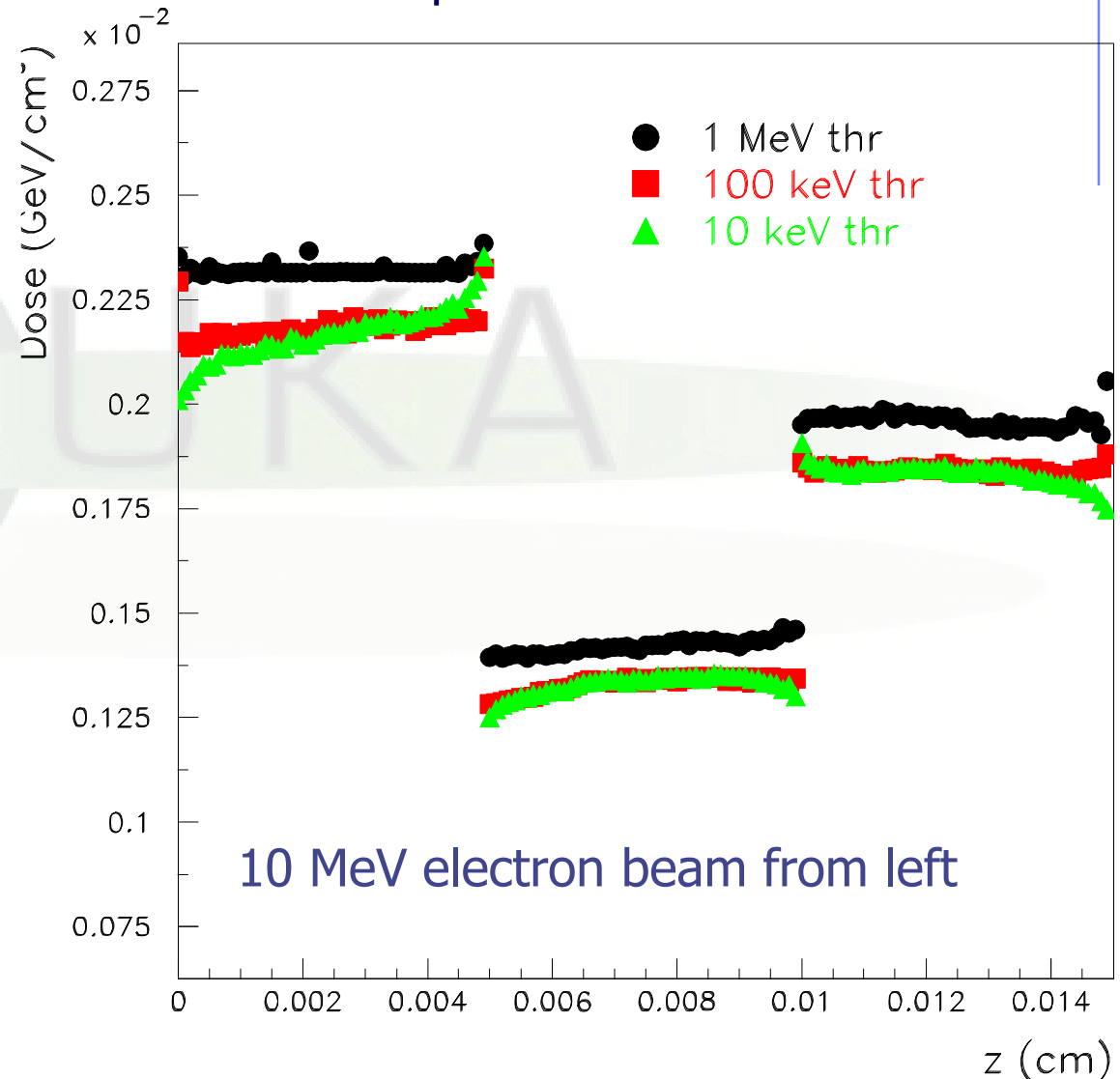
Neutron thresholds

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, $1 \cdot 10^{-5} eV$)

- 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 **DEFAULT**s 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:** phyisical value is $1-\sigma_{abs}/\sigma_{tot}$ default value for thermal groups is 0.95 (**PRECISIO**n and **CALORIME**ter defaults excluded, see next slide)

* A fully analogue event-by-event transport of neutrons below 20 MeV is anyway impossible due to the inclusive nature of the xsec databases

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Differences in the pre-release version for the course the prod. version

- In the pre-release, also **HADRONTHE** does not have non-analogue absorption activated

Neutron setting for full analogue runs -II

- *Pointwise neutron transport* is available for ^{1}H (above 10 eV if bound H requested, down to 10^{-5} eV otherwise) and ^{6}Li

- *Detailed correlated reaction products* are available for ^{1}H , ^{6}Li , ^{10}B (only for the reaction ^{10}B(n,α)^{7}Li), and the ^{14}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}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 (see next slide)

# Differences in the pre-release version for the course the prod. version

- In the pre-release, full pointwise is now available for ^{2}H, ^{3}He and ^{4}He

- same for correlated products

FLUKA

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** utilized for track-length estimators (**USRTRACK**) is the **average one** along the step (E_0-ΔE/2)

- Artifacts can show up if the scoring meshes are inconsistent with the tracking parameters :

USRBIN track apportioning scoring

The energy deposition will be Δl/Δx ΔE

Δl

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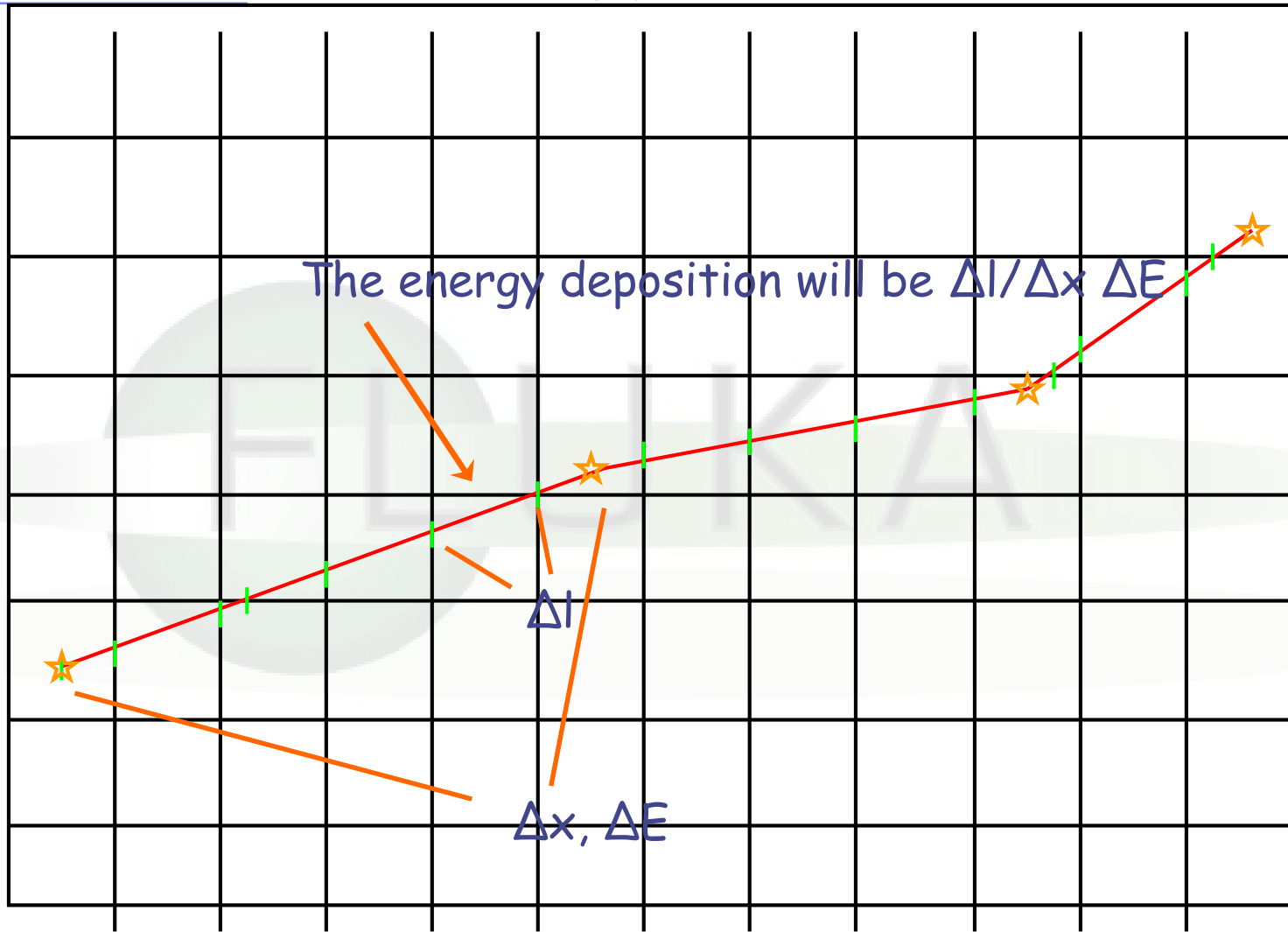
The energy deposited in a single physical step is EQUALLY distributed in the crossed cells (proportionally to dx)

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

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** (Magn. Field lecture)

USRBIN track apportioning scoring

p 48.12 MeV/u
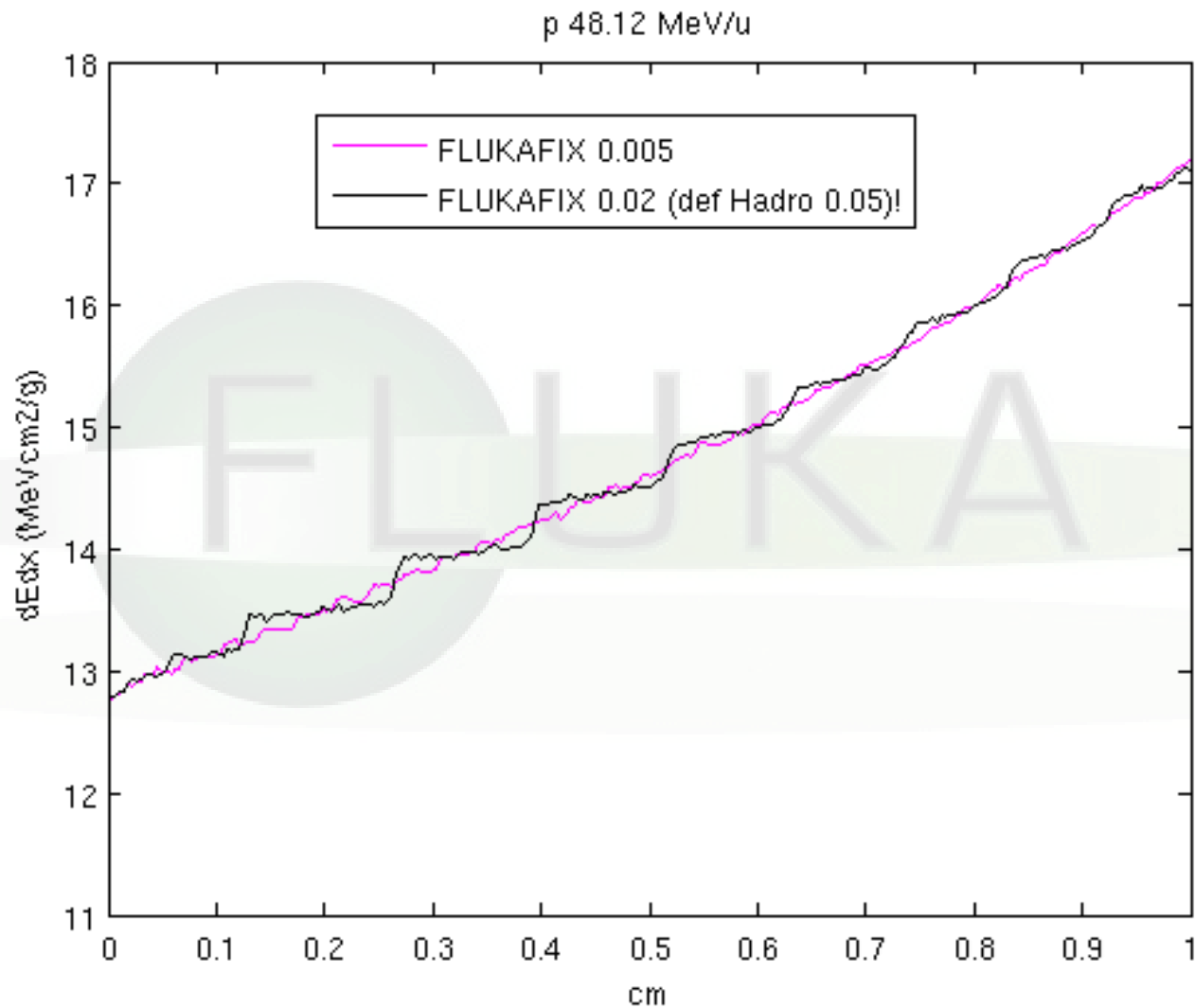
Steps can appear in the scored results

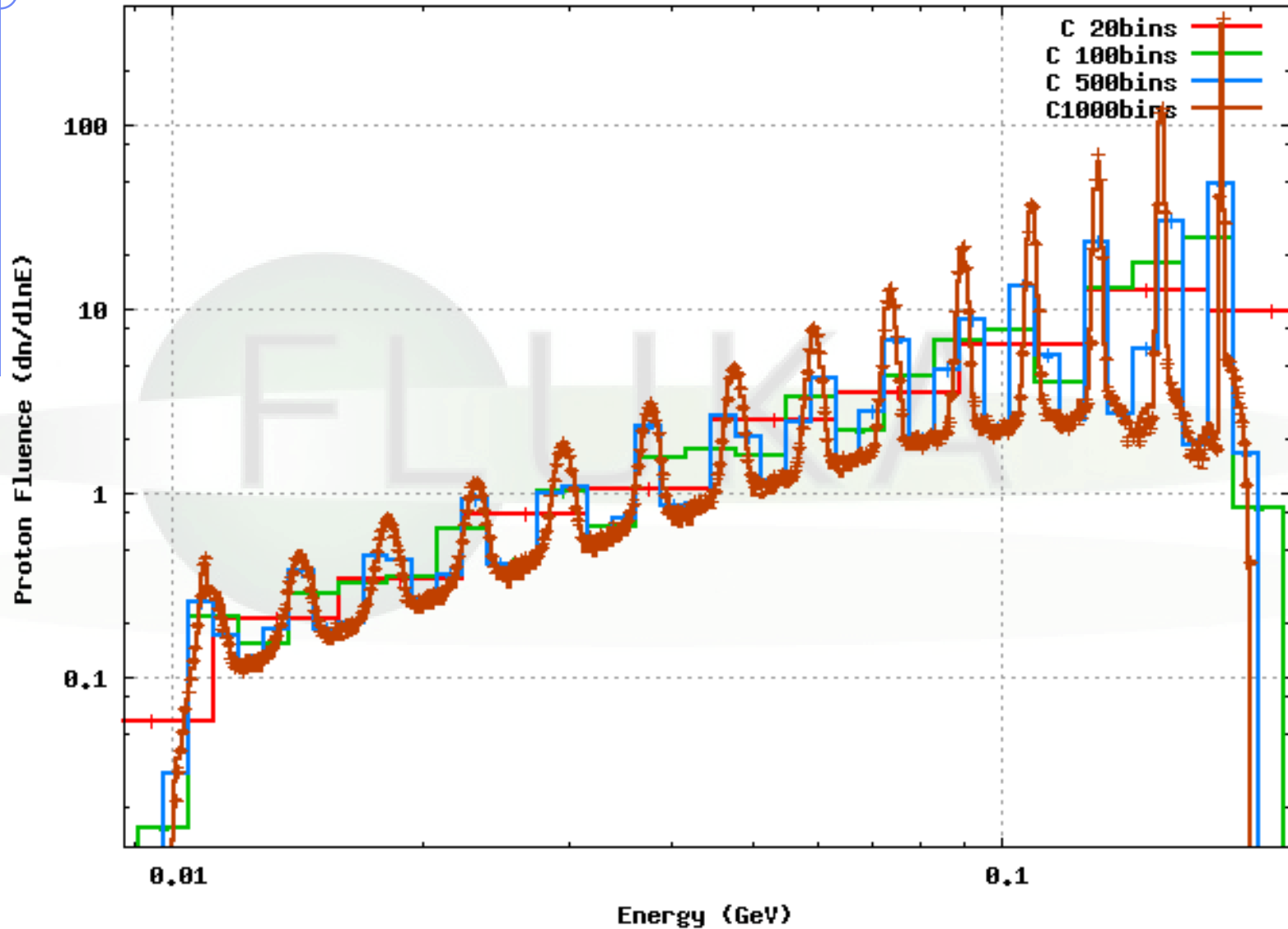Default settings, ≈ 20% energy loss per step

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*

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<3-5GeV/c
Resonance
prod
and decay

Sophisticated
G-Intranuclear Cascade

Gradual onset of
Glauber-Gribov multiple
interactions

hadron

hadron

low E
π,K
Special

High Energy
DPM
hadronizatio
n

Preequilibrium

Coalescence

Evaporation/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 (**IONTRANS***) and link with ldpmqmd when heavy ions are of interested

- For "precision" hadron physics at high energies, residual nuclei, or neutrino beam production: use the extended PEANUT model (**PEATHRESH**)   [**reminder**: in the prod. version the default is to use the old, less refined intranuclear cascade model for projectile momenta $> \approx 5$ 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.
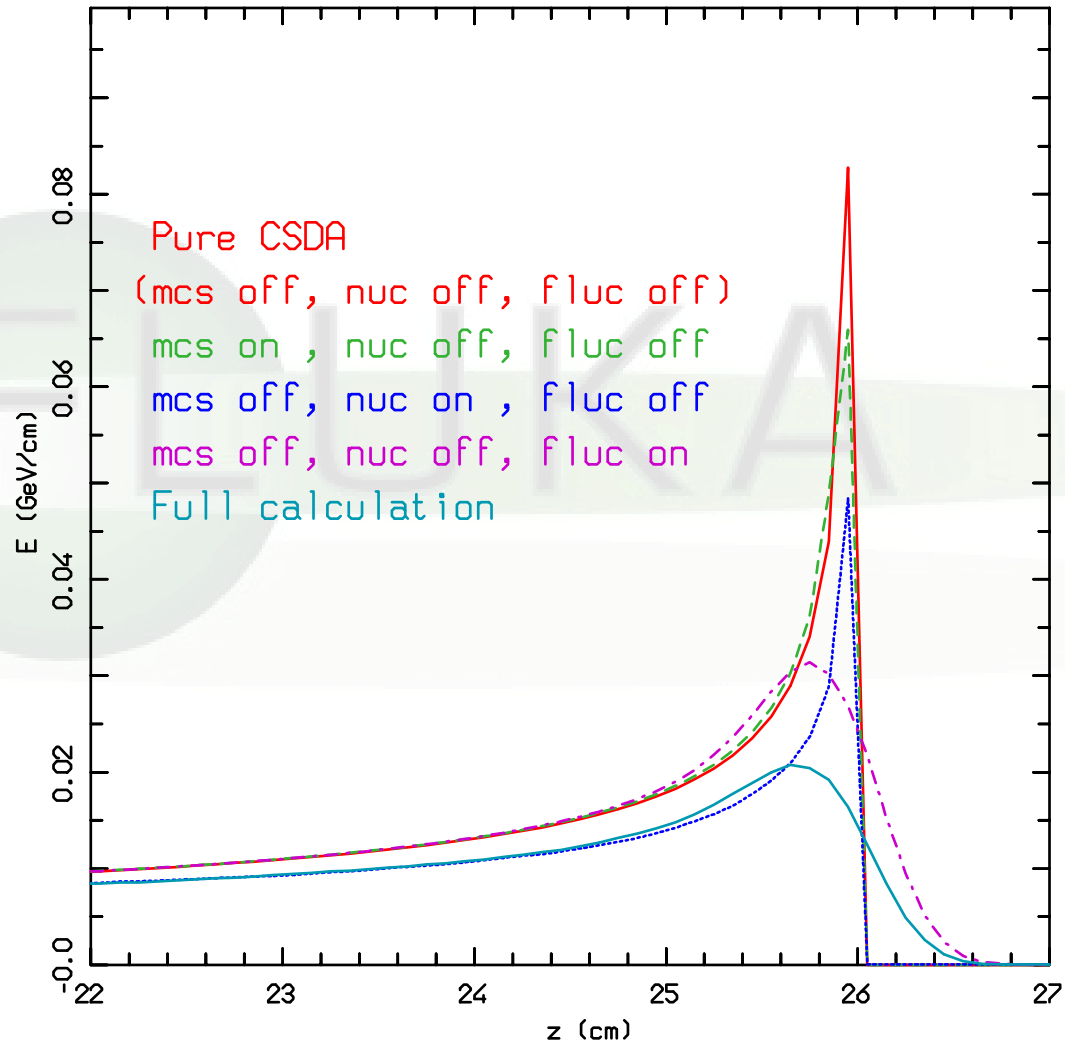
  * No longer EVENTYPE!

Differences in the pre-release version for the course the prod. version

- In the pre-release, **PEANUT** is default at all energies

Bragg peaks: ideal proton case

200 MeV p on water (pencil beam)

Pure CSDA
(mcs off, nuc off, fluc off)
mcs on , nuc off, fluc off
mcs off, nuc on , fluc off
mcs off, nuc off, fluc on
Full calculation

Heavy ion transport and interactions

- The accuracy level of Heavy Ion transport can be set through the **IONTRANS** card:
  - WHAT(3) >= 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,
    - With nuclear interactions up to ~100 MeV/n with BME
    - With nuclear interactions also at higher energies if rQMD and DPMJET are linked
  - 3.0 =< WHAT(3) =< 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 **DEFAULT**s, 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

- Remember to select ion *transport and interactions* if DPA calculations are requested

Heavy ion interactions : warnings

- Interactions of very light ions : d, ^{3}H, ^{3}He in the prod. version are not simulated at low energies (E<100 MeV/A) , where the BME model is used (see next slide)

- The same reactions are performed at higher energies through the RQMD and DPMJET interfaces, in the same way as all other ions. In particular, deuteron stripping is NOT modeled.

→ take with care if specific applications are concerned.

- Work is in progress on this subject

- Remember to build the correct fluka executable if ion interactions above the BME threshold are needed

Differences in the pre-release version for the course the prod. version

- ^{3}H and ^{3}He interactions are now simulated by BME

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

```
IONTRANS -2.0
```

And for energetic heavy ions, activate electromagnetic dissociation

```
PHYSICS  2.                                             EM-DISSO
```
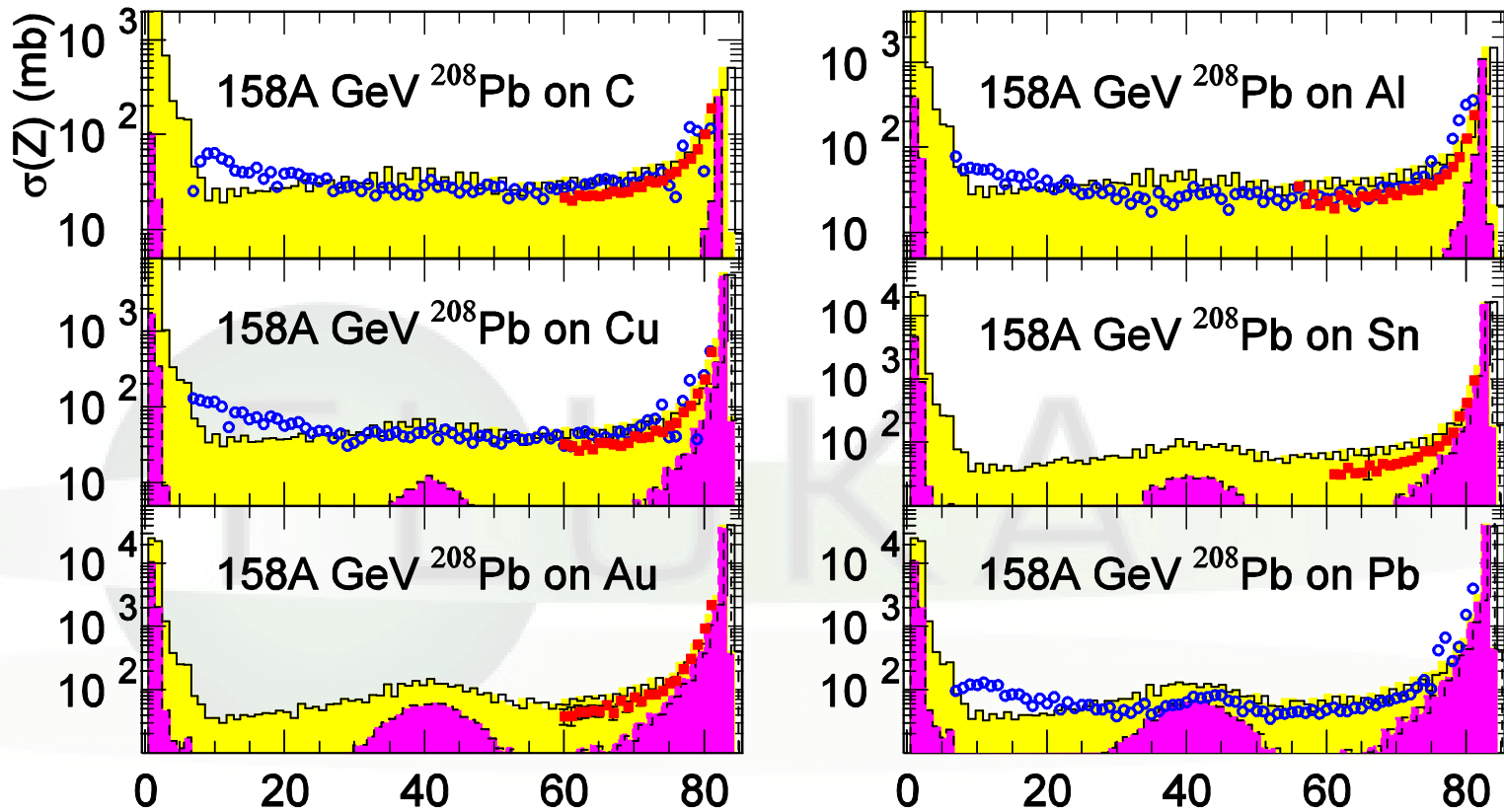
Setting PHYSICS with FLAIR

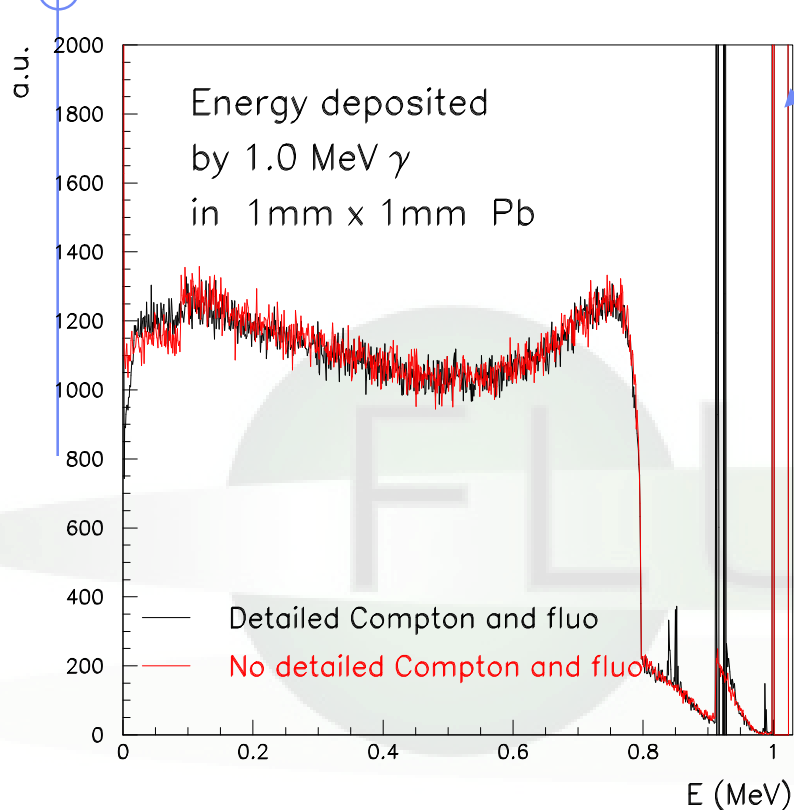# EMD: 158 GeV/n Pb ion fragmentation

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 histos are FLUKA (with DPMJET-III) predictions: purple histos 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) for 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*

Photoelectric effect

Energy deposited
by 1.0 MeV γ
in 1mm x 1mm Pb

Detailed Compton and fluo
No detailed Compton and fluo

a.u.

E (MeV)

Photoelectric
line

Fluorescence after photoelectric is activated only with a subset of **DEFAULT**s
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.

To activate/deactivate fluorescence:
EMFFLUO card, works by material

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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
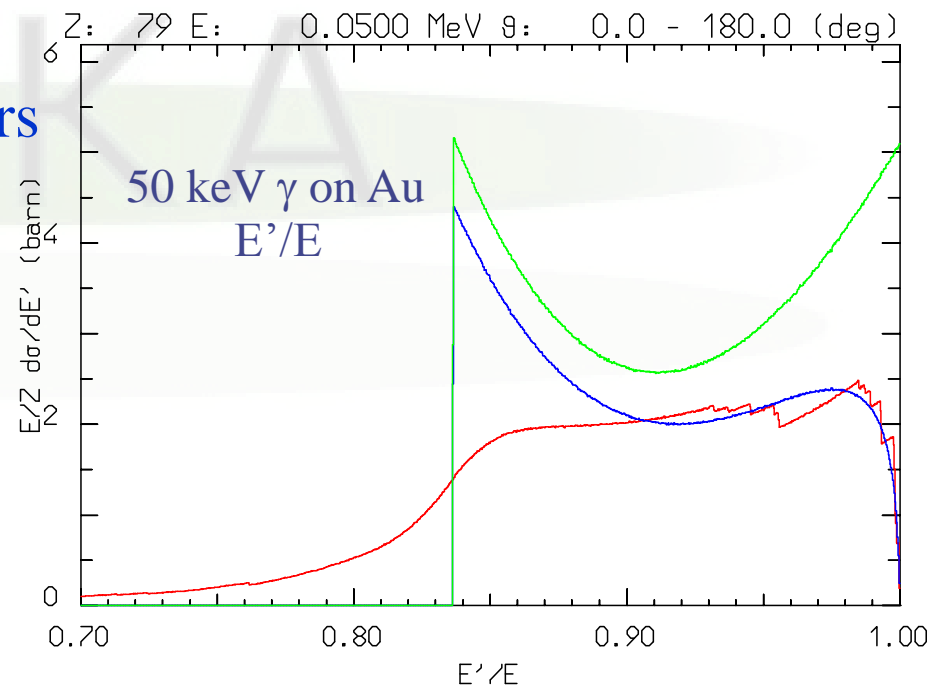blue = binding with form factors
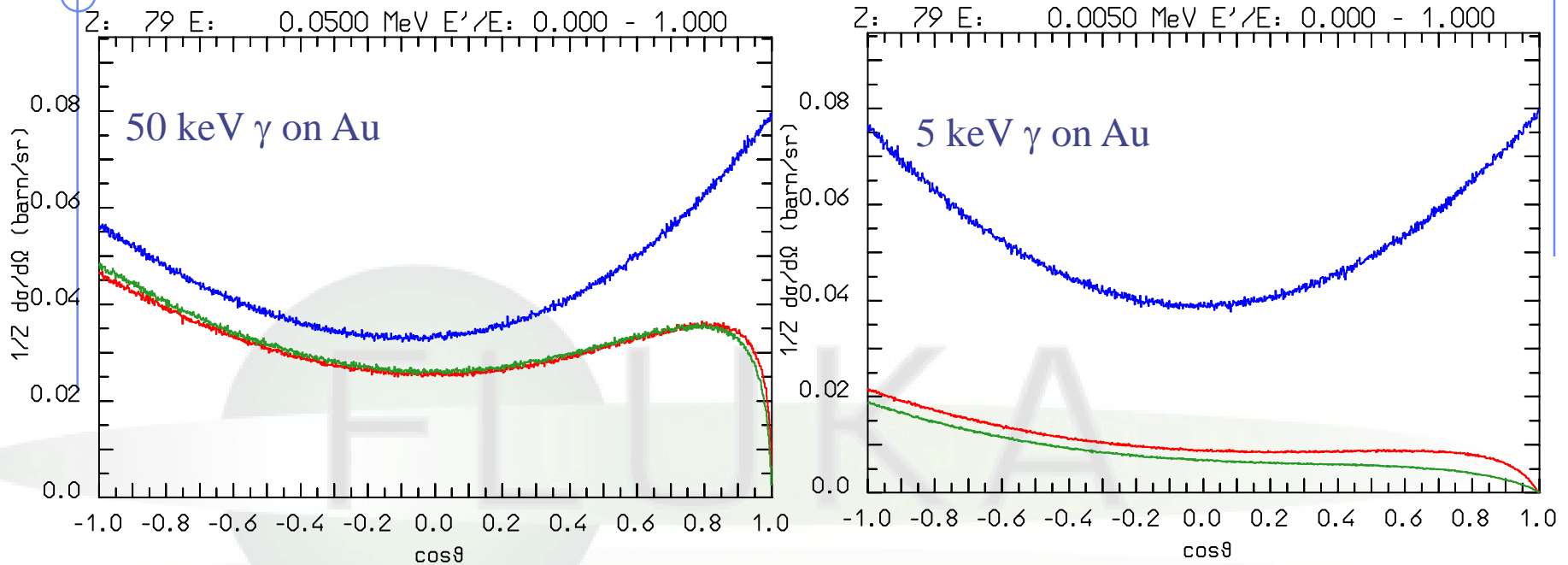red   = binding with shells and
        orbital motion

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….)

Z: 79 E: 0.0500 MeV θ: 0.0 - 180.0 (deg)

50 keV γ on Au
E'/E

E/Z dσ/dE' (barn)

E'/E

Compton ang. distr.: examples II

Z: 79 E: 0.0500 MeV E'/E: 0.000 - 1.000

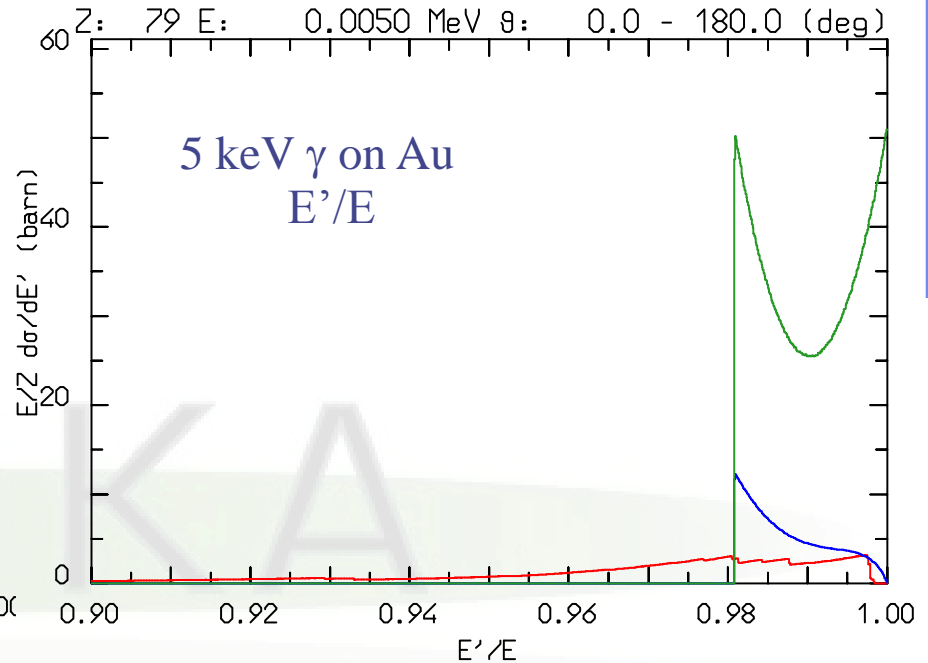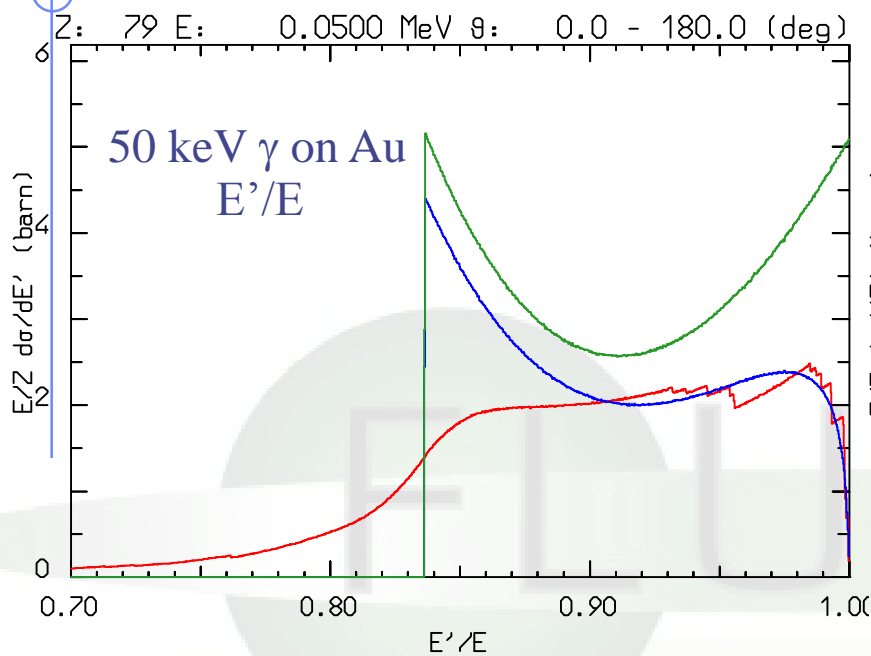Z: 79 E: 0.0050 MeV E'/E: 0.000 - 1.000

50 keV γ on Au

5 keV γ on Au

blue = free electron
green = binding with form factors
red = binding with shells and orbital motion

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

Compton profile: examples II

Z: 79 E: 0.0500 MeV ϑ: 0.0 - 180.0 (deg)

50 keV γ on Au
E'/E

Z: 79 E: 0.0050 MeV ϑ: 0.0 - 180.0 (deg)

5 keV γ on Au
E'/E

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'

Other Photon interactions

- Production of **muon pairs** by photons is off by default. Can be activated through the PHOTONUC card. Biasing of this process is recommended, and is performed with the same PHOTONUC card

- Don't forget that *photon and muon photonuclear interactions are off* by default

- also e^+e^- electronuclear interactions are off by default and **can be activated in the pre-release with PHOTONUC, with SDUM ELECTNUC**

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**

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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 bremss. (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
```