FLUKA

Advanced settings

Advanced transport settings: **FLUKAFIX, EMFFIX, STEPSIZE**

Single scattering: **MULSOPT**

Interaction mechanisms upon user request: **PHYSICS, PHOTONUC**

Outline

- Basics of **condensed history** simulation scheme adopted in FLUKA

- **Simulation parameters** to fine-tune step sizes in pathological situations

- `DEFAULTS` card presets simulation parameter values (not necessarily adequate for all applications). Careless choices may lead to:
  - Wrong results, e.g. premature energy deposition
  - Simulation artefacts, e.g. steps and spikes
  - Low simulation efficiency: relevant interaction mechanisms not sufficiently probed, overbiasing of irrelevant histories, etc.

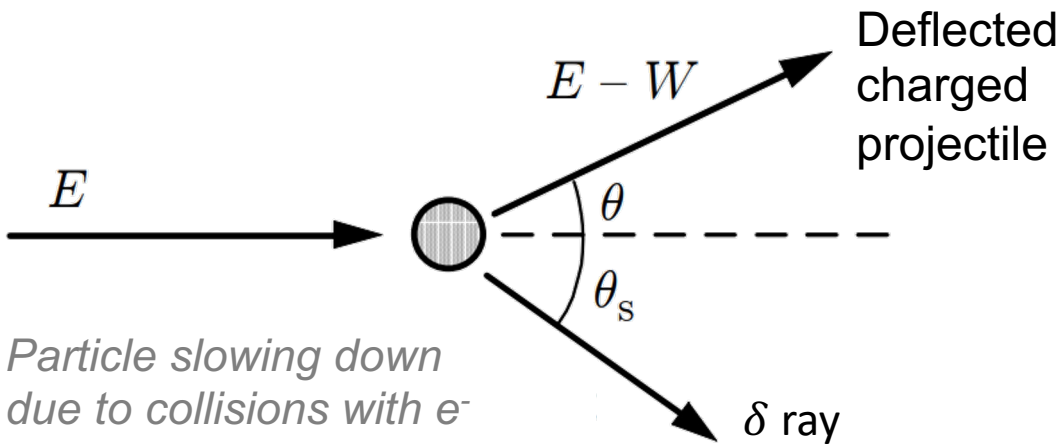
- In this lecture we examine what happens when one does not sufficiently control:
  - Stepsize-related simulation parameters
  - Single scattering in micrometric volumes
  - Lack of physically relevant processes

Condensed-history simulation

Condensed-history MC simulation

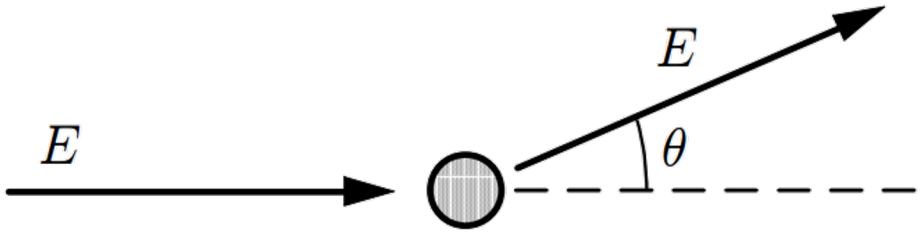
- Basic electromagnetic interaction mechanisms of charged particles in matter:

Ionization



Particle slowing down due to collisions with e^-

Elastic scattering



Particle deflection on electrostatic potential of atom, the latter being left in the ground state

- Mean free paths can be $\ll 1\ \mu$m → **thousands of events** in bulk media
- One cannot afford to sample such interactions individually: general-purpose MC codes perform **macroscopic steps** with longer mean free paths
- FLUKA accounts for the aggregate effect of multiple ionization and elastic scattering events along condensed steps via:

dE/dx model with fluctuations
(explicit δ ray generation above threshold)

Multiple scattering theory of Moliere
(single scattering upon request)

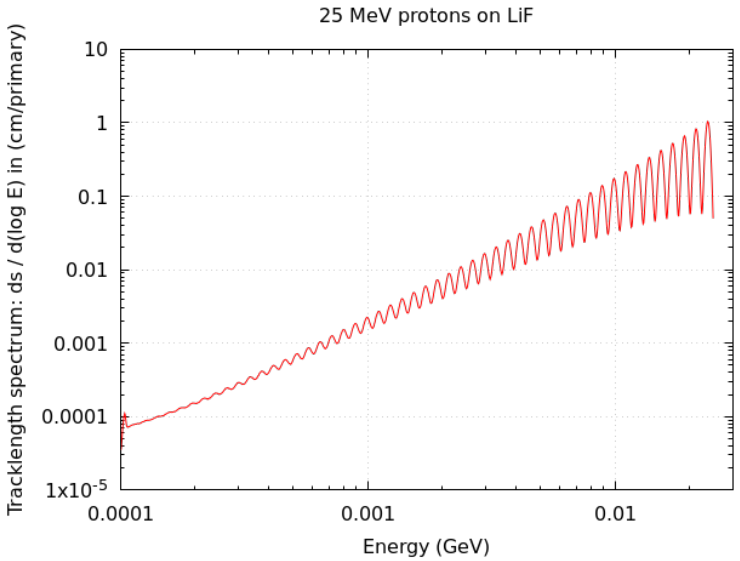
Simulation parameters

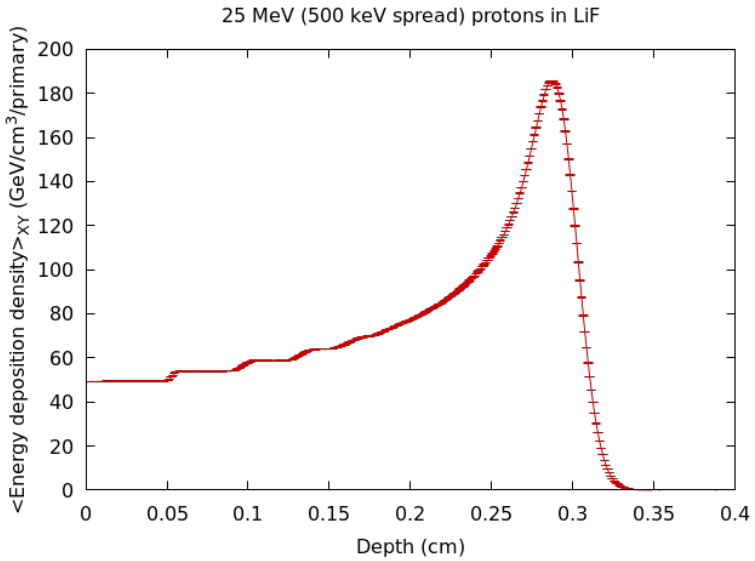
- Macroscopic particle **steps are limited** among other by:
  - Discrete interaction mechanisms: *δ ray production, nuclear interactions, particle decay, absorption, Coulomb single scattering, etc.*
    *(NB: some are **off** - they need to be explicitly requested. See ulterior slides)*
  - Maximum continuous energy loss allowed per particle step
  - Minimum/maximum step size explicitly requested in the simulation
  - Magnetic/electric field tracking accuracy
  - Boundary crossings

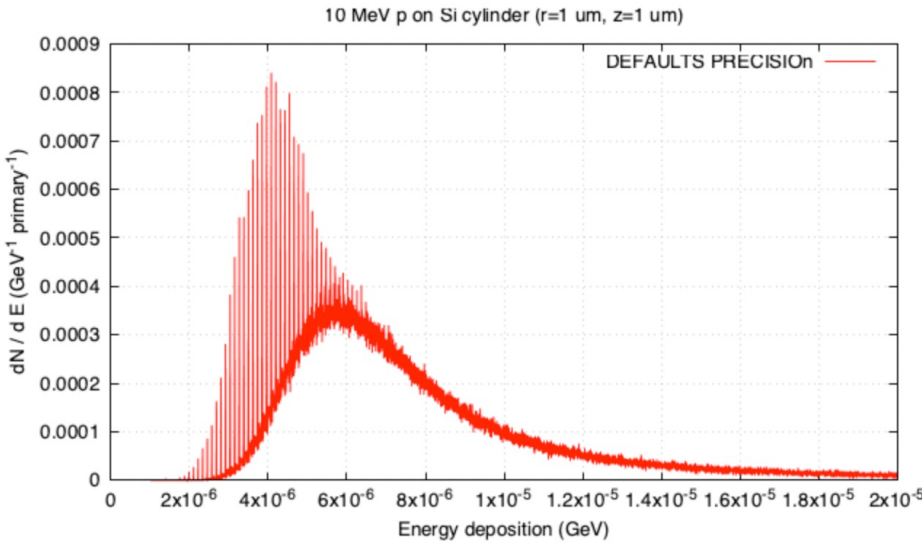
- FLUKA gives access to a series of simulation parameters to the user in order to cope with challenging scenarios, e.g.:
  - Thin layers, dilute gases
  - High spatial/energy resolution in scoring

Simulation artefacts

- Although **default values are provided** for all simulation parameters via the DEFAULTS card, it is ultimately the **user's responsibility to fine-tune** them according to the needs of the specific problem at hand.
- **Simulation artefacts** may appear if one is not careful:







Stepping artefacts

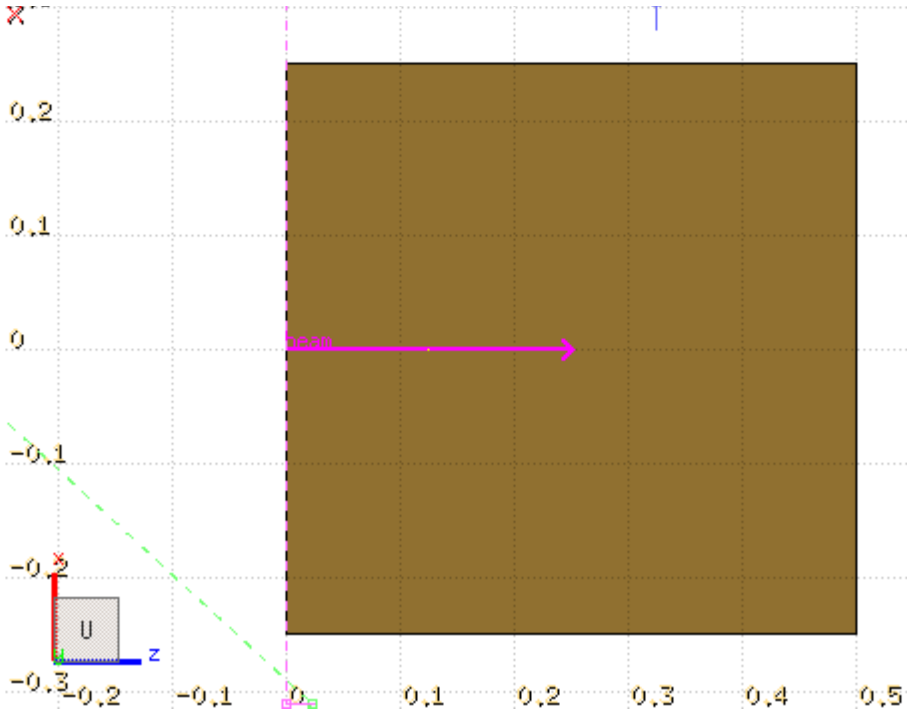
`FLUKAFIX, EMFFIX, STEPSIZE`
`(MGNFIELD, ELCFIELD)`

Example: 25 MeV p on 0.5 cm of LiF

- A fairly straightforward input (just relevant sections displayed here):

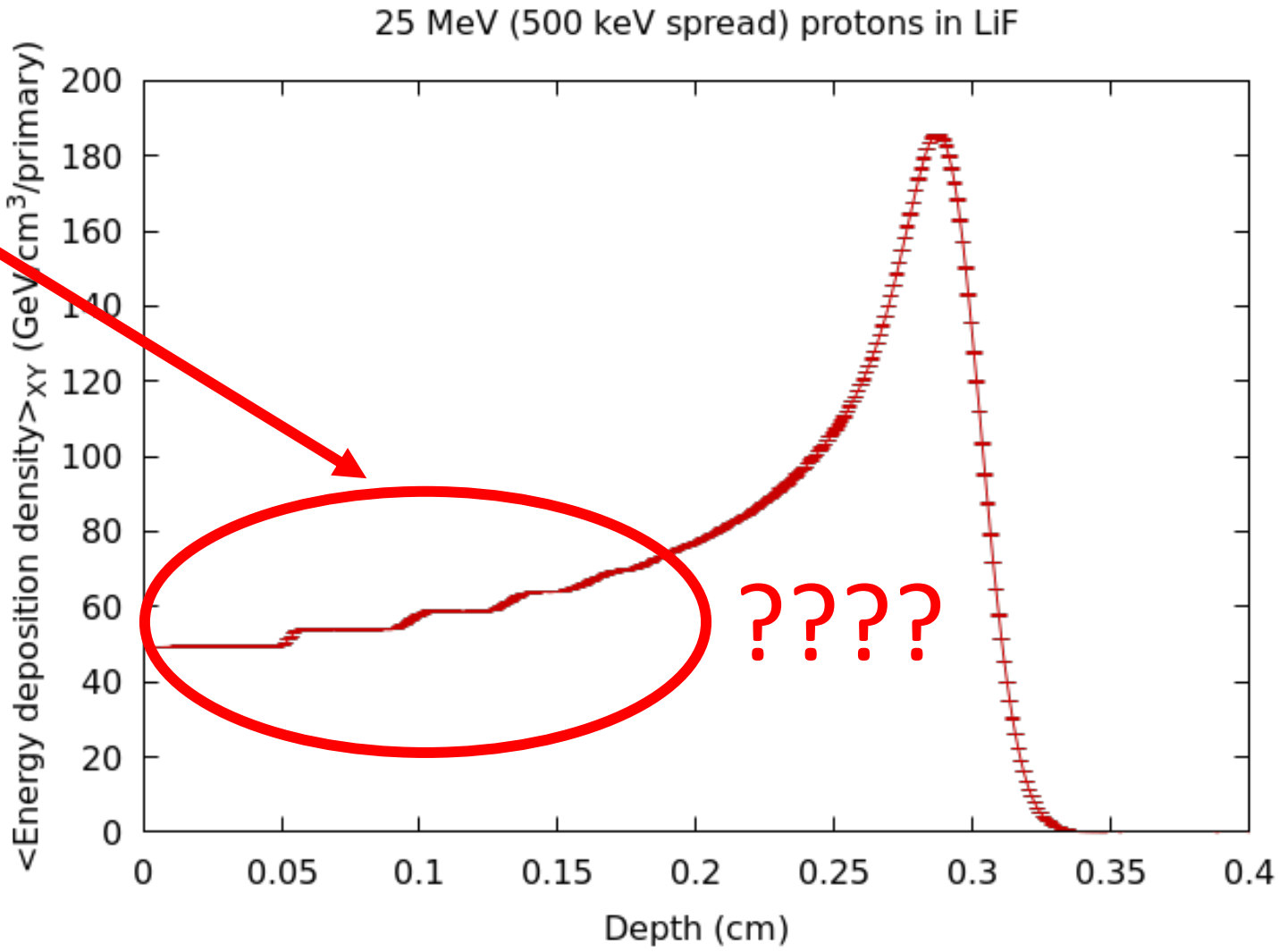
```
Set the defaults for precision simulations
DEFAULTS                                    : PRECISIO ▾
Define the beam characteristics
BEAM                     Beam: Energy ▾             E: 0.025              Part: PROTON ▾
           Δp: Gauss ▾   Δp(FWHM): 0.00520215       Δϕ: Flat ▾            Δϕ: 0.0
   Shape(X): Rectangular ▾       Δx: 0.1     Shape(Y): Rectangular ▾      Δy: 0.1
MATERIAL   LITHIUM                                  #:                    ρ: 0.534
            Z: 3                 Am:                A:                dE/dx: ▾
MATERIAL   FLUORINE                                 #:                    ρ: 0.001696
            Z: 9                 Am:                A:                dE/dx: ▾

MATERIAL   LiF                                      #:                    ρ: 2.635
            Z:                   Am:                A:                dE/dx: ▾
COMPOUND   LiF ▾                                  Mix: Atom ▾      Elements: 1..3 ▾
           f1: 1.0               M1: LITHIUM ▾     f2: 1.0               M2: FLUORINE ▾
           f3:                   M3: ▾
..+....1....+....2....+....3....+....4....+....5....+....6....+....7..
ASSIGNMAT                       Mat: BLCKHOLE ▾    Reg: BLKBODY ▾     to Reg: ▾
                        Mat(Decay): ▾             Step:                Field: ▾
ASSIGNMAT                       Mat: VACUUM ▾      Reg: VOID ▾        to Reg: ▾
                        Mat(Decay): ▾             Step:                Field: ▾
ASSIGNMAT                       Mat: LiF ▾         Reg: TARGET ▾      to Reg: ▾
                        Mat(Decay): ▾             Step:                Field: ▾
USRBIN                                            Unit: 22 BIN ▾        Name: E1000
        Type: X-Y-Z ▾          Xmin: -0.25        Xmax: 0.25              NX: 10
        Part: ENERGY ▾         Ymin: -0.25        Ymax: 0.25              NY: 1
                               Zmin: 0.0          Zmax: 0.5               NZ: 1000
```



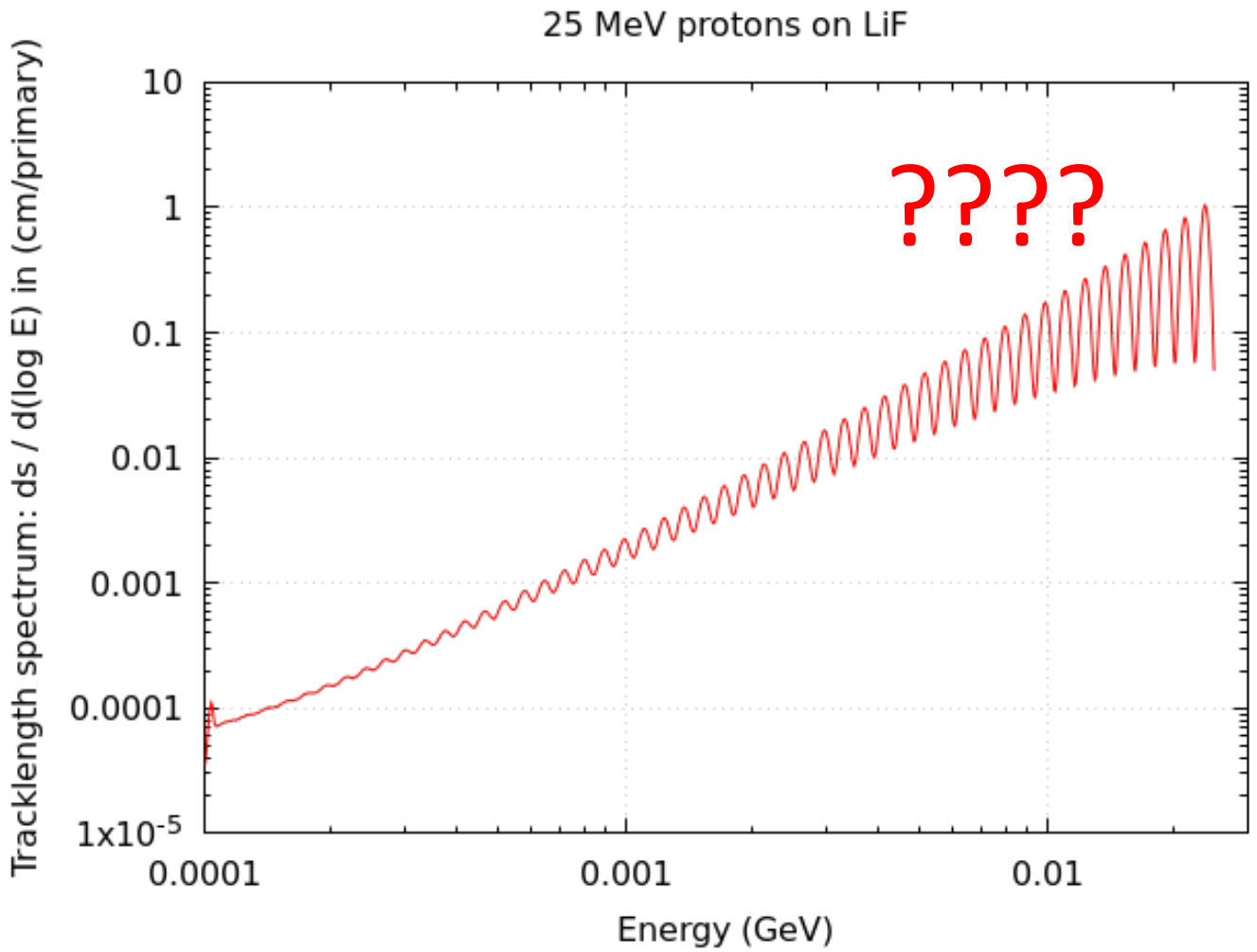
Energy deposition by 25 MeV p on 5 mm of LiF

- **Unexpected steps** witnessed at the beginning of the energy-deposition depth profile
- One may rightfully suspect a particle stepping artefact.
- It is then natural to examine the fluence spectrum (next slide)



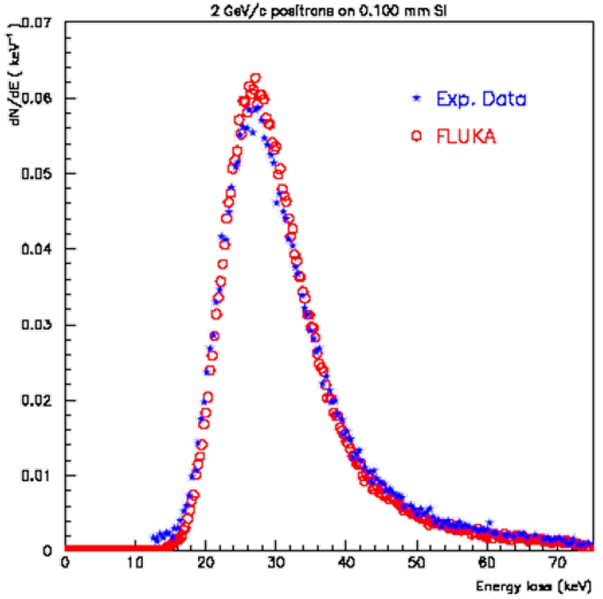
Track-length spectrum of 25 MeV p on 5 mm of LiF

- The artefact is even more spectacular in the fluence spectrum:



Reminder – FLUKA's ionization model

- **Ionization**: collision of a charged projectile with a bound target electron which is promoted to the continuum and transported if above threshold, labelled as a δ ray.
- The charged projectile transfers an energy T to the target electron during the collision
- Collisions with energy transfer $T > T_\delta$:
  - A δ ray is explicitly sampled and tracked
  - FLUKA provides δ-ray production cross sections by $e^{\pm}$, spin-0, spin-1/2 charged projectiles
- Collisions with energy transfer $T < T_\delta$:
  - **Average energy loss along particle step is sampled from the stopping power (dE/dx), restricted to losses smaller than T_δ**
  - Ionization fluctuations are applied on top, so as to reproduce not just the correct average but the first few momenta of the energy-loss distribution
- Example: energy-loss distribution of 2 GeV/c positrons on 0.1 mm Si



Preliminaries to explain the issue

- The **FLUKAFIX** card prescribes, *on a **per-material** basis*, what's the maximum fraction of kinetic energy that can be lost to dE/dx along a particle step:

FLUKAFIX Ekin frac: 0.02 Mat: LiF ▾ to Mat: LiF ▾ Step: 1

- The maximum length of charged-particle steps is limited accordingly
- NB: when you pass a **DEFAULTS** card, you are implicitly selecting the maximum fractional energy loss. From the FLUKA manual:

If option DEFAULTS is used with **SDUM** = `HADROTHErapy`, the default is 0.02.

With **SDUM** = `DAMAGE`, the default is 0.04.

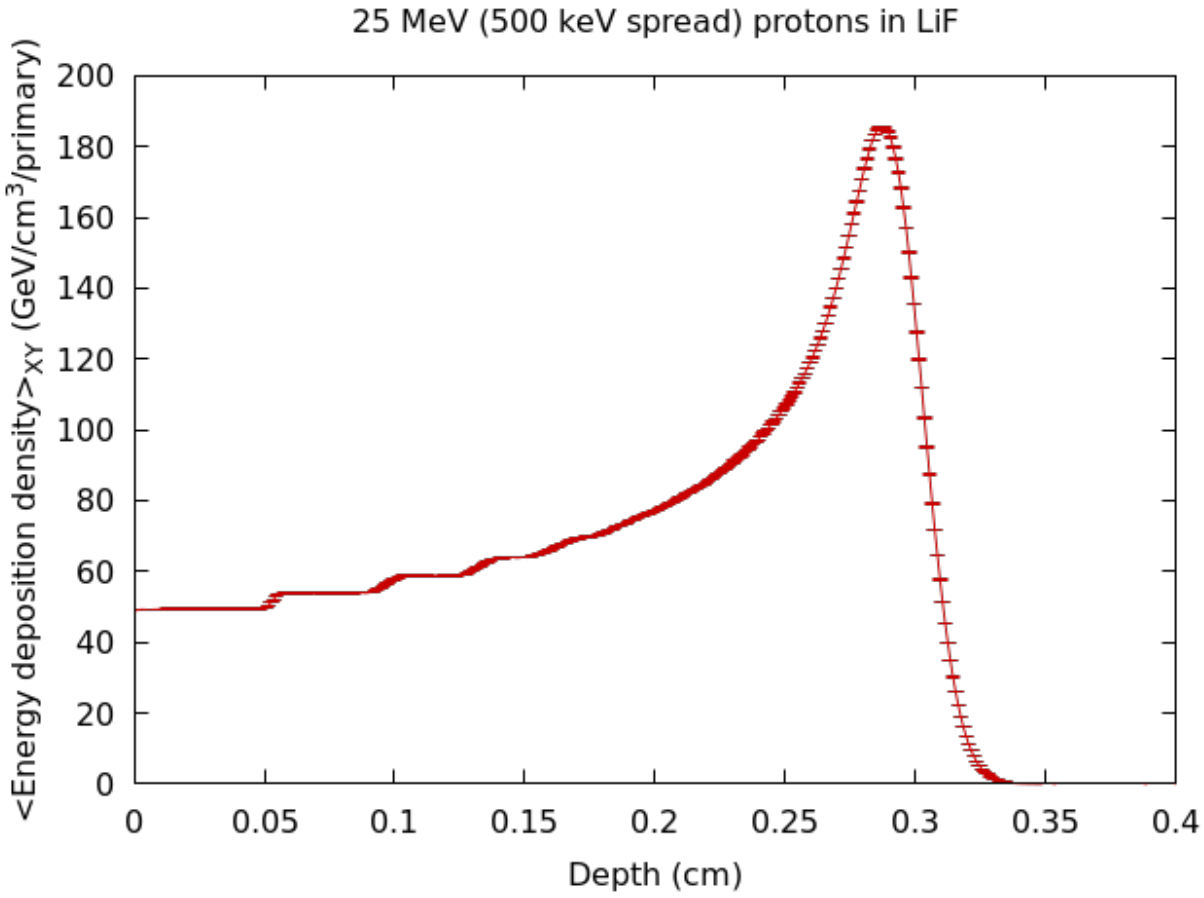
With **SDUM** = `ICARUS` or `PRECISIOn`, the default is 0.05.

If **SDUM** = `CALORIMEtry`, the default is 0.08.

With any other **SDUM** value, or if DEFAULTS is missing, the default is 0.1.

The issue

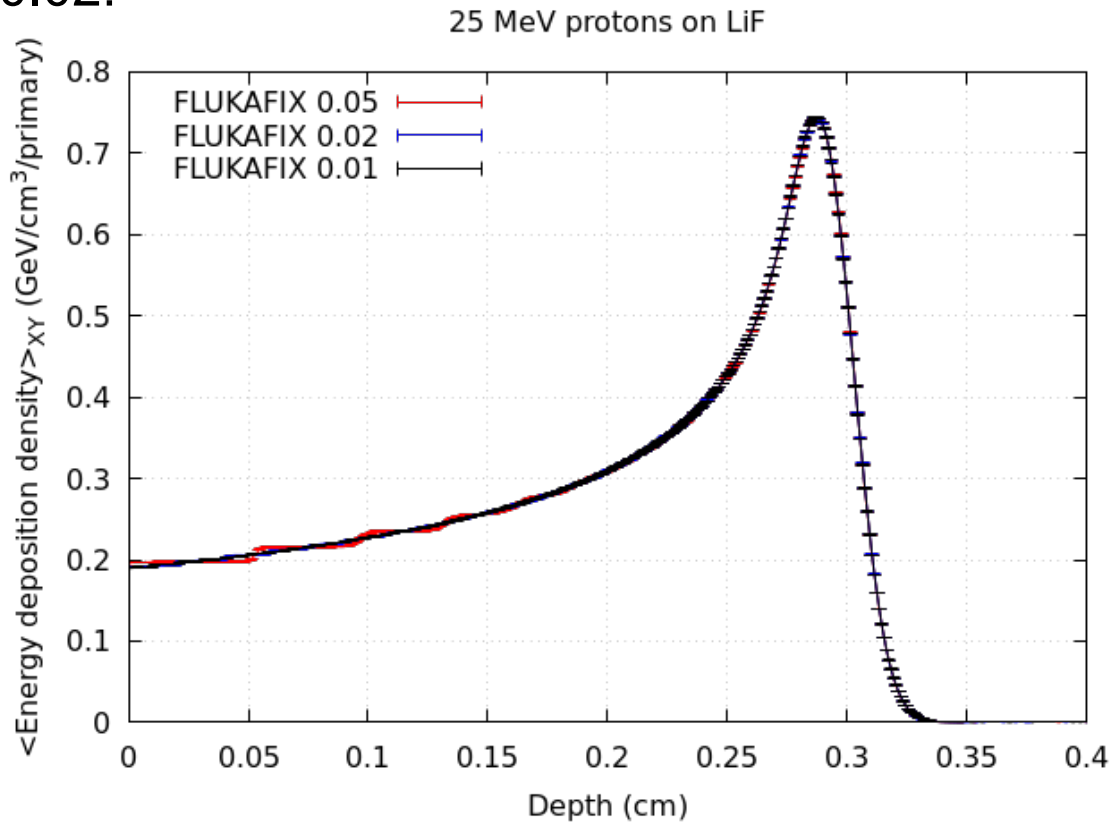
- **FLUKAFIX**=0.05 for 25 MeV p implies a maximum of 1.25 MeV lost in a single step
- The dE/dx for 25 MeV protons in LiF is ~46 MeV/cm
- Protons losing 1.25 MeV travel of the order of 0.03 cm in LiF
- But the resolution of the energy deposition spectrum is 0.001 cm

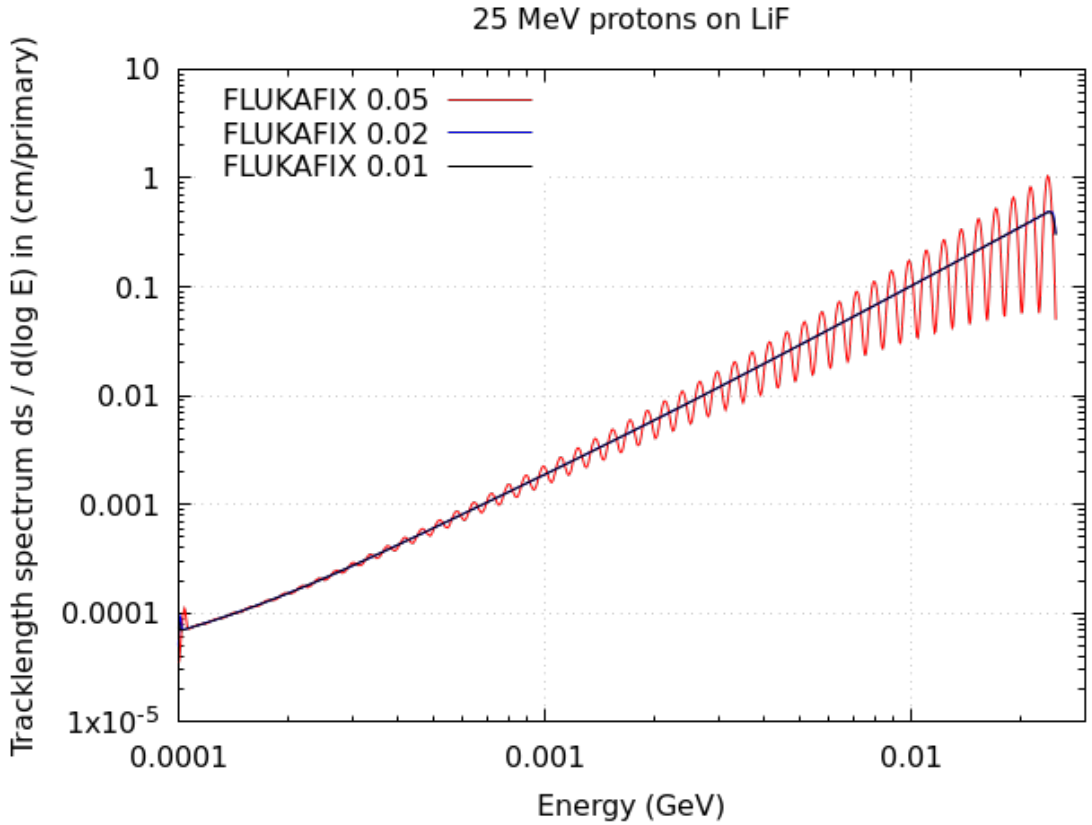


- **We intend to resolve spatial details much smaller than a typical particle step size!!!**
- Not a problem per se (deposited energy is apportioned) unless steps are much longer than scoring resolution.

A solution: reduce FLUKAFIX

- Artefact vanishes if one requests maximum energy loss to be a smaller fraction, e.g. 0.01 or even 0.02:





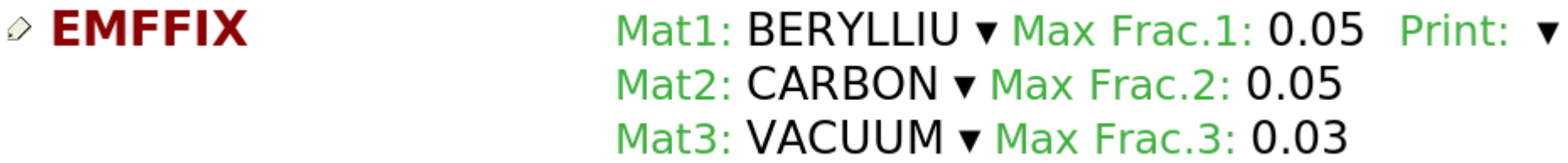
- …at the expense of CPU time:

FLUKAFIX	0.05	0.02	0.01
Average CPU time / p (s)	6.1E-4	1.1E-3	**2.2E-3**

Electromagnetic interlude

- **FLUKAFIX** applies to hadrons, muons, and ions.

- For electrons and positrons, there's the equivalent **EMFFIX** card, also on a per-material basis:



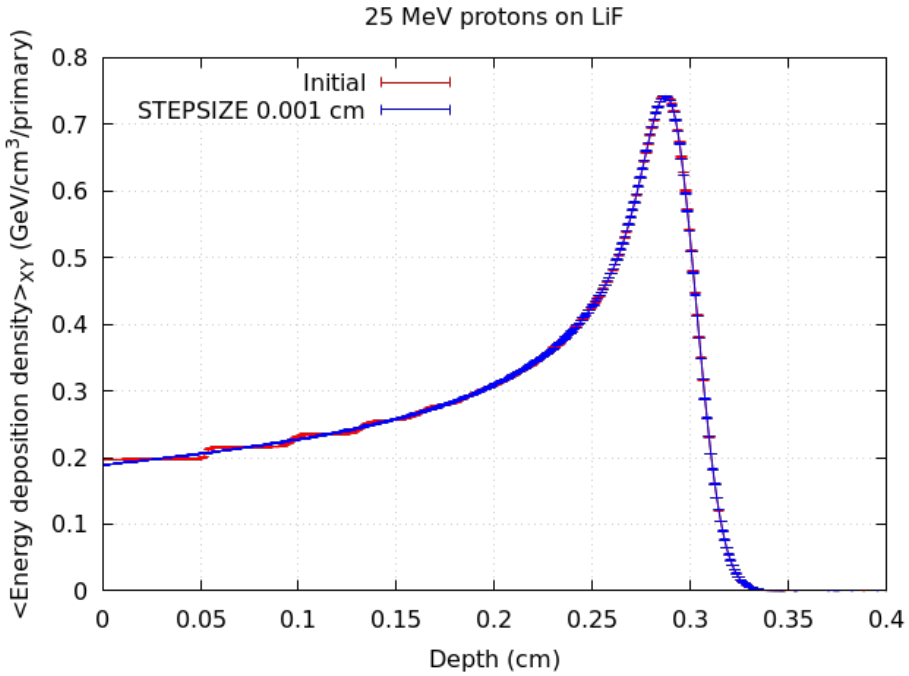
- You can request a printout of electron and positron **restricted** dE/dx in the FLUKA output file via the **PRINT** SDUM

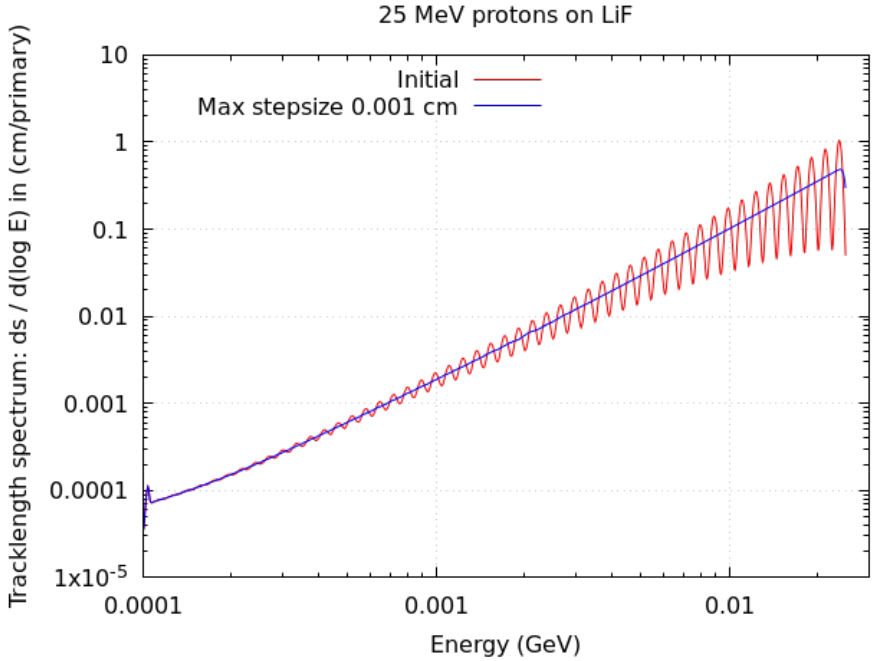
Alternative: STEPSIZE

- The `STEPSIZE` card allows one to
  - Set both maximum and minimum step lengths
  - Set min/max step lengths in an **absolute** manner (not implicitly in terms of dE/dx)
  - One setting directly affects not only hadrons, muons, and ions, but also electrons and positrons
  - Have granularity on a **per-region** (instead of a per-material) basis

Another solution: STEPSIZE

- Back to our 25-MeV p problem on LiF. Passing a **STEPSIZE** to request a maximum step size of, say, 0.001 cm resolves the issue as well



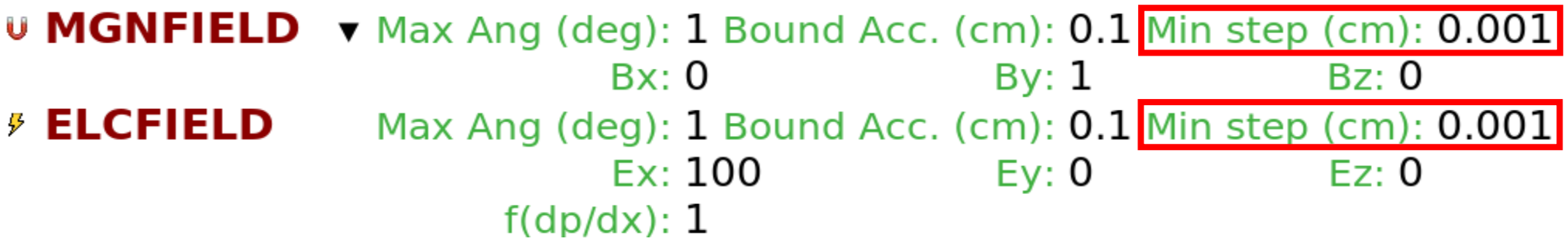


- Naturally, the improvement with shorter steps comes at the expense of longer average CPU times per primary:

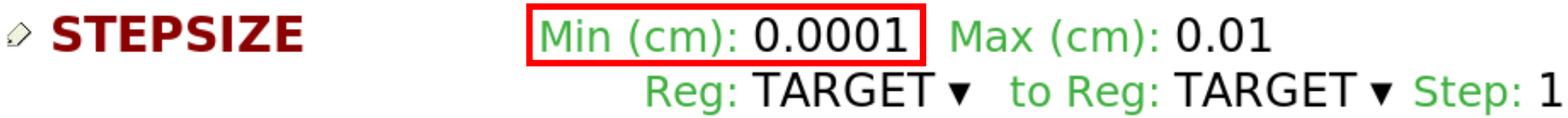
	Initial	Max step size 0.001 cm
Average CPU time / p (s)	6.1E-4	**2.3E-3**

STEPSIZE and B/E-field tracking (1/2)

- In the **MGNFIELD** and **ELCFIELD** FLUKA cards, the user can select a minimum step size (intended to avoid endless tracking if other settings would lead to ridiculously small step sizes):



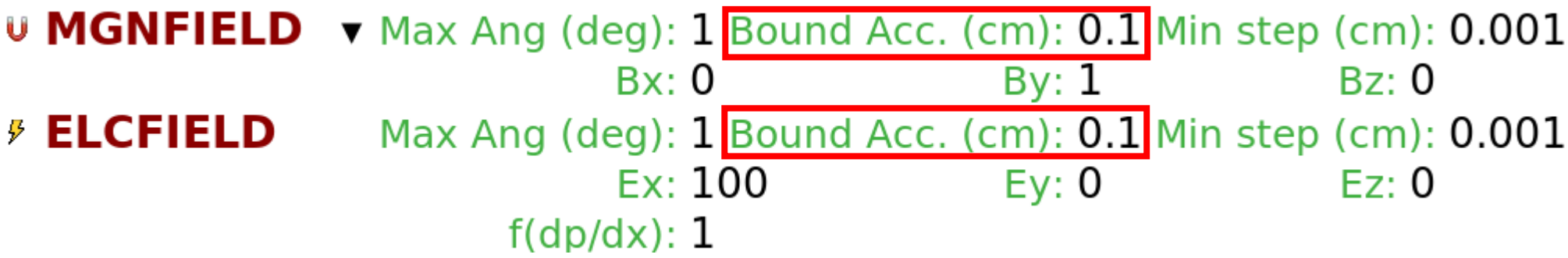
- Assigned **globally**, i.e. for all magnetic/electric fields in your simulation.
- The minimum step setting in **STEPSIZE** provides **region specificity**:



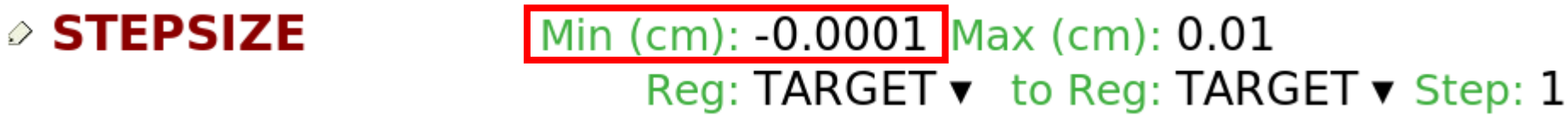
- It overrides **MGNFIELD/ELCFIELD** settings **only if larger!**

STEPSIZE and B/E-field tracking (2/2)

- The **MGNFIELD** and **ELCFIELD** cards have a parameter prescribing the accuracy with which boundary crossings along actually curved trajectory segments should be intercepted:



- Assigned globally, i.e. for all magnetic/electric fields in your simulation.
- The minimum step setting in **STEPSIZE** provides region specificity with a **negative** minimum step:



- Overrides **MGNFIELD/ELCFIELD** settings **always!**

Artefacts related to the breakdown of Moliere multiple-scattering theory

`MULSOPT`

MULSOPT to explicitly request single scattering

- Molière theory of multiple scattering applies for sufficiently long particle steps (accommodating at least a few 10s of individual elastic collisions)
- **Molière theory does not apply in case of very thin layers, wires, or gases (!)**
- FLUKA allows one to switch to single scattering in critical situations:
  - Close to boundaries (to shorten step lengths and apply correct angular deflection from single scattering)
  - When particle energy drops below condition of applicability of Molière
- Card: **MULSOPT** with
  - SDUM: GLOBEMF (e-,e+), GLOBHAD (hadrons, muons, ions), GLOBAL (all)

Toggle single scattering at boundaries and too short steps

Toggle single scattering also when E drops below applicability of Moliere theory

Number of single scatterings when crossing boundaries

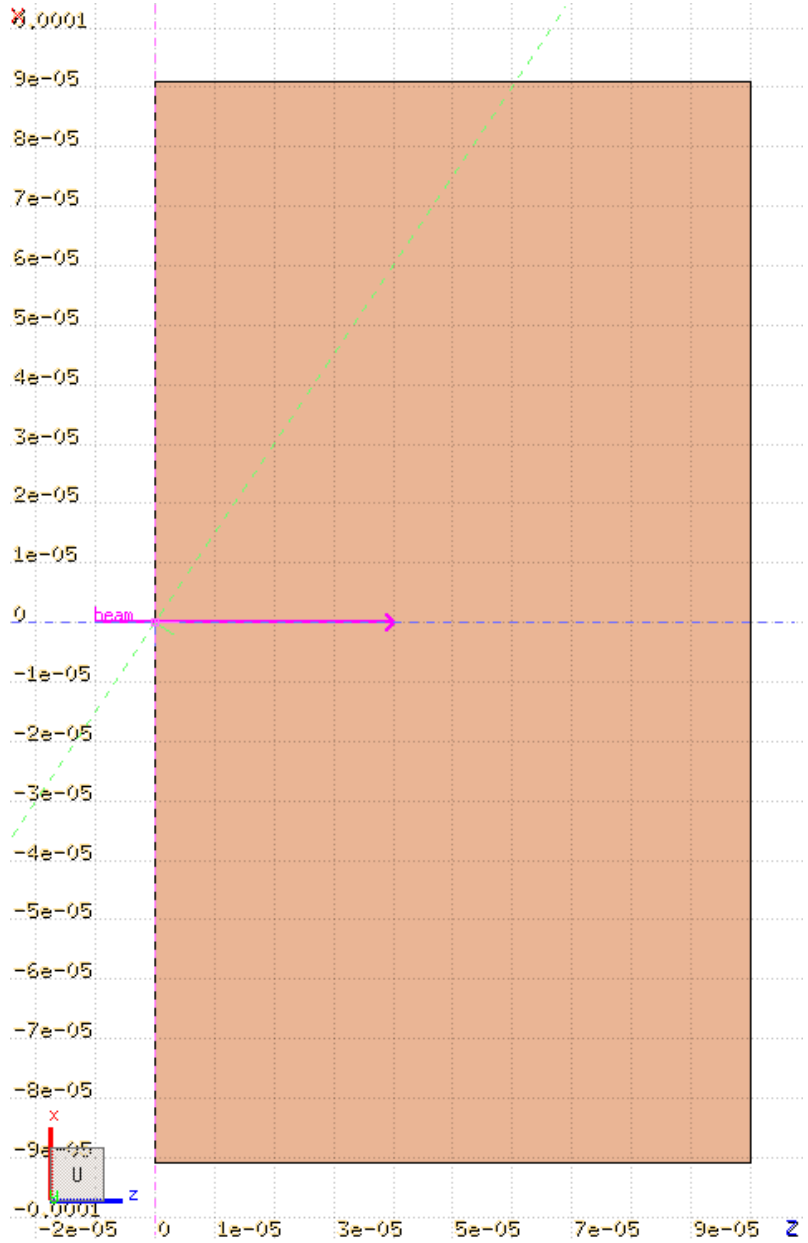
Example: microdosimetry

- Target: Si cylinder
  r = 1 μm
  z = 1 μm

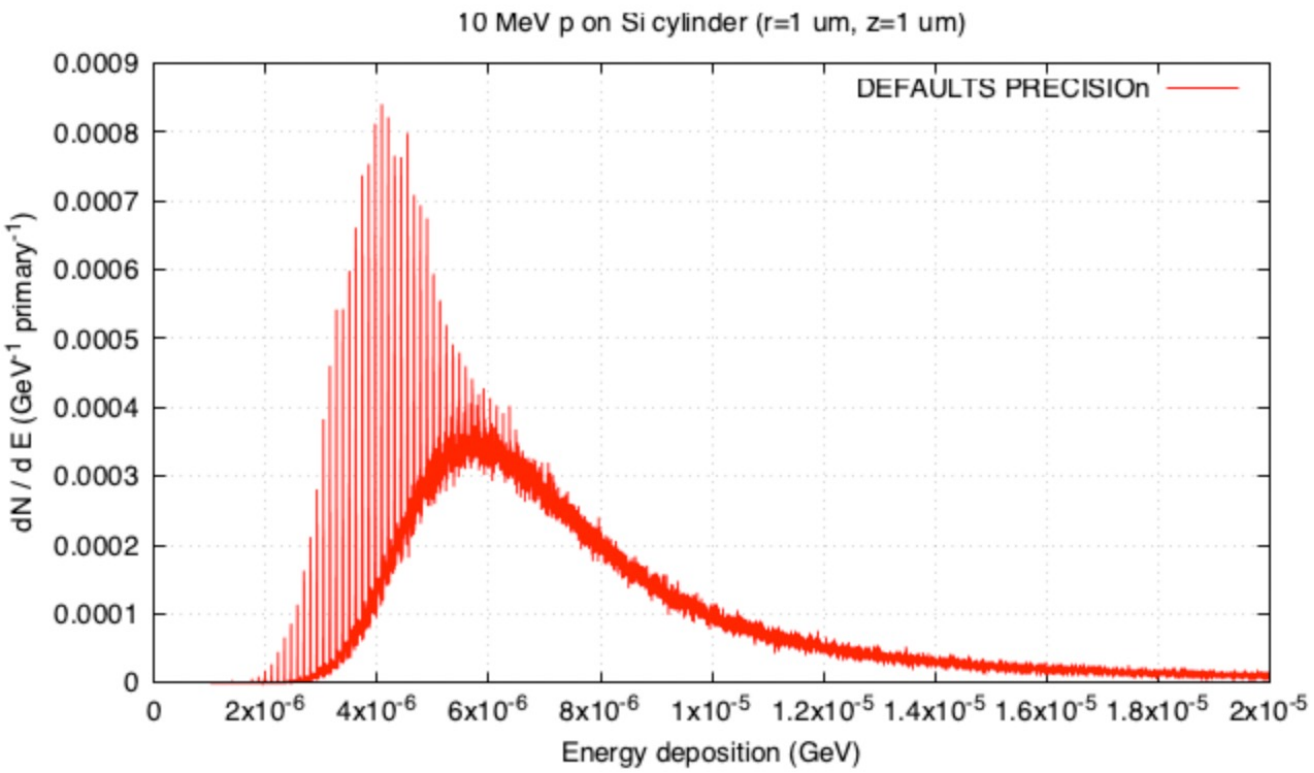
- 10 MeV proton pencil beam

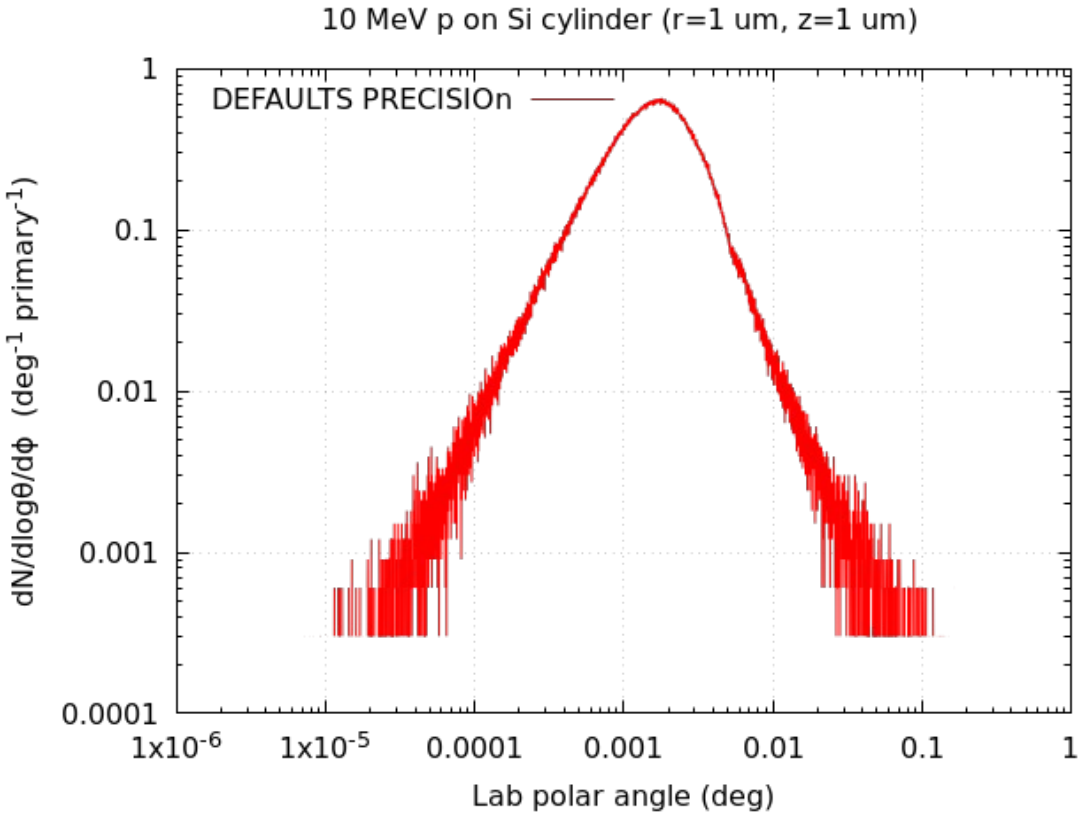
- Impinging along axis of the cylinder (z axis)

- Score:
  - Energy deposition spectrum
  - Angular histogram of protons emerging from the volume



Energy deposition and angular distribution

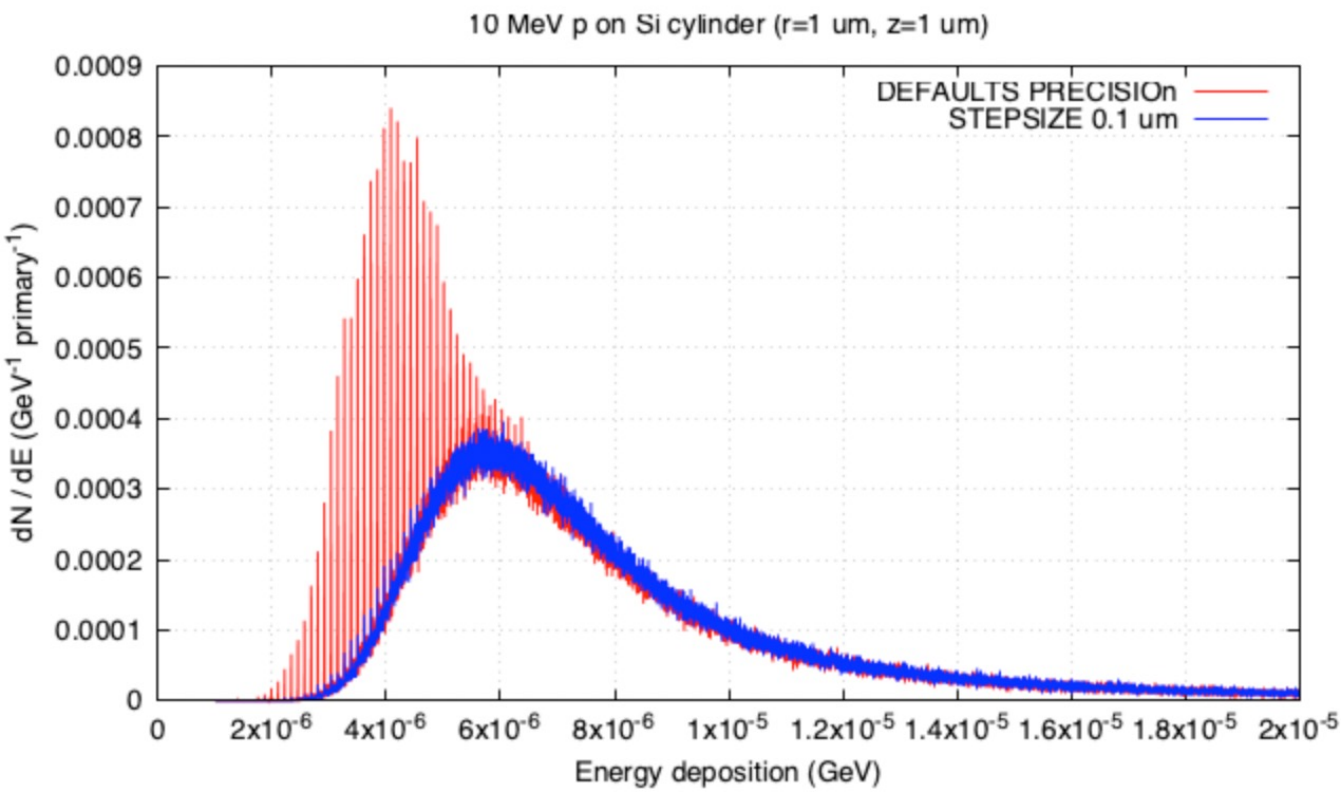


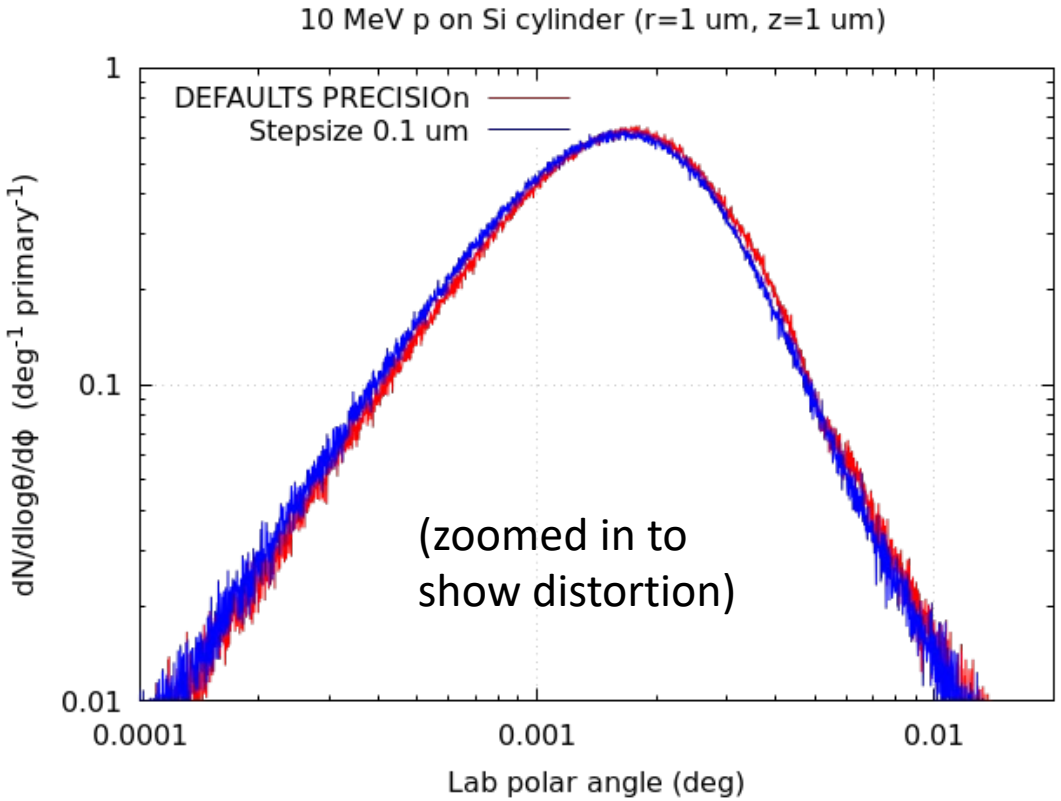


- Spikes in energy deposition spectrum
  - Particle steps are too long to resolve energy-deposition details at the keV level
- Natural solution: shorten step lengths

STEPSIZE shortening

STEPSIZE Min (cm): 1E-6 Max (cm): 1E-5
Reg: TARGET to Reg: TARGET Step: 1

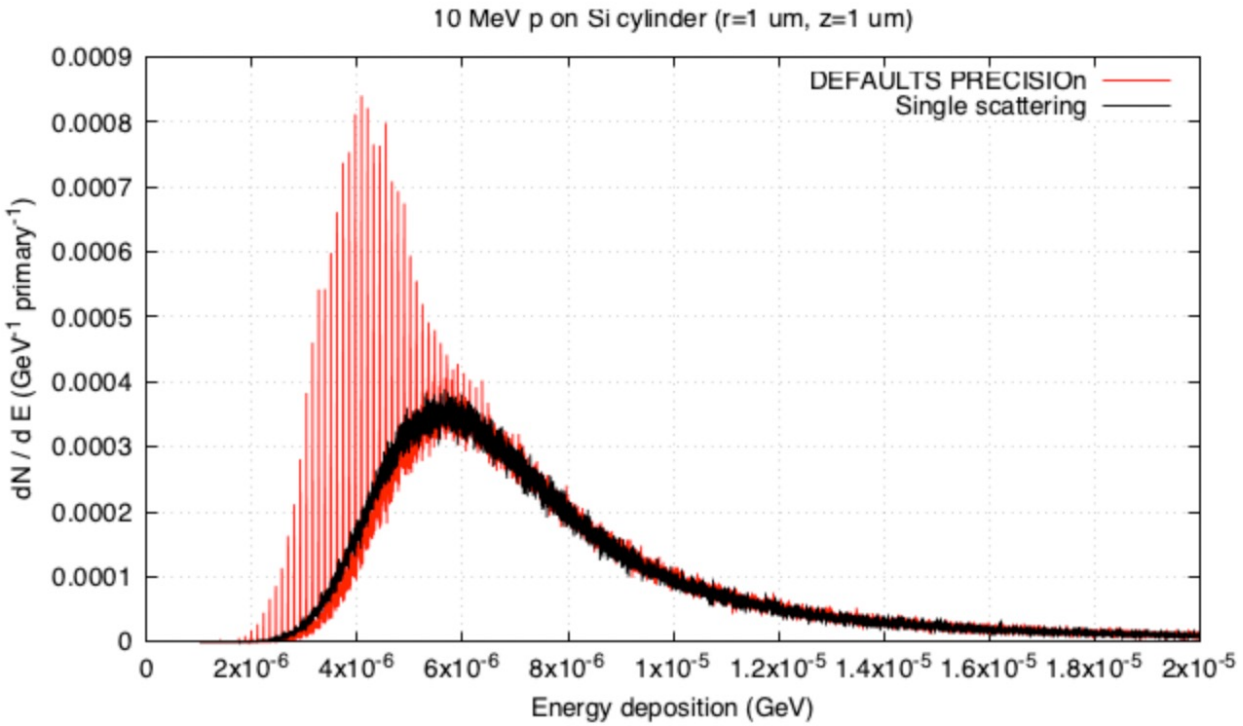


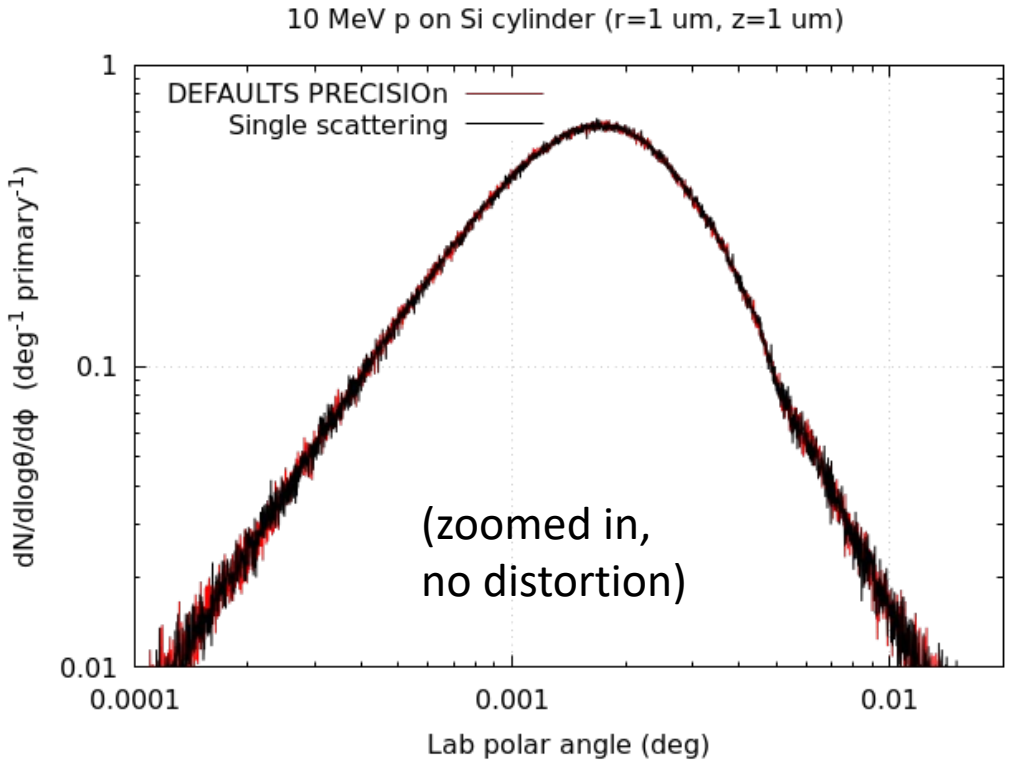


- Steps sizes have now dropped below domain of applicability of Molière theory
- Angular distribution is distorted

Switch to single scattering

MULSOPT
Optimal:
Type: GLOBHAD ▾
Single scat: On ▾
Min step:
E<Moliere: On ▾
Stretching: ▾
scatterings: 10





- Single scattering is now a discrete mechanism that naturally shortens step lengths (and correct angular deflections are applied at each step)

Wrap-up: precautions for thin slabs / micrometric volumes

- Stepping artefacts are likely to occur for thin slabs, dilute gases, micrometric volumes, etc.

- Request single scattering with the **MULSOPT** card (**GLOBAL**, **GLOBHAD**, **GLOBEMF**):
  - At energies below which Molière breaks down
  - Near surfaces (put a large number of events to effectively)
  - NB: this setting is not material/region specific, i.e. it applies to your whole geometry…

- Restrict step sizes, preferably with **EMFFIX, FLUKAFIX**.

- Note that shorter step sizes will lead to a measurable increase in CPU time.

Interaction mechanisms active only upon user request

`PHOTONUC, PHOTONUC (SDUM=ELECTNUC), SYRASTEP`

Interaction mechanisms upon user request

- FLUKA is **not a toolkit**, but a **fully integrated** MC code
- Models for relevant radiation-matter interaction mechanisms are activated by default
- However, **a few interaction mechanisms are not on by default**
- Users have to explicitly request them if they are relevant to their problem

The DEFAULTS card

- Before taking action, one should first at least examine the manual page for the **DEFAULTS** card detailing one's chosen option (typically **PRECISIOn**):

PRECISIOn

- EMF on.
- Rayleigh scattering and inelastic form factor corrections to Compton scattering and Compton profiles activated.
- Detailed photoelectric edge treatment and fluorescence photons activated.
- Low energy neutron transport on down to thermal energies included, (high energy neutron threshold at 20 MeV).
- Fully analogue absorption for low-energy neutrons.
- Particle transport threshold set at 100 keV, except neutrons (1E-5 eV), and (anti)neutrinos (0, but they are discarded by default anyway).
- Multiple scattering threshold at minimum allowed energy, for both primary and secondary charged particles.
- Delta ray production on with threshold 100 keV (see option DELTARAY).
- Restricted ionisation fluctuations on, for both hadrons/muons and EM particles (see option IONFLUCT).
- Tabulation ratio for hadron/muon $\mathrm{d}p/\mathrm{d}x$ set at 1.04, fraction of the kinetic energy to be lost in a step set at 0.05, number of $\mathrm{d}p/\mathrm{d}x$ tabulation points set at 80 (see options DELTARAY, EMFFIX, FLUKAFIX).
- Heavy particle e^+/e^- pair production activated with full explicit production (with the minimum threshold of $2m_e$).
- Heavy particle bremsstrahlung activated with explicit photon production above 300 keV.
- Muon photonuclear interactions activated with explicit generation of secondaries.
- Heavy fragment transport activated.

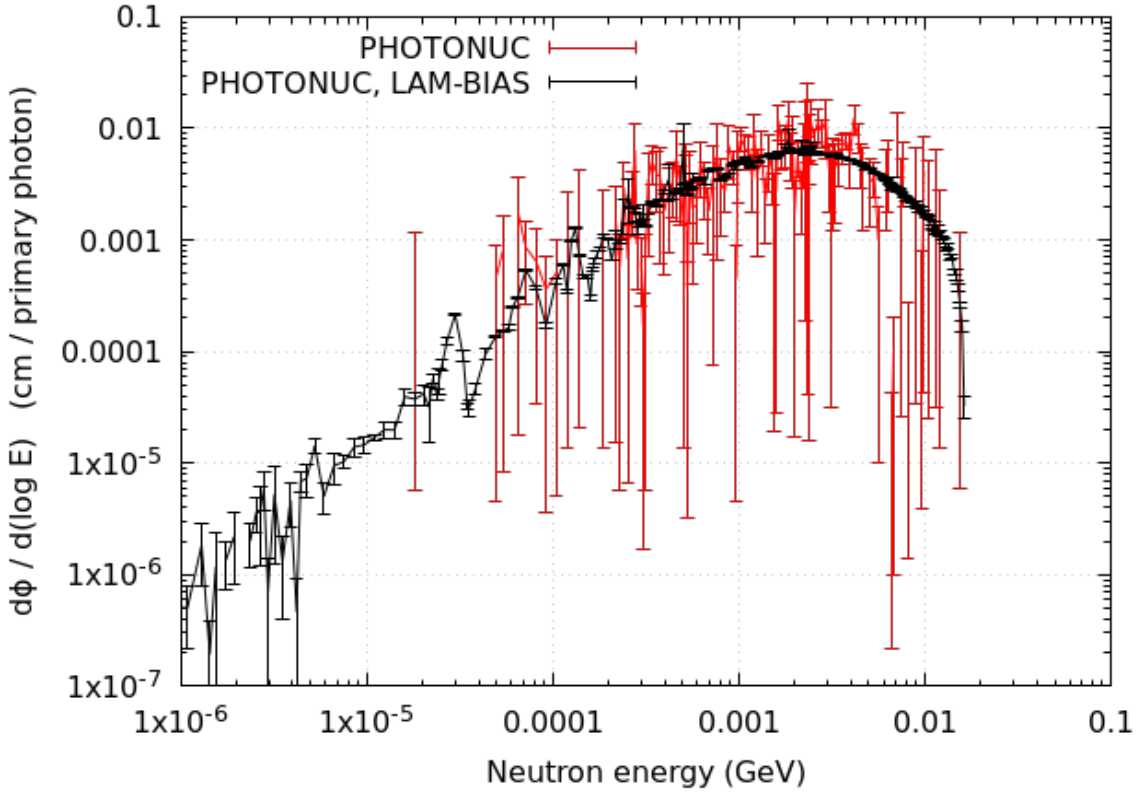
Photonuclear interactions

- Photon absorbed by nucleus, which is promoted to an excited state.
- Interaction driven by PEANUT (intranuclear cascade, pre-equilibrium emission, evaporation/Fermi break-up/fission, gamma-deexcitation)
- **Photonuclear interactions are not on by default in FLUKA**
- Use the `PHOTONUC` card to explicitly request photonuclear interactions at selected/all energy ranges on a per-material basis:

- Inelastic scattering lengths for photonuclear interactions can be very long. One may readily resort to biasing photonuclear interactions, e.g.:

Example: ^{nat}Al(g,n)

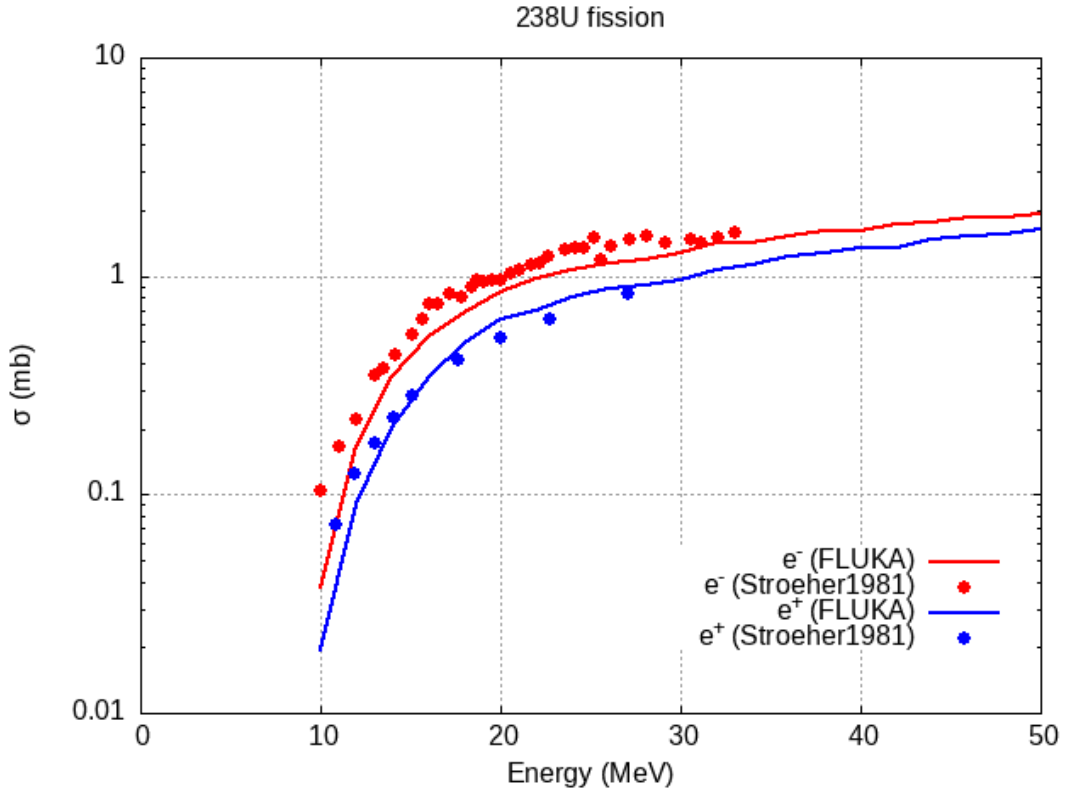
- **30-MeV photons impinging on a cylindrical rod of Al, 10 cm long, 5 cm radius**
- Scoring neutron track-length spectrum.
- **FLUKA without requesting `PHOTONUC`: no spectrum.**
- **Requesting `PHOTONUC`: red curve.**
  Low simulation efficiency. (80000 primaries)
- **`PHOTONUC + LAM-BIAS`: black curve.**
  Inelastic scattering length for 30-MeV photons in Al: 2075 cm
- Shortening the mean free path by e.g. a factor 1000 implies on average one photonuclear interaction every 2 cm (provided the photon has not undergone pair production or Compton meanwhile…)
- Should be reasonable in a target



Electronuclear interactions

- Electron/positron exchanging a *virtual* photon with a target nucleus and triggering a nuclear reaction
- Relevant for $e^{\pm}$ above ~10 MeV in targets thinner than radiation length
- For thicker targets, photonuclear reactions by Bremsstrahlung photons dominate
- **Electronuclear interactions are not on by default**
- They are enabled via the **PHOTONUC** card, with the SDUM **ELECTNUC**, e.g.:

Exp. ref: Stroher et al., Nucl Phys A 378 2 237-250 (1981)

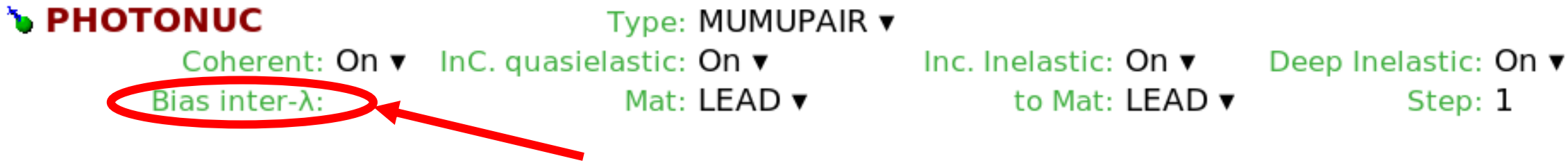


PHOTONUC Type: ELECTNUC ▾ All E: On ▾
E>0.7GeV: off ▾ Δ resonance: off ▾ Quasi D: off ▾ Giant Dipole: off ▾
Mat: GOLD ▾ to Mat: GOLD ▾ Step: 1

- Given the relatively low cross section: **LAM-BIAS**
- NB: electronuclear interactions automatically enable photonuclear reactions if not yet on

Muon pair production

- Photons with an energy above $2m_\mu$ may generate $\mu^+\mu^-$ pairs in the vicinity of a target nucleus
- **Muon pair production is not activated by default**
  (much more suppressed than e^-e^+ pair production –
  but may very well matter when muon backgrounds are of interest!)
- Relevant e.g. for electron accelerators (e- Bremsstrahlung followed by $\mu^+\mu^-$ pair production)
  and for hadronic machines (pion decay into muon is strongly favored over decay into e^{+-})
- Even for hadronic machines (pi0 decay -> high energy photons)
- It is requested by passing **`PHOTONUC`** card with **`SDUM=MUMUPAIR`**:



- Biasing requested in the same card
- NB: one may also request $\mu^+\mu^-$ pair production by just the primary photon with **`SDUM=MUMUPRIM`**

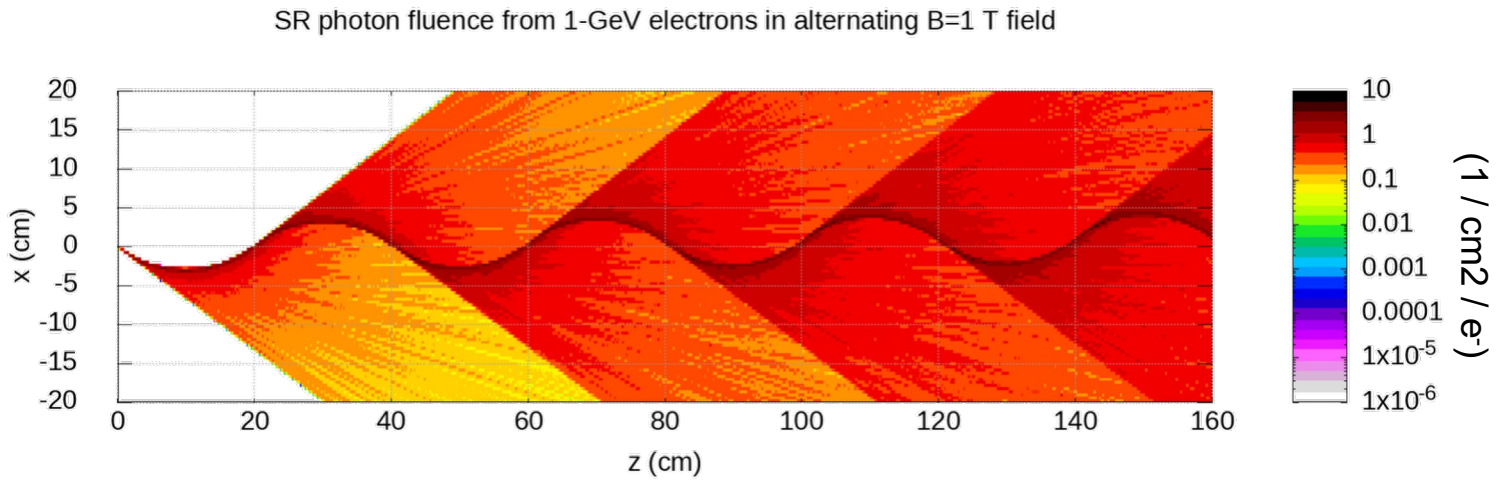
Synchrotron radiation emission

- Synchrotron radiation (SR) emission was available in versions of FLUKA prior to 4-3.0, but as a special source.
- This works for problems where SR by beam particles dominates, but not when SR emission by secondaries is important (e.g. SR emission by e- from muon decay).
- Since FLUKA 4-3.0, SR emission by charged particles *during transport* in B field in vacuum regions can be requested on a per-region basis via the **SYRASTEP** card (**it is not on by default!**):

SYRASTEP

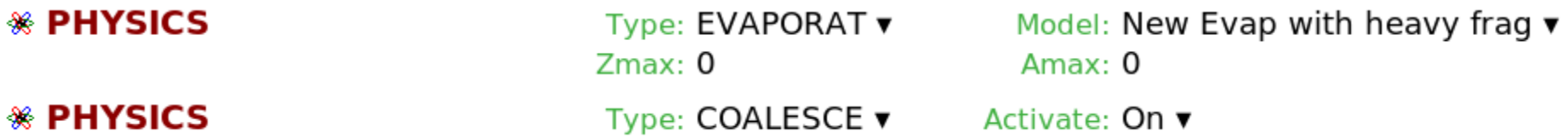
γ Thr: 1e-9 reverse flag:
Reg: TARGET ▾ to Reg: TARGET ▾ Step: 1

- One may use this feature to model e.g. wigglers:

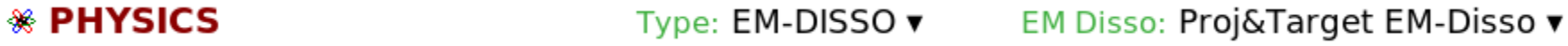


The PHYSICS card

- Request **evaporation** of heavy fragments and **coalescence** if radionuclide inventory/activity is of interest:



- **Electromagnetic dissociation** (very relevant for ultra-relativistic heavy ions, for which it eventually dominates over nuclear inelastic even) is not on by default, it has to be explicitly requested via:



- Note that FLUKA v4-2.0 was equipped with a dedicated model for deuteron nuclear reactions below 150 MeV/n, which is now on by default. Passing an IONSPLIT card as was recommended in the past is no longer adequate nor recommended, as it will switch off the new model in favour of the old crude splitting recipe.

Summary

- Steps, spikes, wiggly curves, and other kinds of artefact may be due to too coarse stepping.
- Resort to **FLUKAFIX, EMFFIX,** and **STEPSIZE** cards to fix them
- In case of thin layers, gases, micrometric volumes, etc., request single scattering with the **MULSOPT** card
- Biasing techniques are powerful simulation efficiency enhancers, but the user is left to their own devices to ensure proper sampling of relevant histories.
- Although FLUKA is a fully integrated package for the MC simulation of particle interactions, there are a handful of interaction mechanisms that are not on by default:
  - Photonuclear interactions: **PHOTONUC** card
  - Electronuclear interactions: **PHOTONUC** card with SDUM=**ELECTNUC**
  - Synchrotron radiation emission: **SYRASTEP** card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