Advanced scoring

DETECT, EVENTBIN, AUXSCORE, DPA calculations, R2E

Outline

- FLUKA Scoring Reminders
  - Various kinds of estimators available to the user
  - Reaction rate and cross section
  - Fluence estimation
- Generalized particles
- Additional scorers
  - **USRYIELD (II)**
  - **DETECT**
  - **AUXSCORE**
  - **EVENTBIN**
  - **RT-DOSE**
- Displacement per atom (DPA)
- Radiation to electronics

FLUKA scoring & results: estimators

- Monte Carlo → **mathematical experiment** (measurement → **estimator**)
- An estimator is obtained by sampling from a statistical distribution and has a **statistical error** (and in general also a systematic one)
- **Different techniques** to measure a given physical quantity ↔ the same quantity can be calculated using **different kinds of estimators**
- FLUKA offers **numerous different estimators**, i.e. users request scorings they are interested in through input cards directly
- For additional requirements, **FLUKA user routines are provided**

FLUKA estimators zoo

Energy deposition	vs. space	**USRBIN**		On a grid
		EVENTBIN		In selected regions
Fluence	vs. space	**USRBIN**		Grid, energy-integrated
	vs. energy	**USRTRACK / USRCOLL**	In a region	Single-differential
		USRBDX	On a surface	Double-differential, E,θ_{surf}
	vs. energy or other	**USRYIELD**	On a surface	Double-differential, single interval on 2^{nd} variable. If angle, θ_{beam}
			At interaction	
Activation	vs. isotope	**RESNUCLE**i		
	vs. space	**USRBIN**		

Reaction rate and cross section

- **Mean free path** *λ*[cm]: average distance travelled by a particle before an interaction. Its inverse, *Σ*[cm^{-1}] is the interaction probability per unit distance, and is called **macroscopic cross section**. Both *λ* and *Σ* depend on the material and particle type/energy

- For *N* identical particles, the number of reactions *R* occurring in a given time interval will be equal to the total distance travelled (*N×l)* times the probability per unit distance *Σ*: $R = N\, l\, \Sigma$

- The reaction rate will be $\dot{R} = \frac{N \mathrm{d}l}{\mathrm{d}t} \Sigma = N v \Sigma$, where v is the average particle velocity

Reaction rate and cross section

- Assume now that $n(\boldsymbol{r}, v) = \frac{\mathrm{d}N}{\mathrm{d}V}$ [cm^{-3}] is the density of particles with velocity $v = \frac{\mathrm{d}l}{\mathrm{d}t}$ [cm/s], at a spatial position $\boldsymbol{r}$

The **reaction rate** inside the volume element dV will be: $\frac{\mathrm{d}\dot{R}}{\mathrm{d}V} = n(\boldsymbol{r}, v)v\Sigma$

- $\dot{\Phi}(\boldsymbol{r}, v) = n(\boldsymbol{r}, v)v$ is called fluence rate or flux density and has dimensions [cm^{-3} cm s^{-1}]
- The time integral of the flux density $\Phi(\boldsymbol{r}, v) = n(\boldsymbol{r}, v)\mathrm{d}l$ is **the fluence** [cm^{-2}]

Fluence is measured in particles per cm^{-2} but in reality it describes a density of particle tracks!

- The number of reactions inside a volume V is given by the formula: $R = \Sigma\Phi V$ (where the product $\Sigma\Phi$ is integrated over energy or velocity)

Reaction rate and cross section

- Dividing the macroscopic cross section by N_0 (atoms per unit volume), one obtains the microscopic cross section σ [barn=10^{-24} cm^2]

$$\frac{\mathbf{probability/m}}{\mathbf{atoms/m^3}} = \frac{\mathbf{probability\,.\,m^2}}{\mathbf{atoms}} = \mathbf{atom\ effective\ area}$$

i.e. the **area of an atom weighted with the probability of interaction** (hence the name "cross section")

- But it can also be understood as the **probability of interaction per unit length**, with the length measured in atoms/m^2 (number of atoms contained in a 1m^2-base cylinder)
- In this way, both microscopic and macroscopic cross section are shown to have a similar physical meaning of "**probability of interaction per unit length**", with length measured in different units. Thus, the number of interactions can be obtained from both, by multiplying them by the corresponding particle track-length

Fluence estimation

- **Track length** estimation:

USRTRACK

$$\dot{\Phi}(v)\,\mathrm{d}t = n(v)v\,\mathrm{d}t = \frac{\mathrm{d}N(v)}{\mathrm{d}V}\frac{\mathrm{d}l(v)}{\mathrm{d}t}\mathrm{d}t = \lim_{\Delta V \to 0}\frac{\sum_i l_i(v)}{\Delta V}$$

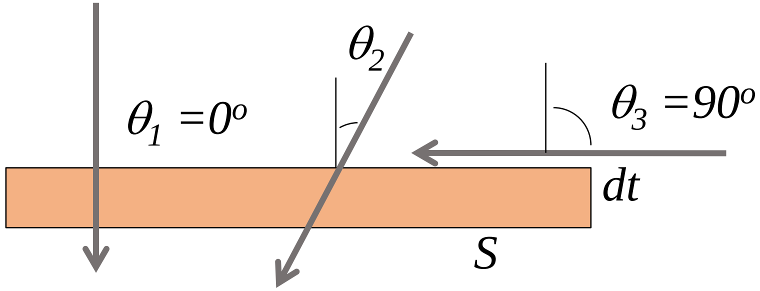
- **Collision density** estimation **(NOT IN VACUUM*)**:

(USRCOLL)

$$\dot{\Phi}(v) = \frac{\mathrm{d}\dot{R}(v)}{\mathrm{d}V}\,\lambda(v)$$

*: $0 \cdot \infty$ indetermination

Fluence vs Current



Consider the volume generated by a surface S and infinitesimal thickness dt.
A particle incident with *an angle θ wrt the normal to the surface S* travels a segment $dt/\cos\theta$ inside the volume.

The **average fluence** Φ over the surface S is defined as*:*

The total length of particle trajectory inside a unit volume

<u>*Unit*</u>*: m / m³ → [m⁻²]*

total track length inside the volume

$$\Phi = \lim_{dt \to 0} \frac{\sum_i \frac{dt}{\cos\theta_i}}{S\, dt}$$

volume

While the **average current** J over the surface S is given by the number of particles crossing the surface N divided by the surface area:

$$J = \frac{N}{S}$$

Reminder: normalization

- Beware! FLUKA **does not know the intensity** of the beam. It only knows how many events were run in the simulation
- All FLUKA intrinsic scorings are normalized « **per primary event** » or better, « **per unit primary weight** » if the source is biased
- Normalization to experimental conditions has to be applied by the user

Warning: Activation is an exception to this, as the beam intensity is provided by the user in the `IRRPROFI` card

Generalised particles

Generalised particles are **categories of particles**, or **quantities exclusively used in scoring**

They provide various easy-to-use options for built-in results filtering on particle basis, or scoring derived quantities

The most common GP filtering on particle type ←

ALL-PART	All transportable particles
NUCLEONS	protons and neutrons
BEAMPART	Primary (source/beam) particle
E+&E-	Electrons and positrons
MUONS	Muons and antimuons
KAONS	All kaons

ENERGY	Dose sc: Deposited energy / Energy fluence sc: Kinetic energy
DOSE	Dose (energy deposited per unit mass GeV/g)
ACTIVITY	Activity per unit volume (Bq/cm^3) (requires DCYTIMES option)
ACTOMASS	Activity per unit mass (Bq/g) (requires DCYTIMES option)
DOSE-EQ	Dose equivalent (pSv)
DOSEQLET	Dose equivalent with Q(LET) (GeV/g)
RES-NUCL	Residual Nuclei
SI1MEVNE	Silicon 1MeV-neutron equivalent fluence (cm^{-2})
HADGT20M	Fluence of hadrons above 20 MeV (cm^{-2})
DPA-NRT	Norgett-Robinson-Torrens DPA
ARC-DPA	Athermal recombination-corrected DPA

→ Some extensively used quantities available as GP across various fields

[See whole list in the manual]

Advanced scoring options

USRYIELD, DETECT, AUXSCORE, EVENTBIN, TPSSCORE

Outline - Additional scoring cards

- **USRYIELD** – Double-differential particle yield
- **DETECT** scores energy deposition in coincidence or anti-coincidence with a trigger, separately for each «event» (primary history). Dedicated post-processing routine available
- **AUXSCORE** defines filters and conversion coefficients and apply them to other scoring cards
- **EVENTBIN** is similar to **USRBIN** but prints the binning output after each event instead of an average over histories
- **RT-DOSE**

Input option: USRYIELD (1/2)

We remind you that **USRYIELD** is useful for scoring

- what comes out of nuclear inelastic events (**EMERGING option**)
- what goes from one region to another **BUT** different to a USRBDX because
  - More quantities available to score
  - Angles calculated wrt beam orientation and NOT the normal to the boundary

USRYIELD always needs two quantities!

Results must always be normalized by the size of the second quantity interval

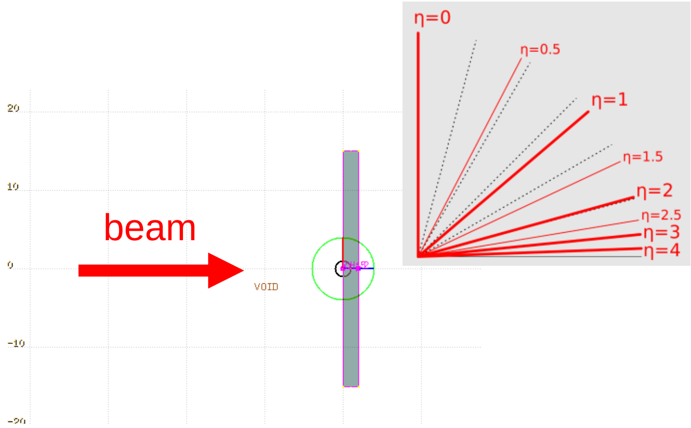
Tip: If no need for 2nd quantity:

- Choose one that does not filter anything
- Make sure it has an interval of size 1 so you don’t need any normalization
- Example: filtering a proton USRYIELD scoring with « charge inside [0.5 , 1.5] »

Input option: `USRYIELD` (2/2)

<u>Example</u>: 400 GeV/c proton beam on a tungsten target

We want to illustrate the link between emerging particle energy and its pseudorapidity η → 1 USRYIELD for each pseudorapidity interval under consideration



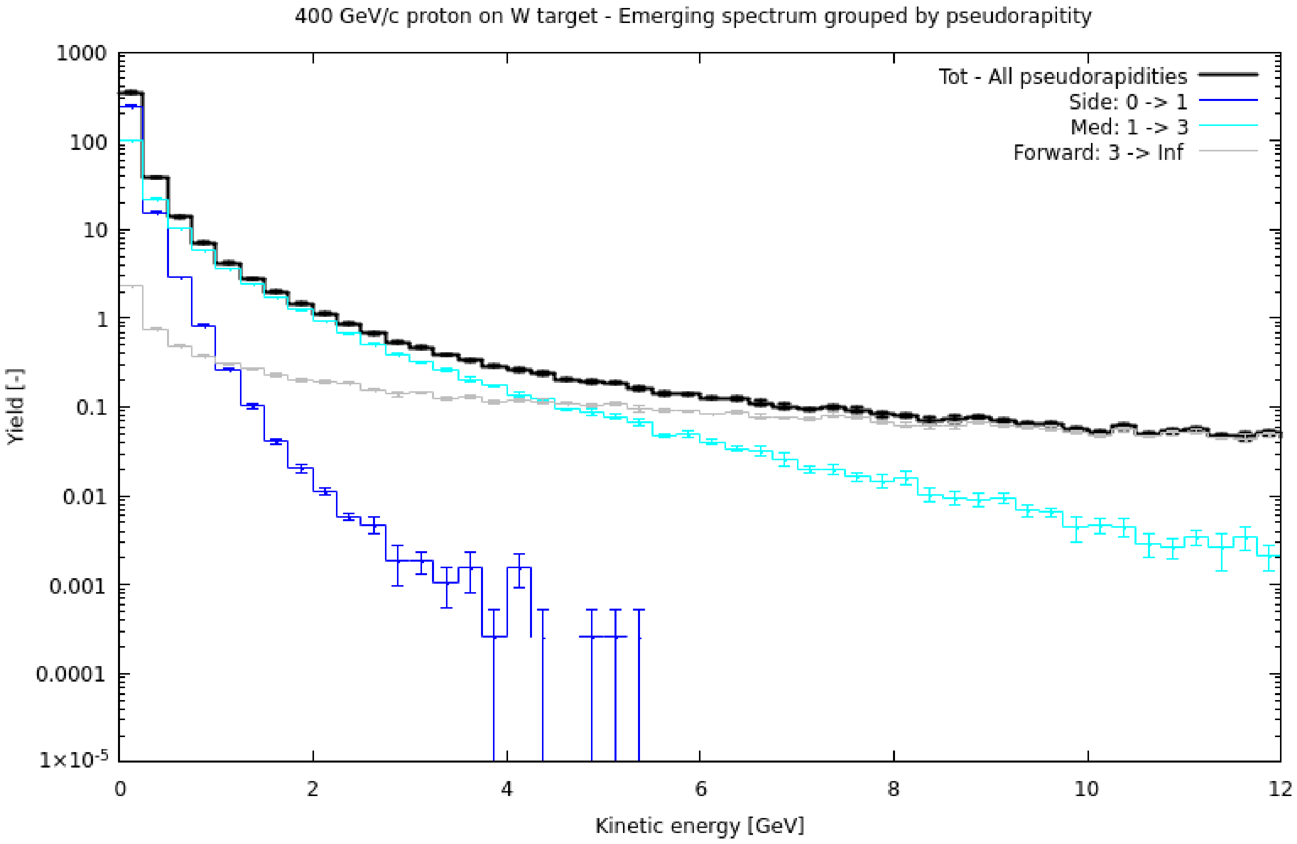
Note the normalization factors

USRYIELD Type: Yield ▾ Unit: 24 BIN ▾ Name: targ_tot
ie: Ekin GeV ▾ ia: Pseudorap. lab ▾ Log: Linear ▾ Norm: 1.0E-6
Part: PROTON ▾ Yield: EMERGING ▾
Min1: 0 Max1: 50 Nbins1: 200
Min2: 0 Max2: 1.0E6 Kind: d2σ/dx1dx2 ▾ Mat: ▾

USRYIELD Type: Yield ▾ Unit: 24 BIN ▾ Name: targ_sid
ie: Ekin GeV ▾ ia: Pseudorap. lab ▾ Log: Linear ▾ Norm: 1.0
Part: PROTON ▾ Yield: EMERGING ▾
Min1: 0 Max1: 50 Nbins1: 200
Min2: 0 Max2: 1 Kind: d2σ/dx1dx2 ▾ Mat: ▾

USRYIELD Type: Yield ▾ Unit: 24 BIN ▾ Name: targ_med
ie: Ekin GeV ▾ ia: Pseudorap. lab ▾ Log: Linear ▾ Norm: 0.5
Part: PROTON ▾ Yield: EMERGING ▾
Min1: 0 Max1: 50 Nbins1: 200
Min2: 1 Max2: 3 Kind: d2σ/dx1dx2 ▾ Mat: ▾

USRYIELD Type: Yield ▾ Unit: 24 BIN ▾ Name: targ_fw
ie: Ekin GeV ▾ ia: Pseudorap. lab ▾ Log: Linear ▾ Norm: 1.0E-6
Part: PROTON ▾ Yield: EMERGING ▾
Min1: 0 Max1: 50 Nbins1: 200
Min2: 3 Max2: 1.0E6 Kind: d2σ/dx1dx2 ▾ Mat: ▾



Input option: DETECT (1/3)

- Scores energy deposition on an **event by event basis**
- Useful for assessing detector response from single event
- Can also reproduce **coincidence** or **anti-coincidence** trigger, separately for each « event » (primary history)

- Output → Unit 17, to be processed by **DETSUW,** then read through (for instance – see manual for details):

```
CHARACTER*80 RUNTIT, RUNTIM*32, CHNAME*10
INTEGER*4 NCASE, NDET, NBIN, IV(1024)
REAL EMIN, EBIN, ECUT
...
READ(17) RUNTIT, RUNTIM, WEIPRI, NCASE
READ(17) NDET, CHNAME, NBIN, EMIN, EBIN, ECUT
READ(17) (IV(I), I = 1, NBIN)
```

IMPORTANT: DETECT should only be used in fully analogous mode (i.e. without biasing) as particle weights different than 1 are not accounted for properly

Input option: DETECT (2/3)

Use case: Quantification of detector response

- 4/6/8 MeV Proton beam (1MeV FWHM) impacting a thin Si target
- 1024 energy bins (channels)

DETECT Type: Detector ▾ Channels: 1024 Name: Edet
Emin: 1E-4 Emax: 10E-3 Ecut: Trigger: ▾
Regions: 1 ▾ Reg1: TARGET ▾

Output → histogram of energy deposition in considered region

Overall results normalized by total number of histories in the run

In some cases, users need to apply a smearing to reproduce real detector response

DETGEB allows to apply the following FWHM to each signal

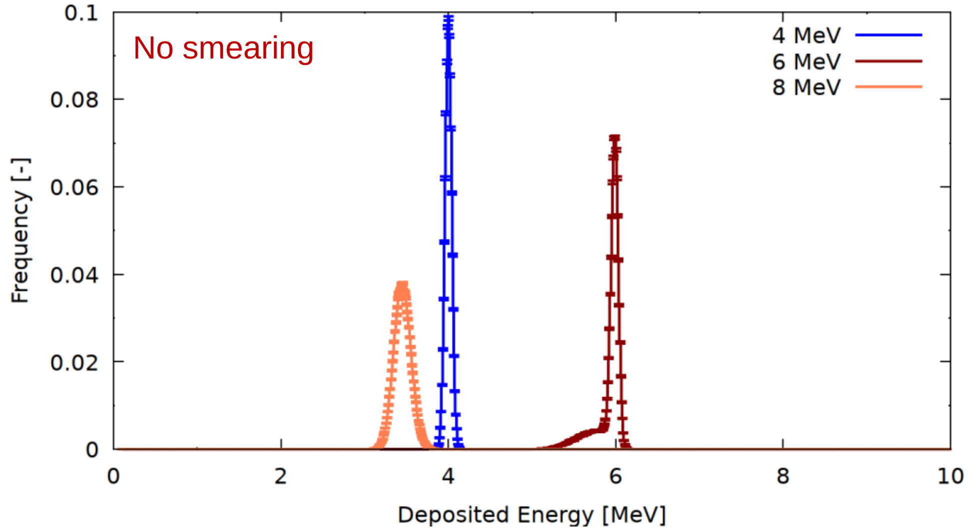
$$FWHM = a + b\sqrt{\Delta E + c(\Delta E)^2}$$

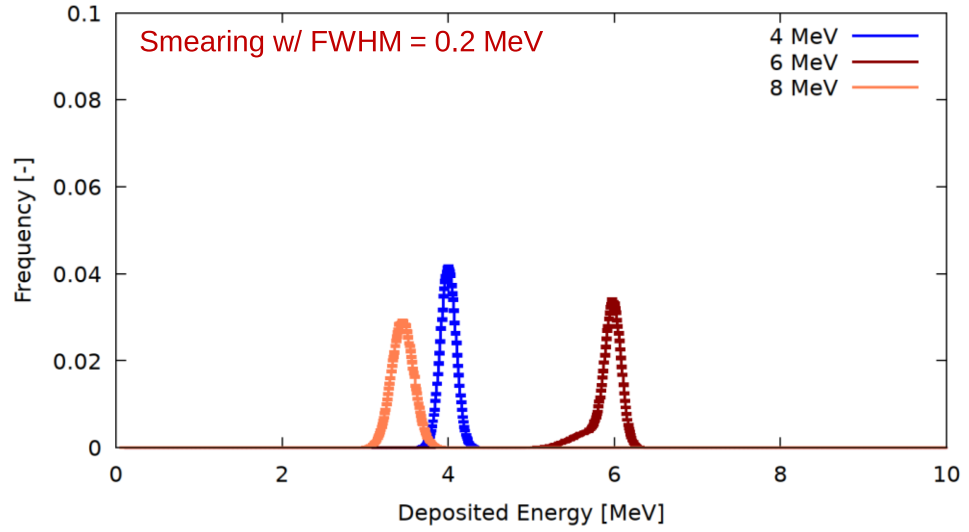
where

WHAT(1) = a [GeV] WHAT(2) = b [$GeV^{1/2}$] WHAT(3) = c [GeV^{-1}]

Illustration of energy-independent case:

DETGEB a: 0.0002 b: c:
Det: ▾ to Det: ▾ Step:

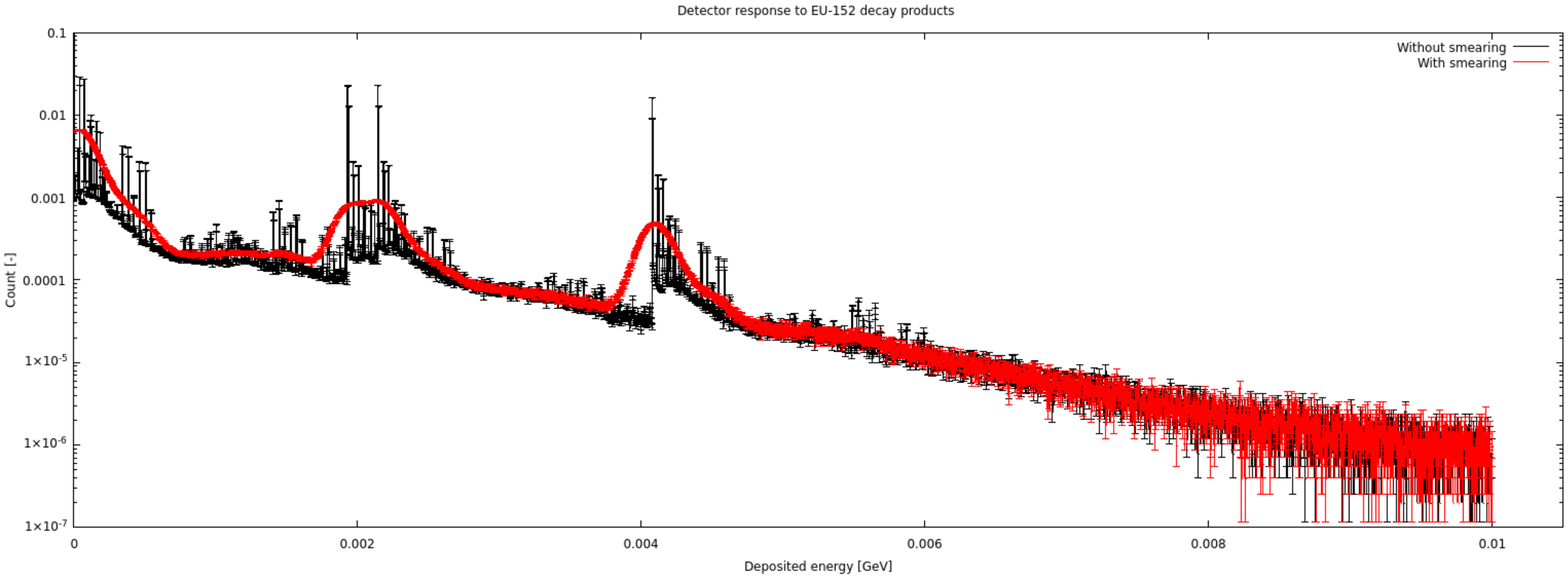




Input option: DETECT (3/3)

Example: Isotope source (Eu-152) in front of a Ge detector (6cm thickness)

```
DETECT        Type: Detector ▾   Channels: 3000      Name: Det
    Emin: 0.00000001   Emax: 0.01   Ecut:            Trigger: ▾
  Regions: 1 ▾        Reg1: TARGET ▾
#if      detgeb ▾
    DETGEB        a: 0.0002         b: 0.0002           c: 0.001
                Det: Det ▾     to Det: Det ▾          Step:
#endif
```



Input option: AUXSCORE (1/2)

Provides the option to associate a dose equivalent conversion factor to a scorer, or
to apply a filter to highlight contribution by given set of particles

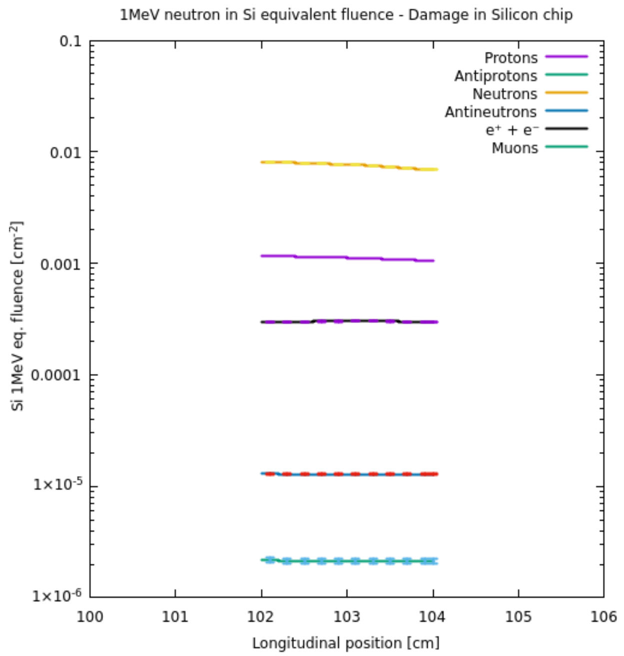
Type	**Type of estimator to associate with** drop down list of estimator types (USRBIN, USRBDX…)
Part	**Particle or isotope to filter for scoring** Particle or particle family list
Det .. to Det	**Detector range** Drop down list to select detector range of type **Type**
Step	**Step in assigning indices of detector range**
Set	**Conversion factor set for dose equivalent (DOSE-EQ) scoring** Drop down list of available dose conversion sets

Warning : Some quantities (such as energy deposition) are technically ultimately caused by electrons, coming from interactions of other particle types with the considered medium. In that case, be very careful in using AUXSCORE to isolate contributions of said particles, as the result WILL depend on the value of the EM threshold, and therefore on the electron being explicitly produced and transported or not.
In the former case, the scored quantity is attributed to the electron; in the latter, to the leading particle.

Input option: AUXSCORE (2/2)

Example 1: Damage estimation in 2cm thick Si slab

- Using AUXSCORE to discriminate contributions by various particle types to SI1MEVEQ scoring

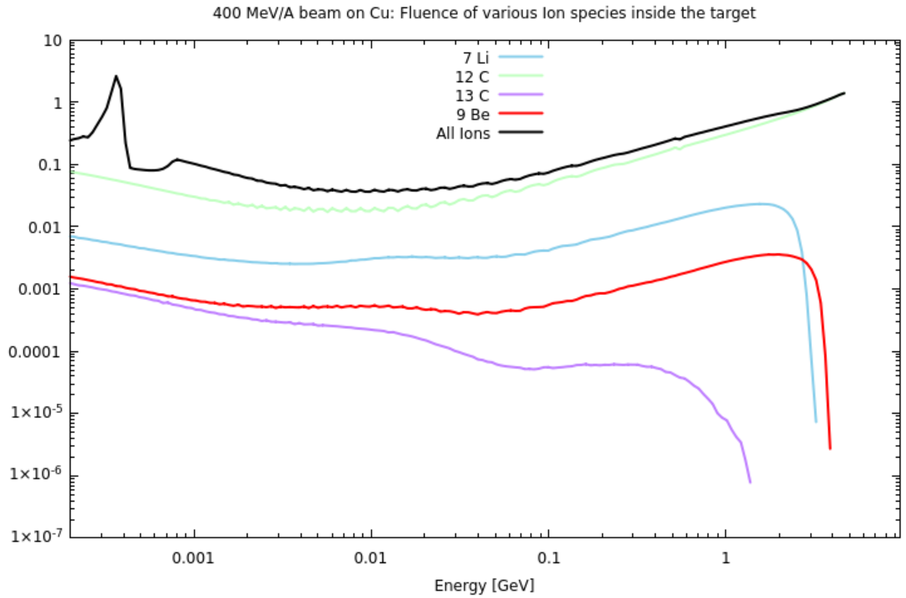


USRBIN
Type: X-Y-Z ▾ Part: SI1MEVNE ▾
Xmin: 10 Ymin: -20 Zmin: 102
Unit: 22 BIN ▾ Xmax: 30 Ymax: 20 Zmax: 104
Name: chipscon NX: 20 NY: 20 NZ: 10

AUXSCORE
Delta Ray: ▾
Type: USRBIN ▾ Det: chipscon ▾
Part: NEUTRON ▾ to Det: ▾
Set: ▾ Step:

Example 2: Filtering a scoring option by ion species

- 400 AMeV Carbon beam impacting a Cu target. HEAVYION GP regroups all species of all elements (A>6)
- AUXSCORE can be used to get scoring from a single species



Delta Ray: ▾ Z: 6 Det: 13C ▾ A: 13 to Det: ▾ Isomer: 0 Step:

USRTRACK
Type: Log ▾ Part: HEAVYION ▾
Reg: TARGET ▾ Emin: 0.000001
Unit: 36 BIN ▾ Emax: 10
Name: 9Be Vol: Bins: 220

AUXSCORE
Delta Ray: ▾
Type: USRTRACK ▾ Z: 4 Det: 9Be ▾
Part: ▾ A: 9 to Det: ▾
Set: ▾ Isomer: 0 Step:

USRTRACK
Type: Log ▾ Part: HEAVYION ▾
Reg: TARGET ▾ Emin: 0.000001
Unit: 36 BIN ▾ Emax: 10
Name: tot Vol: Bins: 220

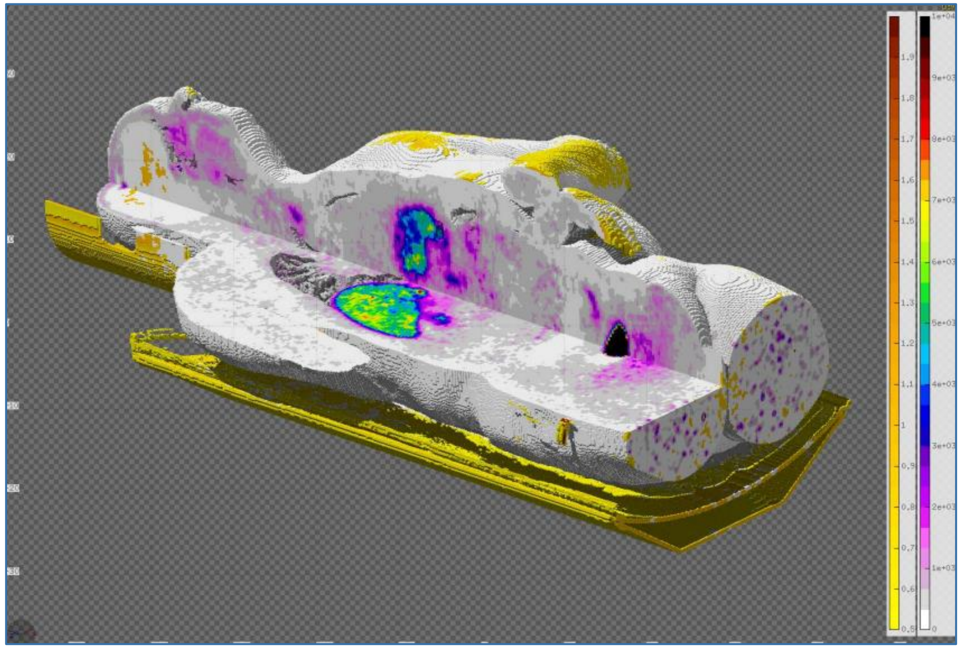
Input option: **`EVENTBIN`**

- Superimposes a binning to the geometry and prints requested results after each event
- Card works similarly to USRBIN (except WHAT(1) < 0 indicates that only non-zero data is printed)
- Output: akin to USRBIN's, but binning data printed at the end of each event (primary history), **without any normalization**
  - Energy in a bin : In a USRBIN → energy density per unit volume (normalized by bin volume)
    In a EVENTBIN → total energy per bin
- Notes :
  - Can be applied to regions, in which case it is equivalent to DETECT (DETECT results being easier to process)
  - Again, event-by-event scoring → only meaningful in fully analogue runs i.e. without biasing
    - Biasing leads to events being correlated
  - Recommended DEFAULTS: CALORIMEtry or PRECISIOn
  - In case of sparse outputs, consider printing only non-empty bins!

Input option: RADBIOL & TPSSCORE

Flair is fully equipped to work on medical applications

- CT scan view
- Voxel geometries
- D-V histograms, and more…



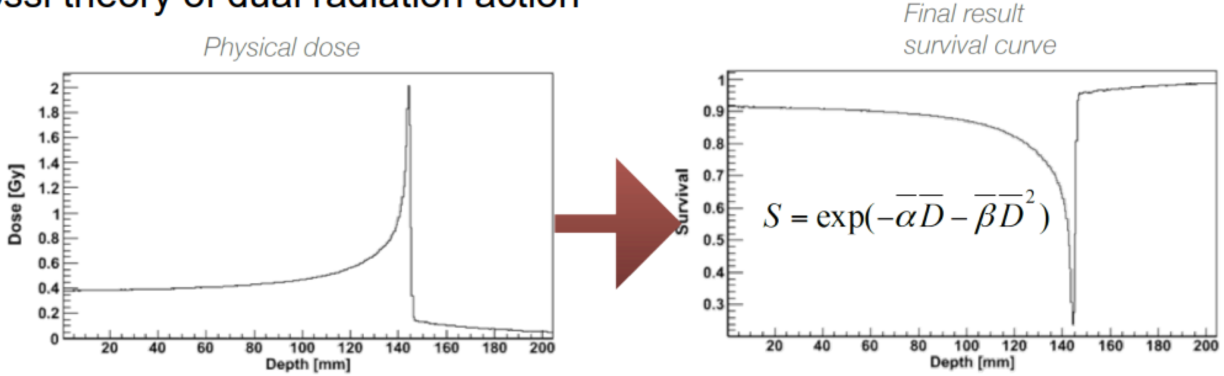
Related scoring options:

TPSSCORE is a scoring option giving the surviving cell probability in a spatial binning

Using **RAD-BIOL** to define conversion coefficients between dose and cell damage

Attention: these coefficients are proprietary → not distributed as part of the code

Rossi theory of dual radiation action



270 MeV/u 12C ions on V79 cell line

Displacement per Atom (DPA)

In crystalline materials, interaction of HE particles can lead to lattice defects (from energy deposited to the atomic centres) quantified through the concept of **DPA**

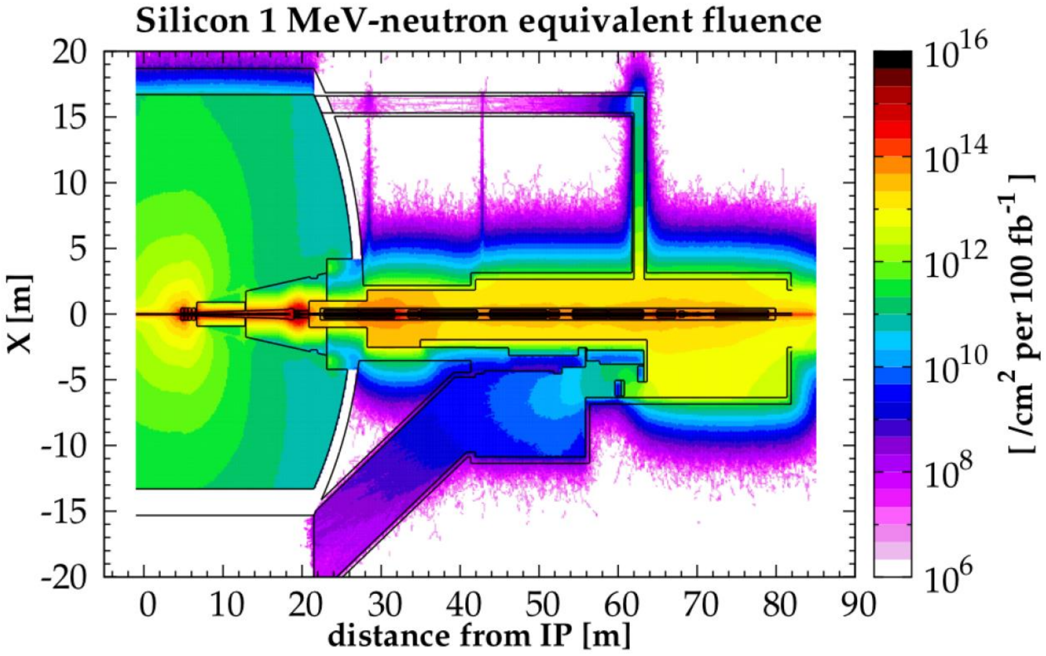
Important quantity in the fields of **material damage** (e.g. damage to electronics, or to mechanical properties of materials)

- Multiple DPA formalisms exist (generalised particles in FLUKA):
  - DPA-SCO: DPA scoring specific to FLUKA – **RETROCOMPATIBILITY ONLY**
    - Developed prior to the following alternatives
    - For graphite only
  - **DPA-NRT**: DPA in the Norgett-Robinson-Torrens model
    - Model used extensively in the literature for the past ~20 years
    - BUT: overestimates heavily the actual damage, as recombinations are totally ignored!
  - **ARC-DPA**: athermal recombination-corrected DPA
    - conceived to improve dpa models and get a better estimate of defect production in irradiated materials
    - **RECOMMENDED FOR MOST USES**

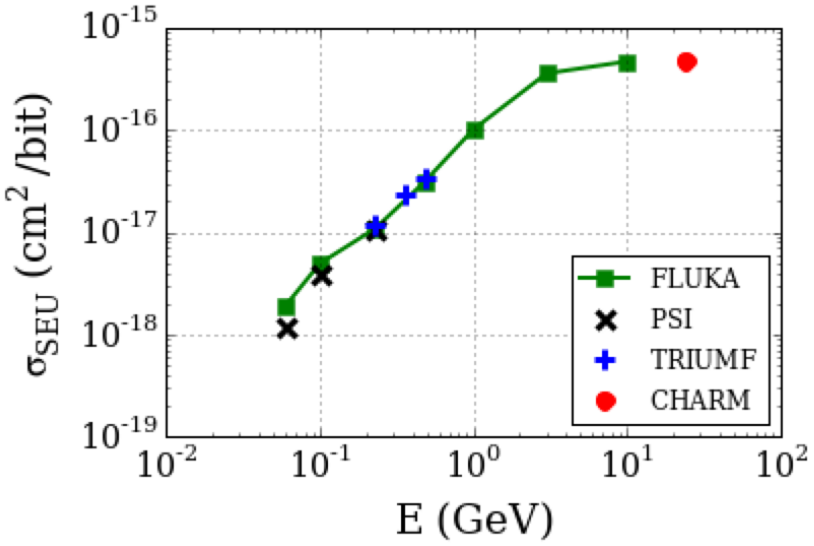
For more information: Radiation damage to materials [OECD note]
https://inis.iaea.org/collection/NCLCollectionStore/_Public/46/066/46066650.pdf

FLUKA simulations for radiation damage on electronics

- Particle-matter interaction Monte Carlo codes are very useful in the context of radiation damage to electronics, mainly linked to (i) the calculation of the radiation environment and (ii) the analysis of the effects on electronics.



Example of simulation of radiation environment: 1-MeV silicon neutron equivalent fluence in LHC interaction point



Example of simulation of radiation effect: Single Event Upset probability as a function of proton energy

[Note: often not only based on Monte Carlo simulations, but relying on coupling with other simulation tools (e.g. semiconductor or circuit level) and/or additional modeling aspects of the response of electronics to a given physical quantity simulated in FLUKA. More on that later…]

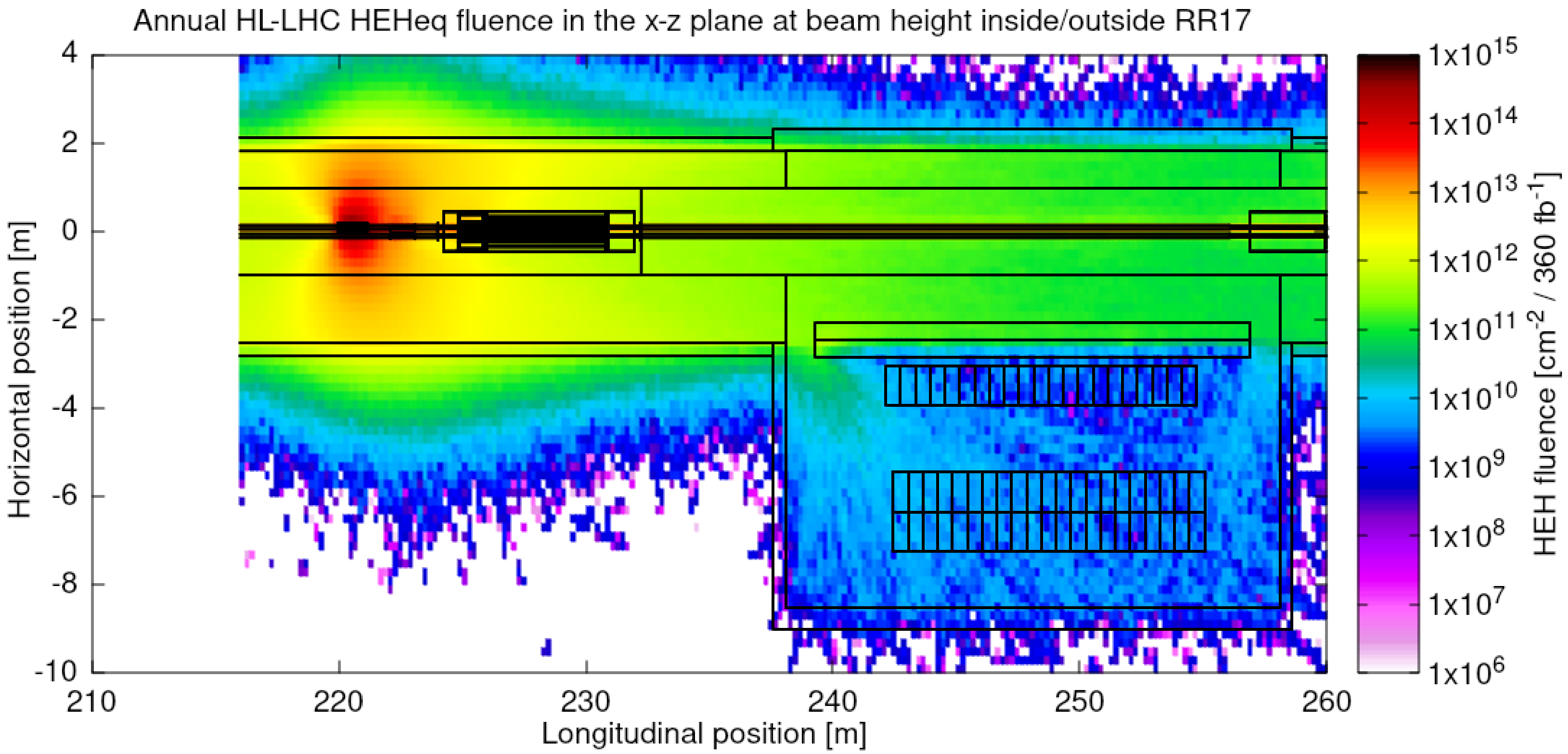
Main radiation effects in electronics

Category	Sub-category	Example of effect	Associated scorings
Stochastic	Non-destructive Single Event Effects (SEEs)	Single Event Upset (SEU): Bit flip in SRAM memory	**USRTRACK, USRBDX USRYIELD**
	Destructive SEEs	Single Event Latchup (SEL): Overcurrent, which can lead to thermal breakdown	**USRTRACK, USRBDX USRYIELD**
Cumulative	Total Ionizing Dose (TID)	Charge build up in oxide, leading to increased leakage current and/or threshold voltage shift	**USRBIN**
	Displacement Damage (DD)	Atomic displacement leading to dark current increase in CMOS imagers	**USRTRACK, USRBDX, USRBIN**

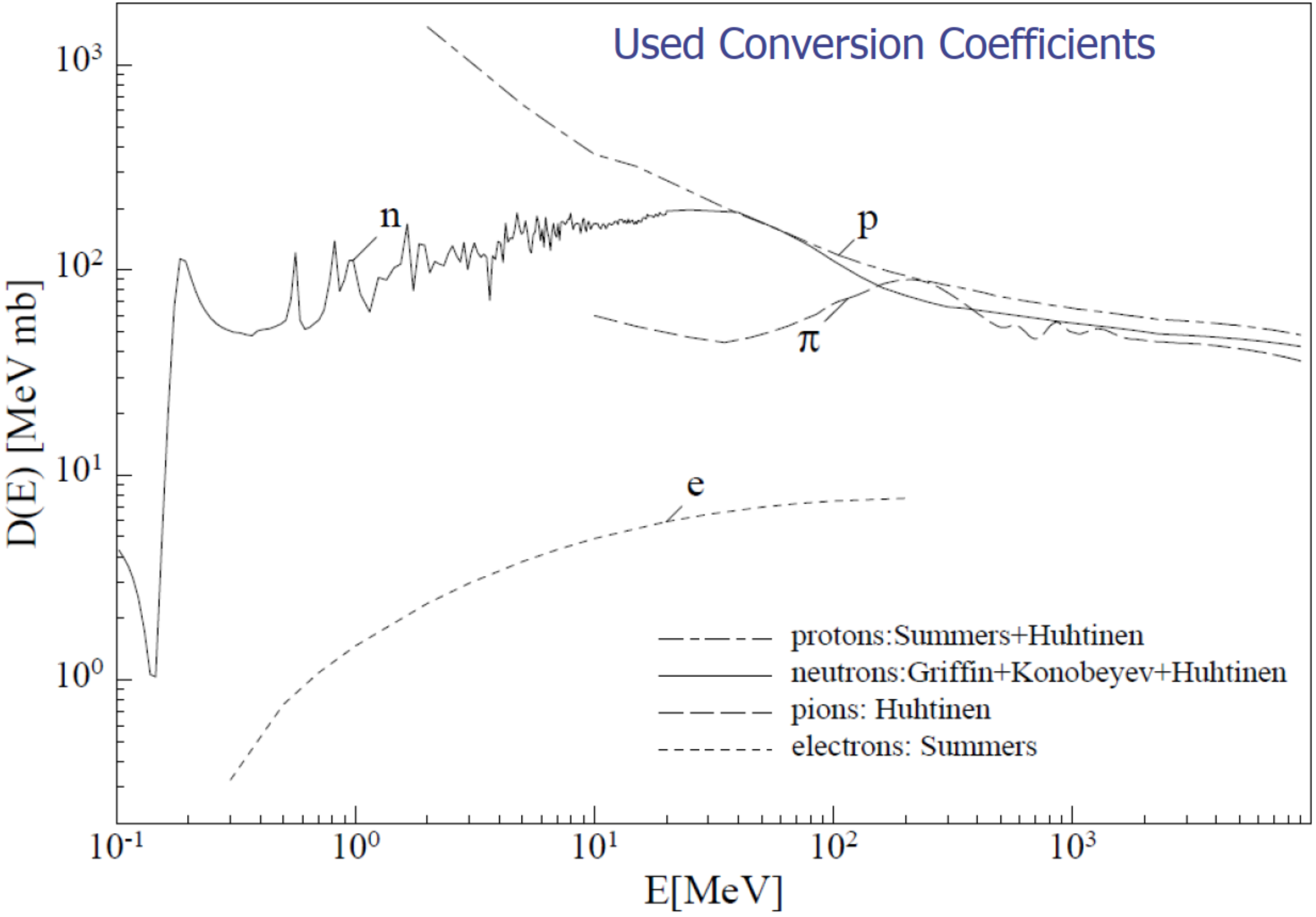
Radiation damage scoring in FLUKA

- All important quantities used to estimate radiation damage on electronics can be retrieved in FLUKA
  - Cumulative damage:
    - Energy deposition (total ionizing dose) by scoring **DOSE** in `USRBIN` (you will need to convert from GeV/g to Gy or rad!)
    - Silicon lattice displacement: 1-MeV neutron equivalent fluences (**SI1MEVNE**), with any related estimator (e.g. `USRTRACK, USRBDX`) or, more commonly, directly in integral form (e.g. `USRBIN`)
  - Stochastic failures (SEEs):
    - Depending on the environment, the particle energy (e.g. `USRTRACK, USRBDX`) or LET spectra (e.g. `USRYIELD`) can be scored and convoluted with the device's response function (i.e. SEE cross section as a function of energy or LET)
    - In FLUKA, three relative response functions are already implemented by default:
      - Hadrons above 20 MeV (**HADGT20M**)
      - Hadrons above 20 MeV, plus weighted neutron contribution in 0.2-20 MeV range (**HEHAD-EQ**)
      - Equivalent thermal neutron flux, weighted as 1/v (**THNEU-EQ**)

Example of high-energy hadron equivalent scoring in the LHC

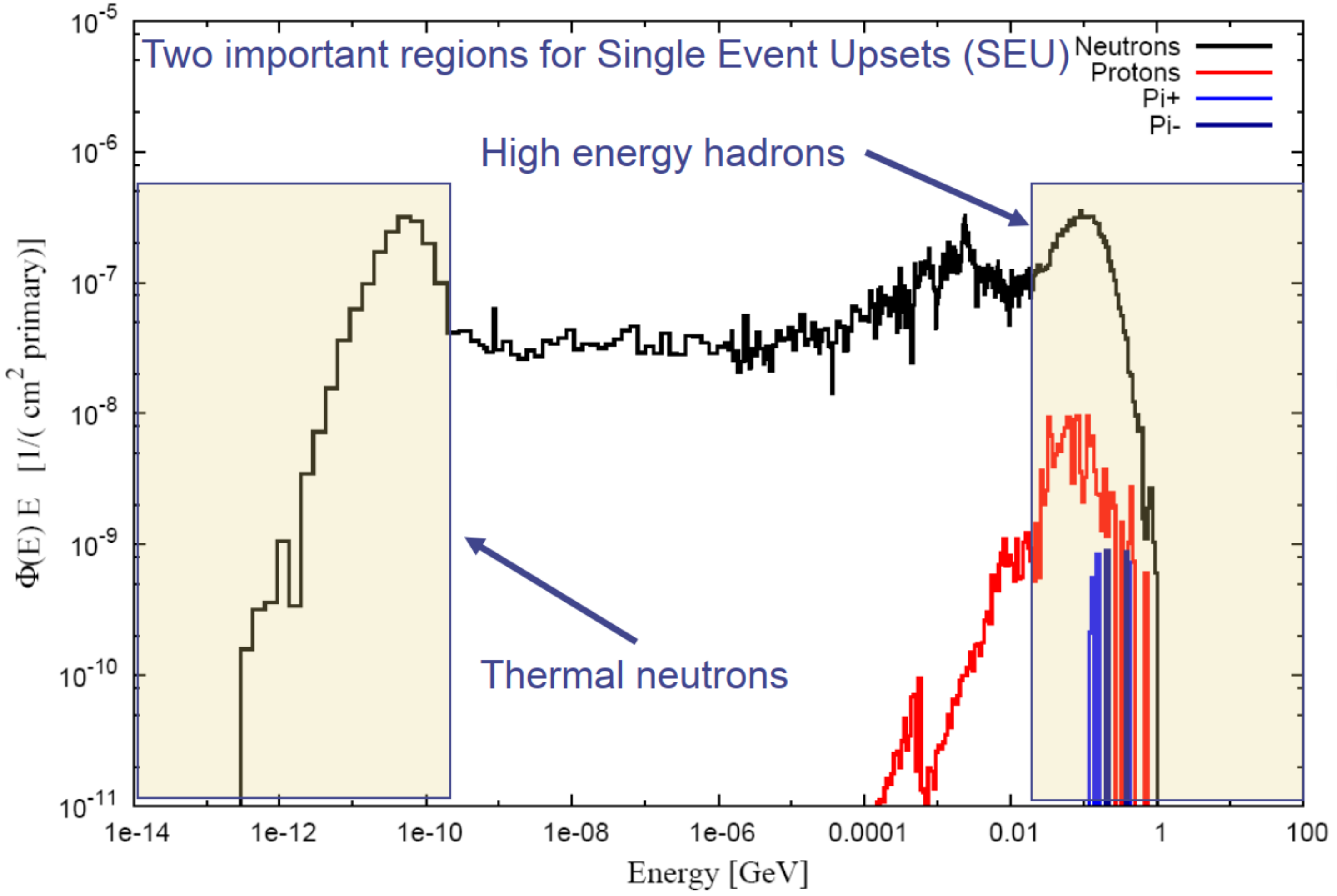


1-MeV neutron equivalent in silicon



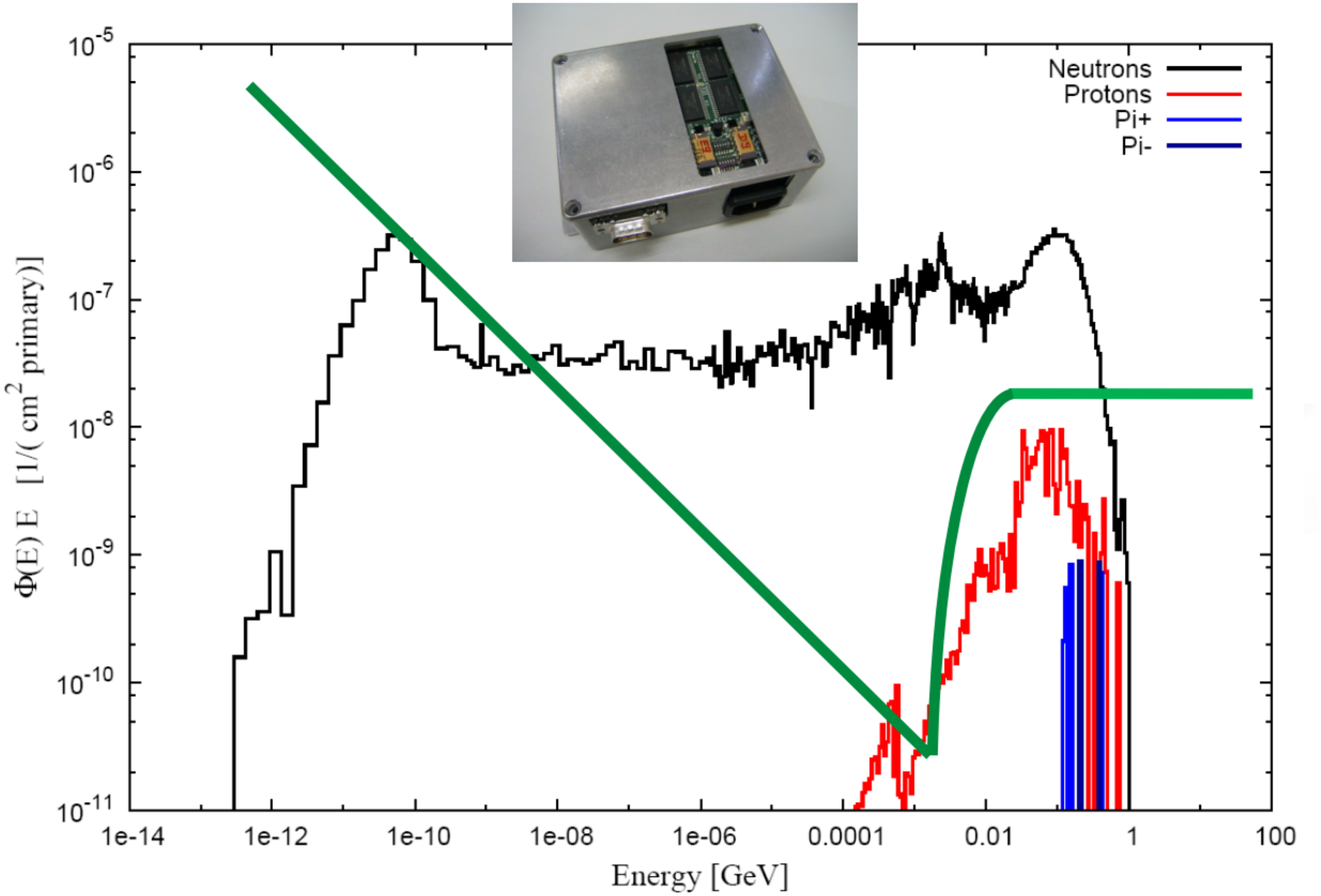
SEUs in mixed radiation field

$$\#SEU = \sigma_{Th.\,n.} \cdot \Phi_{Th.\,n.} + \sigma_{HEH} \cdot \Phi_{HEH}$$



SEUs in mixed radiation fields

e.g. LHC RadMon



FLUKA