

Estimators and Scorings

FLUKA Beginner's Course

Reaction Rate and Cross Section (1/3)

- We call mean free path $\lambda[cm]$ the average distance travelled by a particle in a material before an interaction. Its inverse, $\Sigma[cm^{-1}]$ is the probability of interaction per unit distance, and is called macroscopic cross section. Both λ and Σ depend on the material and on the particle type and energy.
- For N identical particles, the number of reactions R occurring in a given time interval will be equal to the total distance travelled Nl times the probability per unit distance Σ : $R = Nl\Sigma$
- The reaction rate will be $\dot{R} = N \mathrm{d}l/\mathrm{d}t$ $\Sigma = N v \Sigma$, where v is the average particle velocity.

Reaction Rate and Cross Section (2/3)

- Assume now that n(r,v)=dN/dV [cm^{-3}] be the density of particles with velocity v=dl/dt [cm/s], at a spatial position r. The reaction rate inside the volume element dV will be: $d\dot{R}/dV = n(r,v)v\Sigma$
- The quantity $\dot{\Phi}(\mathbf{r}, v) = n(\mathbf{r}, v)v$ is called fluence rate or flux density and has dimensions $[cm^{-3} cm s^{-1}] = [cm^{-2} s^{-1}].$
- The time integral of the flux density $\Phi(\mathbf{r}, v) = n(\mathbf{r}, v) dl$ is the fluence $[cm^{-2}]$
- Fluence is measured in particles per cm² but in reality it describes the 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 (3/3)

• Dividing the macroscopic cross section by N_0 , the number of atoms per unit volume, one obtains the microscopic cross section: $\sigma[barn=10^{-24}cm^2]$

$$\frac{\text{probability/cm}}{\text{atoms/cm}^3} = \frac{\text{probability} \times \text{cm}^2}{\text{atom}} = \text{atom effective area}$$

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/cm² (the number of atoms contained in a cylinder with a 1 cm² base).
- 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 interaction can be obtained by both by multiplying by the corresponding particle track-length.

Fluence estimation (1/2)

Track length estimation:

USRTRACK

$$\dot{\Phi}(v) dt = n(v) v dt = \frac{dN(v)}{dV} \frac{dl(v)}{dt} dt = \lim_{\Delta V \to 0} \frac{\sum_{i} l_{i}(v)}{\Delta V}$$

Collision density estimation:

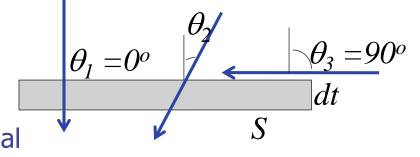
USRCOLL

$$\dot{\Phi}(v) = \frac{\dot{R}(v)}{\sigma(v) N_o \Delta V} = \frac{\dot{R}(v)}{\Sigma(v) \Delta V} = \frac{\dot{R}(v) \lambda(v)}{\Delta V}$$

Fluence estimation (2/2)

Surface crossing estimation

• Imagine a surface having an infinitesimal thickness dtA particle incident with an angle θ with respect to the normal of the surface S will travel a segment $dt/cos\theta$.



Therefore, we can calculate an average surface fluence by adding $dt/cos \theta$ for each particle crossing the surface, and dividing by the volume S dt:

$$\Phi = \lim_{dt \to 0} \frac{\sum_{i} \frac{ai}{\cos \theta_{i}}}{Sdt}$$

• While the current *J* counts the number of particles crossing the surface divided by the surface:

$$J = dN/dS$$

The fluence is independent from the orientation of surface *S*, while the current is NOT!

In an isotropic field can be easily seen that on a flat surface $J = \Phi/2$

FLUKA Scoring & Results - Estimators

- It is often said that Monte Carlo (MC) is a "mathematical experiment"
 The MC equivalent of the result of a real experiment (i.e., of a measurement) is called an estimator.
- Just as a real measurement, an estimator is obtained by sampling from a statistical distribution and has a statistical error (and in general also a systematic one).
- There are often several different techniques to measure the same physical quantity: in the same way the same quantity can be calculated using different kinds of estimators.
- FLUKA offers numerous different estimators, *i.e.*, directly from the input file the users can request scoring the respective quantities they are interested in.
- As the latter is implemented in a very complete way, users are strongly encouraged to preferably use the built-in estimators with respect to user-defined scoring
- For additional requirements FLUKA user routines are provided

Built-In and User Scoring

- Several pre-defined estimators can be activated in FLUKA.
- One usually refers to these estimators as "scoring" capabilities
- Users have also the possibility to build their own scoring through user routines, HOWEVER:
 - Built-in scoring covers most of the common needs
 - Built-in scoring has been extensively tested
 - Built-in scoring takes BIASING weights automatically into account
 - Built-in scoring has refined algorithms for track subdivision
 - Built-in scoring comes with utility programs that allow to evaluate statistical errors
- Scoring can be geometry dependent AND/OR geometry independent FLUKA can score particle fluences, current, track length, energy spectra, Z spectra, energy deposition...
- Either integrated over the "run", with proper normalization, OR event-by event
- Standard scoring can be weighted by means of simple user routines (fluscw, comscw)

Related Scoring Commands

- USRTRACK, USRCOLL score average $d\Phi/dE$ (differential fluence) of a given type or family of particles in a given region;
- USRBDX scores average $d^2\Phi/dEd\Omega$ (double-differential fluence or current) of a given type or family of particles on a given surface;
- USRBIN scores the spatial distribution of energy deposited, or total fluence (or star density, or momentum transfer) in a regular mesh (cylindrical, Cartesian o per region) described by the user;
- USRYIELD scores a double differential yield of particles escaping from a surface. The distribution can be with respect to energy and angle, but also other more "exotic" quantities;
- SCORE scores energy deposited (or star density) in all regions;
- The output of SCORE will be printed in the main (standard) output, written on logical output unit LUNOUT (pre-defined as 11 by default)
- All other detectors write their results into logical output units assigned by the user (the unit numbers must be >20)

More "Special" Scoring

- RESNUCLEi scores residual nuclei in a given region (more details are given in the respective lecture on activation);
- DETECT scores energy deposition in coincidence or anti-coincidence with a trigger, separately for each "event" (primary history);
- EVENTBIN is like USRBIN, but prints the binning output after each event instead of an average over histories;
- ROTPRBIN sets the storage precision (single or double) and assigns rotations/translations for a given user-defined binning (USRBIN or EVENTBIN). Useful in case of LATTICEs;
- TCQUENCH sets scoring time cut-offs and/or Birks quenching parameters for binnings (USRBIN or EVENTBIN) indicated by the user;
- USERDUMP defines the events to be written onto a "collision tape" file;
- AUXSCORE defines filters and conversion coefficients.

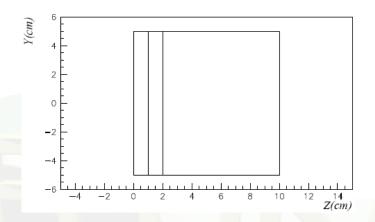
The FLUKA Output Files

The respective Fluka output consists of:

- A main (standard) output, written on logical output unit LUNOUT (predefined as 11 by default) [.out]
 - for details refer to the lecture explaining the FLUKA output
- A file with the last random number seeds, unit LUNRAN (2 by default) [ran*]
- A file of error messages, unit LUNERR (15 by default) [.err]
- Any number (including zero) of estimator output files. Their logical unit number is defined by the user [*fort_xx*]
- The available range of logical output numbers is: 21-99
- Generally, the user can choose between formatted (ASCII) and unformatted (binary) scoring (negative or positive sign in the logical unit number). Unformatted scoring is mandatory for the use of provided post-processing utilities.
- Possible additional output generated by the user in any user routine;

Extending the example with Scoring

Cylinder along Z, filled by water-aluminum-lead and surrounded by Air



- The USRBIN command allows to <u>define</u> a 3-D grid, either cartesian, cylindrical (R-Z-Φ) or by region.
- On this grid, one can score energy deposition, particle fluence (total or by particle type), as well as the density of interactions;
- There is an equivalent EVENTBIN command, that outputs the same quantities event-by-event;
- Using USERWEIG the results can be weighted by the comscw.f or fluscw.f external routines (Advanced).

USRBIN

```
* Energy deposition [GeV/cm<sup>3</sup>]
                      11.0
                                                               10.0
                                                -40.0
                                                                                           15.0TargEne
USRBIN
                                 ENERGY
                       0.0
                                                 -5.0
                                                                                         200.0&
USRBIN
                                                              100.0
USRBIN
                                                      Unit: 40 BIN ▼
                                                                                Name: TargEne
                                                     Bmax: 10
   Туре: R-Ф-Z ▼
                           Bmin: 0
                                                                                  NR: 100
                                                        Y:
                             X:
                                                                                  NΦ:
    Part: ENERGY ▼
                            Zmin: -5.0
                                                                                  NZ: 200
                                                     Zmax: 15.0
```

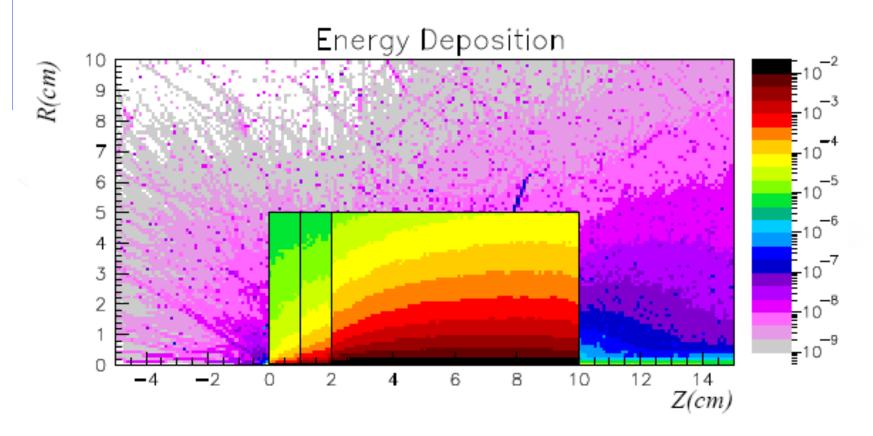
• This is an R-Z- Φ binning (what(1)=11), scoring energy density (generalized particle ENERGY, or 208), writing the unformatted output on unit 40, spanning 0<R<10 in 100 bins, 0< Φ <2 π in 1 bin (default), -5<z<15 in 200 bins.

```
* Neutron fluence [cm<sup>-2</sup>]
                      11.0
                                                -40.0
                                                                                           15.0TarqNeu
USRBIN
                               NEUTRON
                                                               10.0
USRBIN
                       0.0
                                                  -5.0
                                                              100.0
                                                                                          200.0&
                                                                                   Name: TargNeu
USRBIN
                                                         Unit: 40 BIN ▼
    Туре: R-Ф-Z ▼
                             Bmin: 0
                                                       Rmax: 10
                                                                                     NR: 100
                               X:
                                                          Y:
                                                                                     NΦ:
     Part: NEUTRON ▼
                             Zmin: -5.0
                                                                                     NZ: 200
                                                       Zmax: 15.0
```

• This is a R-Z- Φ binning (what(1)=11), scoring neutron fluence, writing the unformatted output on unit 40, spanning 0<R<10 in 100 bins, 0< Φ <2 π in 1 bin (default), -5<z<15 in 200 bins.

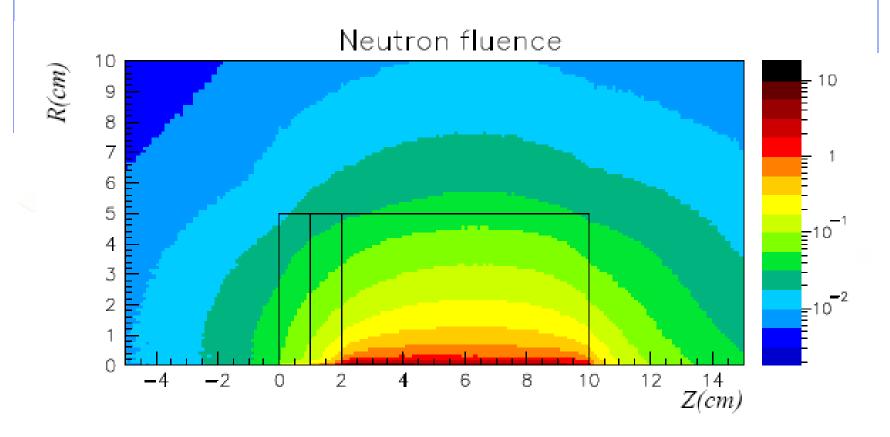
USRBIN → The Result

WHAT(2) = ENERGY: Energy deposition from a 3.5 GeV proton beam hitting at [0.,0.,0.] directed along z results are normalized to GeV/cm³ per primary



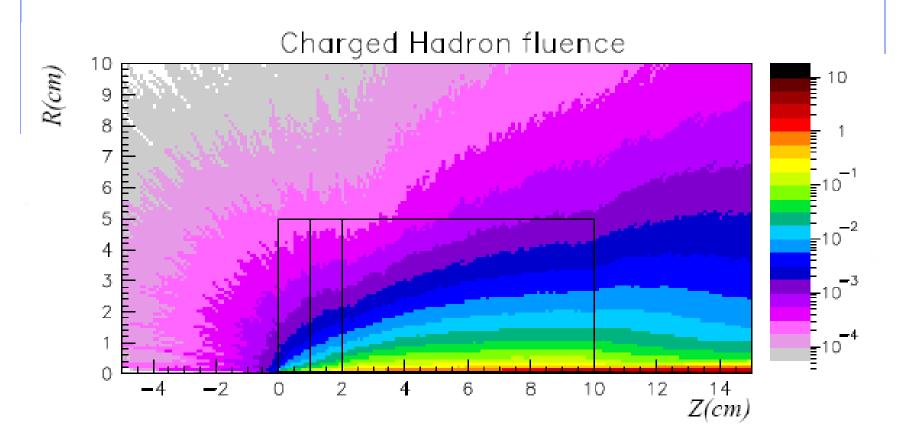
USRBIN → The Result

Same, WHAT(2)= NEUTRON to get neutron fluence results are normalized to particles/cm² per primary



USRBIN → The Result

Same, WHAT(2)= HAD-CHAR to get charged hadron fluence results are normalized to particles/cm² per primary



USRBIN – more quantities

USRBIN can score Particle fluence as well as "Generalized particles", either fluence-like or energy-like, for instance with what(2) =

DOSE: Energy/unit mass (GeV/g)

DPA-SCO: Displacements per atom (see the lecture on

Ionization and transport)

X-MOMENT: x-component of momentum transfer (GeV/c)

ACTIVITY: activity per unit volume (Bq/cm³)

(see lecture on radioactivity)

... and more (see in the manual)

USRBDX

* in this case post-processed results are single differential (already integrated over the solid angle)

USRBDX scores double differential (energy and angle) particle distributions across a boundary surface. The angle is with respect to the normal of the surface. The distribution can be fluence or current, one-way or two-ways, according to WHAT(1)

• Score charged hadrons at the outer surface of the lead segment (from TARGS3 to INAIR). WHAT(1)=99 means: fluence, one-way only, log. intervals in energy. From 1 MeV to 10 GeV in 40 intervals, and *one angular interval (default)**. WHAT(6) is a normalization factor: setting it equal to the surface area provides results normalized to cm⁻² (fluence unit) GeV⁻¹ sr⁻¹. Output to unformatted unit 50

∆ USRBDX			^{Unit:} 50 BIN ▼		Name: S	p3ChH
USRBDX	10.0	0.001	40.			&
USRBDX	99.0	HAD-CHAR	-50.	TARGS3	INAIR	329.87Sp3ChH
* out from 1	.ead					
~ + 1	T 2	т 3	T 4	т 5	т о	т / т

USRBDX		Unit: 50 BIN ▼	Name: Sp3ChH
Type: Φ1,LogE,LinΩ ▼	Reg: TARGS3 ▼	to Reg: INAIR ▼	Area: 329.87
Part: HAD-CHAR ▼	Emin: 0.001	Emax: 10.	Boins: 40
	Ωmin:	Ωmax:	Ωbins:

• Score at the surface between 2nd and 3rd target section, same as before but in 3 angular bins.

*	+	1	+	2	+	3	+	4	+	5	+	6	+	7	+
USF	RBDX		9	9.0	HAD-C	HAR	_	54.	TAR	GS2	TAR	GS3	78.5	398 <mark>S</mark> p	2ChHA
USF	RBDX		1	0.0	0.	001		40.						3.0&	

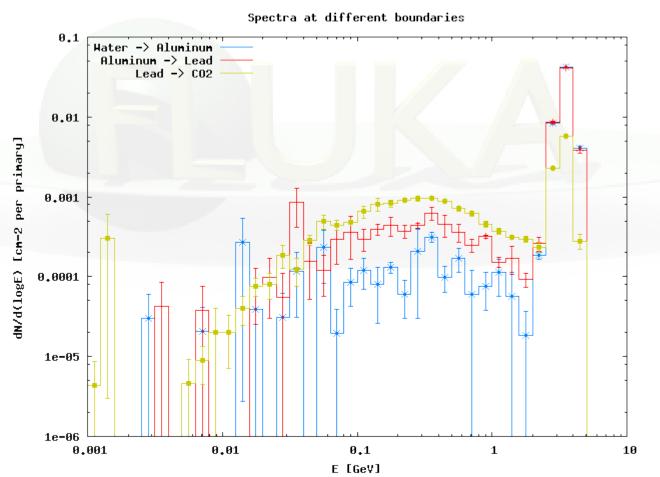
A USRBDX		^{Unit} : 54 BIN ▼	Name: Sp2ChHA	
Type: Φ1,LogE,LinΩ ▼	Reg: TARGS2 ▼	10 Reg: TARGS3 ▼	Area: 78.5398	
Part: HAD-CHAR ▼	Emin: 0.001	Emax: 10.	Boins: 40	18
	Omin:	Omax:	Ωbins: 3	

USRBDX → The Result

This is true only if the surface area is explicitly given

Evolution of charged hadron spectra at the various surfaces post-processed results are normalized to GeV⁻¹ cm⁻² per primary

From post-processing we get **single** differential spectra since we asked for one angular bin only



USRBDX → The Result

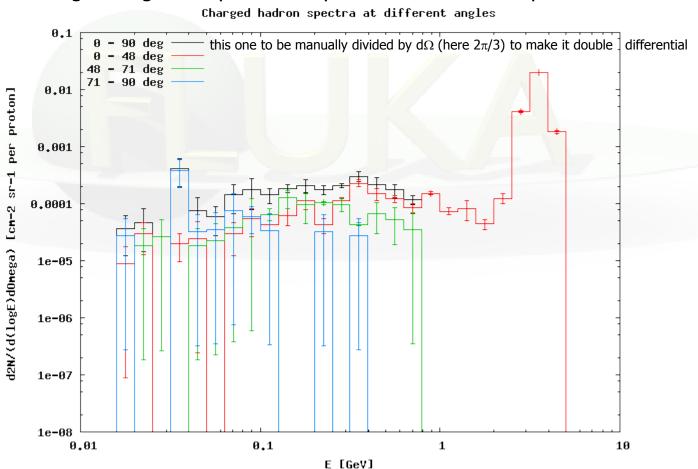
This is true only if the surface area is explicitly given

20

Double differential charged hadron spectra for consecutive solid angle portions results are normalized to GeV⁻¹ sr⁻¹ (cm⁻²) per primary

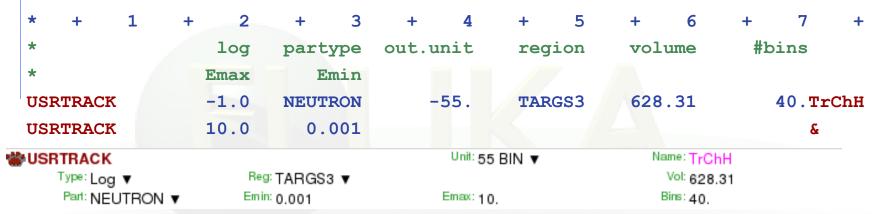
From post-processing we get **double** differential spectra since we asked for more than one angular bin,

but the angle-integrated spectrum is provided as well on top



USRTRACK

• Calculates differential fluence as a function of energy by scoring tracklength in a given region. Results are normalized to *GeV*¹ *cm*⁻² *per primary* if the region volume is provided (otherwise should be intended as *GeV*¹ *cm per primary*, i.e. differential track-length)



- remember: USRBDX scores on a surface, while USRBIN scores fluence in volumes and gives no differential information
- WHAT(4) = @ALLREGS activates scoring over all regions

USRYIELD

- Scores a double-differential particle yield across a boundary surface or at interaction points
- "Energy-like" quantities

```
Kinetic energy , total momentum , total energy , longitudinal momentum in the lab frame , longitudinal momentum in the c.m.s. frame
```

"Angle-like" quantities

```
Rapidity in the lab frame , rapidity in the c.m.s. frame , pseudorapidity in the lab frame , pseudorapidity in the c.m.s. frame , Feynman-x in the lab frame , Feynman-x in the c.m.s. frame , transverse momentum , transverse mass , polar angle (*) in the lab frame , polar angle (*) in the c.m.s. frame , square transverse momentum , charge , weighted angle in the lab frame , weighted transverse momentum
```

USRYIELD

WARNING!! calculating a cross section has no meaning in case of a thick target.

option USRBDX calculates angular distributions WITH RESPECT TO THE NORMAL to the boundary at the point of crossing, USRYIELD's distributions are calculated WITH RESPECT TO THE BEAM DIRECTION, as defined by BEAMPOS (or a different direction specified with SDUM=BEAMDEF).

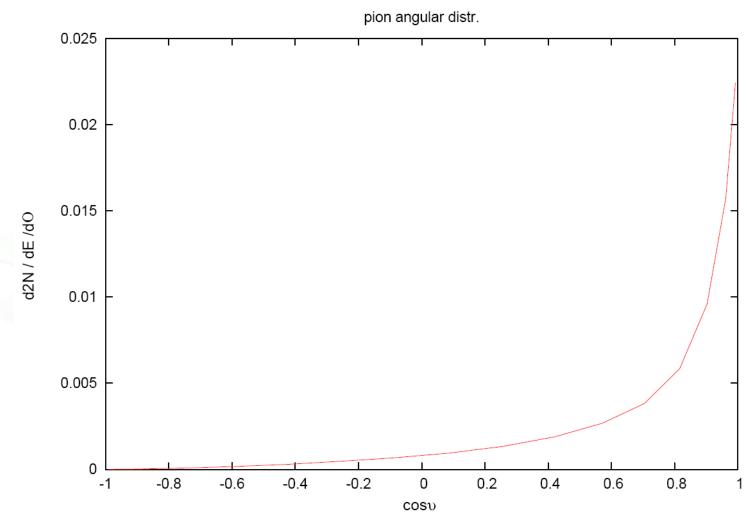
```
124 = 24 + 1 * 100 => polar angle (in degrees) and kinetic energy
                                     out.unit
                                                      Reg1
                                                                 Reg2
                                                                             Norm
                                       #Abins
                                                     Emax
                                                                 Emin dbl.differential
                               Amin
                    Amax
                  124.0 PIONS+- -57. TARGS3
 USRYTELD
                                                                 INAIR
                                                                              1.0YieAng
                                0.0
                                        18. 10.0
                                                               0.0
                                                                              3.0&
 USRYIELD
                  180.0
                         Type: Yield ▼
WUSRYIELD
                                                 Unit: 57 BIN ▼
                                                                       Name: Yie And
                                                                       Norm: 1.0
       ie:Polarθ lab deg ▼
                         ia:Ek in GeV ▼
                                               <sup>Log:</sup>Linear ▼
     Part: PIONS+- ▼
                                               Reg: TARGS3 ▼
                         Yield: ▼
                                                                      to Reg: INA R ▼
     Min1: 0.0
                         Max1: 180.0
                                               Nbins1: 18.0
     Min2: 0.0
                         Max2: 10.0
                                                Kind: d2N/dx1dx2 ▼
```

Only one interval is possible for the second variable, BUT results are normalized as Double Differential (in this case, charged pions GeV⁻¹ sr⁻¹ per primary) **WARNING!!**

Use WHAT(6) = 3 for plain double differential yield, the DEFAULT is plain double-differential cross section !! 23

USRYIELD -> The Result

pion angular distribution



Standard Postprocessing Programs

- To analyze the results of the different scoring options, several programs are made available
- The most natural ones are kept in \$FLUPRO/flutil.
- They assume that the <u>estimator files are unformatted</u>, and can calculate standard deviations and average values over many cycles:
 - ustsuw.f to analyze USRTRACK and USRCOLL outputs
 - usxsuw.f to analyze USRBDX outputs
 - usysuw.f to analyze USRYIELD outputs
 - usbsuw.f to analyze USRBIN outputs
 - usrsuw.f to analyze RESNUCLEi outputs
- Each of these programs (except usbsuw) produces three files:
 - a text file with extension _sum.lis which contains averaged distributions, standard deviations, cumulative (integral) quantities
 - an unformatted file which can replace the N unformatted estimator files in further postprocessing
 - a text file with extension _tab.lis to be easily readout by graphics codes

[Simpler programs are also provided in the manual, as guide for users who would like to write their own analysis program].

Standard Postprocessing Programs

Example of sum.lis from USRYIELD

```
Detector n: 1 YieAng
(User norm: 1.
sigma: 1. mb
distr. scored: 209 , PIONS+-
from reg. 4 to reg. 5)
linear 1st variable (x1) binning from 0.0000E+00 to 3.1416E+00 18 bins
(1.7453E-01 wide)
2nd variable (x2) ranges from 0.0000E+00 to 1.0000E+01
1st variable (x1) is: Laboratory Angle (radians)
2nd variable (x2) is: Laboratory Kinetic Energy
The scored double differential yield is (normalized per primary particle):
plain d2 N / dx1 dx2 where x1, x2 are the first and second variables
```

Tot. response (integrated over x1) 2.6339998E-02 +/- 3.883959 %

WARNING!! The Tot. response is NOT integrate over the second quantity !! in this case it turns out to be *particles/GeV per primary* (to be multiplied by the energy width interval of 10GeV)

Standard Postprocessing Programs

Example of tab.lis for USRYIELD

```
# Detector n: 1 YieAng # N. of x1 intervals 18
```

Thetamin	Thetamax	Result	Error (%)
0.000000	0.1745329	2.0742605E-02	10.87912
0.1745329	0.3490658	1.4 <mark>4</mark> 63779E-02	10.65940
0.3490658	0.5235988	9.8084798E-03	7.649231
0.5235988	0.6981317	5.8580171E-03	4.966214
0.6981317	0.8726646	3.8220894E-03	10.60832
0.8726646	1.047198	2.6973977E-03	5.450788

. . .

FILTERS: AUXSCORE

There is the possibility to filter the estimators, restricting the scoring to a selected subset of particles.

For instance: USRBIN energy deposition by muons only:

	*	+	1	+	2	+	3	+	4	+	5	+	6	+	7	+	
	USR	BIN		1	1.0	ENE	RGY	-4	0.0	1	0.0			1	5.0 T a	rgEne	<u> </u>
	USR	BIN			0.0		†	_	5.0	10	0.0			20	3 0.0		
	AUX	SCORE	2	USR	BIN	MU	ONS			Targ	Ene	Targ	Ene				
-	USR	BIN							Uni	t: 40 BIN	▼		Name	TargEn	e		
		Type: R-	Ф-Z ▼		Rm	in: 0	\		Rma	C 10			NB	100			
		Part: EN	NERGY	•		X:	\	\	,	Y:			NΦ	:			
					Zm	in: -5.0		\	Zma	C15.0			NZ	200			
7	AUX	SCORE	E		Тур	∞:USRE	BIN ▼		Par	t: MUON:	S▼		Set	: ▼			
_		Delta: ▼			D	et: TargE	ne ▼	\	to De	t:TargEn	e ▼		Step):			

Assign the "muons" filter to the USRBIN estimator named TargEne

WARNING!!

In reality energy is eventually deposited by electrons only.

This way it is retained the fraction due to ionization by muons, in fact depending on the arbitrary delta ray threshold

FILTERS: AUXSCORE

Another example: score the yield of 56-Iron ions (very useful: there is no separate name for each ion specie, except light ones. HEAVYION score all isotopes heavier than alpha's together!)

```
124.0
                                                       -87.
                                                                                                     1.0Fe56
                                 ALI - PART
                                                                  TARGS3
 USRYIELD
                                                                                   INAIR
                                                        18.
                                                                                                     3.0&
                       180.0
                                         0.0
                                                                     10.0
                                                                                     0.0
 USRYIELD
                   USRYIELD -5602600.
                                                                     Fe56
                                                                                    Fe56
 AUXSCORE
USRYIELD
                              Type: Yield ▼
                                                          Unit: 87 BIN ▼
                                                                                      Name: Fe56
                                 ia:Ekin GeV ▼
                                                           <sup>Log:</sup>Linear ▼
                                                                                      Norm: 1.0
        ie: Polar θ lab deg ▼
      Part: ALL-PART ▼
                              Yield: ▼
                                                          Reg: TARGS3 ▼
                                                                                     to Reg: INAIR ▼
                                                        Nbins1: 18.0
     Mint: 0.0
                              Max1: 180.0
     Min2: 0.0
                              Max2: 10.0
                                                          Kind: d2N/dx1dx2 ▼
                                                                                       Mat: 🔻
                              Type: USRYIELD ▼
                                                          Part: 🔻
   UXSCORE
                                                                                        Set: 🔻
     Delta: 🔻
                                 Z: 26
                                                            A: 56
                                                                                     lsomer: n
                                Det: Fe56 ▼
                                                         to Det: Fe56 ▼
                                                                                       Step:
```

The requested ion is coded in what(2) according to its **A**, **Z** and (optionally) isomeric state **m**:

what(2) =
$$-(100*Z + 100000*A + m*100000000)$$

Z,A,m=0 means all , e.g. $-2600 ==$ all Iron isotopes

Built-in Conversions and AUXSCORE

For some quantities, there is the possibility to get built-in conversions, without the need for user routines: done with generalized particles

For example:

SI1MEVNE Silicon 1 MeV-neutron equivalent fluence

DOSE-EQ Dose Equivalent (pSv)

The set of conversion coefficients used to calculate DOSE-EQ can be selected by the user among a list (see manual) with AUXSCORE:



Scores equivalent dose by folding the particle fluences with the "AMB74" conversion coefficients