

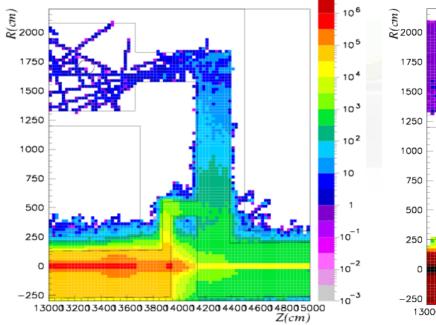
Simulation Optimization

Advanced FLUKA Course

Concept

 Variance reduction techniques in Monte Carlo calculations reduce the computer time or the opposite to obtain results of sufficient precision in the phase-space region of interest.

 Remember: that precision is not the only requirement for a Good Monte Carlo calculation. Even a zero variance calculation cannot accurately predict natural behavior if other sources of error are not minimized.



No Bias and no maze

Region Biasing + maze

Is optimization necessary?

- Visual inspection of histograms (specially 2D maps) is a powerful way to determine if simulations have NOT converged in the area of interest. Big fluctuation in colors between neighboring voxels warn of potential systematic errors.
- However, even in smooth 2D histograms lack of convergence may be present, e.g.:
 - If the scoring scale spans over many orders of magnitude significant differences may are hard to spot
 - 2-step simulations may give a false sense of convergence if first step has not converged but 2nd step has. Plot also maps for the 1st step!
 - Relatively smooth maps may have some 'hard'-tracks overlaid typically indicating strong energy dependent weight dispersion

Monte Carlo Flavors

	Microscopic Analog	Microscopic Biased	Macroscopic Analog
Physics Models	Theoretical	Theoretical	Parameterizations
PDF sampling	Physical processes	Artificial distributions	Fits & Data
Predict Average	Yes	Yes	Yes
Predict Higher Moments	Yes	-	-
Preserves Correlations	Yes	-	-
Reproduces Fluctuations	Yes	-	-
Rare events	-	Yes	-
Predictability	Yes	Yes	-
Convergence	Slow	Fast privileged regions	Fast
Safe	Yes	Almost	-

Analog vs. Biased - 1

Analog Monte Carlo

- samples from actual phase space distributions
- predicts average quantities and all statistical moments of any order
- preserves correlations and reproduces fluctuations (provided the physics is correct...)
- is (almost) safe and can (sometimes) be used as "black box"

BUT

- is inefficient and converges very slowly
- fails to predict important contributions due to rare events

Analog vs. Biased - 2

Biased Monte Carlo

- samples from artificial distributions and applies a weight to the particles to correct for the bias
- predicts average quantities, but not the higher moments (on the contrary, its goal is to minimize the second moment)
- same mean with smaller variance, i.e., faster convergence

BUT

- cannot reproduce correlations and fluctuations
- requires physical judgment, experience and a good understanding of the problem (it is not a "black box"!)
- in general, a user does not get the definitive result after the first run, but needs to do a series of test runs in order to optimize the biasing parameters



Figure of Merit

Computer cost of an estimator

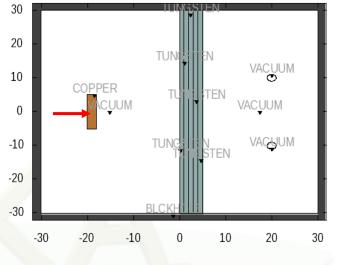
$$FOM = \sigma^2 \times t$$

$$\sigma^2 = \text{Variance } \propto 1/N, \quad t = \text{CPU time } \propto N$$

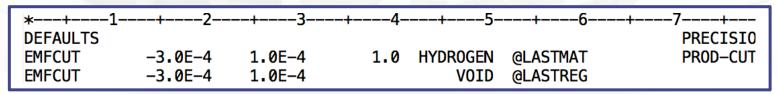
- some biasing techniques are aiming at reducing the σ^2 , others at reducing t
- often reducing σ^2 increase t, and vice versa
- therefore, minimizing $\sigma^2 \times t$ means to reduce σ at a faster rate than t increases, or vice versa
- ⇒ the choice depends on the problem, and sometimes a combination of several techniques is most effective
- bad judgment, or excessive "forcing" on one of the two variables, can have catastrophic consequences on the other one, making computer cost "explode"

Figure of Merit - Example

- 5 MeV/c e⁻ beam on 2-cm long 4 cm radius Cu disk
- 1 cm radius sphere detector (scoring ¹⁰ total fluence) 10 cm off-axis, 20 cm ⁰ behind a 5 cm thick W shielding, ¹⁰ which is in turn 20 cm away from ²⁰ the target

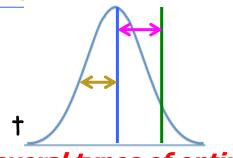


Analogue simulation



- Used 8 detectors at equivalent locations to (symmetry)
- Analogue: N = 1E6; t = 217s; FOM \approx 3.6E-10; $\sigma/\mu \approx$ 57%

Optimization strategies and cost



Optimization consists in focusing CPU use towards the area of interest so that statistical error is reduced with minimal no increase of systematic errors

Several types of optimization...

No biasing: no/insignificant systematic error, preserves correlations

Code & optimization: e.g. less use of memory: use 2D USRBIN in stead of 3D, read data at initialization, ...

Geometry optimization: Choice of body types, definition of geometry logics, number of neighboring regions (avoid NAS>>), avoid unnecessary/excessive transformation directives

Scoring/transport choice: energy deposition or fluence, *single scattering vs. multiple scattering, run-time processing

Biasing M1: Energy thresholds, blackhole outside of region of interest, detail of geometry, number of processes considered (e.g. neglect photonuc for hadron beams), granularity of scoring histograms...

Biasing Mn (n>1): Importance biasing, LAM-BIAS, EMF-BIAS

Biasing Techniques

FLUKA offers the following possibilities for biasing

- Importance Biasing (BIASING)
- Weight window (WW-FACTOr, WW-THRESh, WW-PROFIle)
- Leading Particle Biasing (EMF-BIAS)
- Multiplicity Tuning (BIASING)
- Biased down scattering for neutrons, only for experts (LOW-DOWN)
- Non analogue absorption (LOW-BIAS)
- Biasing Mean free paths (LAM-BIAS)
- User defined biasing (usbset.f, usimbs.f)

Other optimization checks

CPU intensive consuming physics options and uses

User written biasing

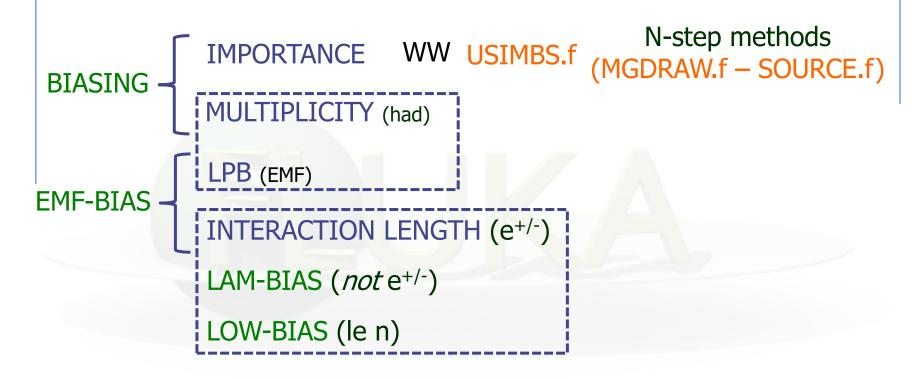
FLUKA offers the following routines for user-written biasing

- ubsset.f: User BiaSing SETting
 - called after reading in the input file and before the first event
 - allows to alter almost any biasing weight on a region-dependent basis
- usimbs.f: USer defined IMportance BiaSing
 - if activated, called at every particle step
 - allows to implement any importance biasing scheme based on region number and/or phase space coordinates
- udcdrl.f: User defined DeCay DiRection biasing and Lambda
 - only for neutrinos emitted in decays: bias the direction of emitted neutrino

Not biasing by itself, but it could be used for generating biased runs

- source.f: User written source
 - to sample primary particle properties from distribution in space, energy, time...

Summary Biasing Techniques



Reduce memory / check requirements
Use *physics process* and *thresholds* relevant to the problem

Importance Biasing

- Importance biasing combines two techniques:
 - Surface splitting: Reduces σ but increases t
 - Russian roulette: which does the opposite
- It is the simplest, most safe and easiest to use of all biasing
- The user assigns a relative importance to each geometry region (the absolute value doesn't matter) based on:
 - expected fluence attenuation with respect to other regions
 - probability of contribution to score by particles entering the region
- Importance biasing is commonly used to maintain a constant particle population, compensating for attenuation due to absorption or distance.
- In FLUKA it can be tuned per type of particle

Importance biasing - 2

Surface Splitting

A particle crosses a region boundary, coming from a region of importance I_1 and entering a region of *higher* importance $I_2 > I_1$:

- the particle is replaced on average by $n=I_2/I_1$ identical particles with the same characteristics
- the weight of each "daughter" is multiplied by I₁/I₂

If I_2/I_1 is too large, excessive splitting may occur with codes which do not provide an appropriate protection .

An internal limit in FLUKA prevents excessive splitting if I_2/I_1 is too large (> 5), a problem found in many biased codes.

Importance biasing - 3

Russian Roulette

A particle crosses a region boundary, coming from a region of importance I_1 and entering a region of *lower* importance $I_2 < I_1$:

- the particle is submitted to a random survival test: with a chance I_2/I_1 the particle survives with its weight increased by a factor I_1/I_2
- with a chance (1 I₂/I₁) the particle is killed

Importance biasing is commonly used to maintain a uniform particle population, compensating for attenuation due to absorption or distance. In FLUKA it can be tuned per particle type.

Importance biasing - 4

Note:

In FLUKA, for technical reasons, importances are internally stored as integers. Therefore, importances can only take values between 0.0001 and 100000. An input values 0.00015 is read as 0.0001, 0.00234 is read as 0.0023, etc.

There is also a user routine **USIMBS** which allows to assign importances not only at boundaries, but at each step, according to any logic desired by the user (as a function of position, direction, energy,...).

Very powerful, but *time-consuming* (it is called at each step!). The user must balance the time gained by biasing with that wasted by calls.

Importance biasing – 5

BIASING 0.0 0.0 4.64 8. 18. 2.PRINT

| BIASING | Type: ▼ | RR: | Imp: | Imp: | Step: | Step:

The meaning of WHAT(1)...WHAT(6) and SDUM is different depending on the sign of WHAT(1):

```
If WHAT(1) >= 0.0 :

WHAT(1) specifies the particles to be biased

= 0.0 : all particles
= 1.0 : hadrons and muons
= 2.0 : electrons, positrons and photons
= 3.0 : low energy neutrons

WHAT(2) = (see multiplicity tuning)

WHAT(3) = region importance (Default = 1.0)
Allowed values range from 0.0001 to 100000.
```

Importance biasing - 6

```
If WHAT(1) >= 0.0:
     WHAT (4) = lower bound of the region indices/names (Default = 2.0)
     WHAT (5) = upper bound of the region indices/names (Default = WHAT(4))
     WHAT (6) = step length in assigning indices (Default = 1.0)
                             importance biasing counters are printed
               = PRINT :
      SDUM
                             counters are not printed
               = NOPRINT:
                              (cancels any previous PRINT request)
                             importance biasing
               = USER:
                              according to the user defined routine USIMBS
                             reset to default (cancels any previous USER request)
               = NOUSER:
                             multiplicity biasing for primary particles only
               = RRPRONLY:
                             ignored
               = (blank):
```

(Default: NOPRINT, NOUSER, multiplicity biasing for all generations)

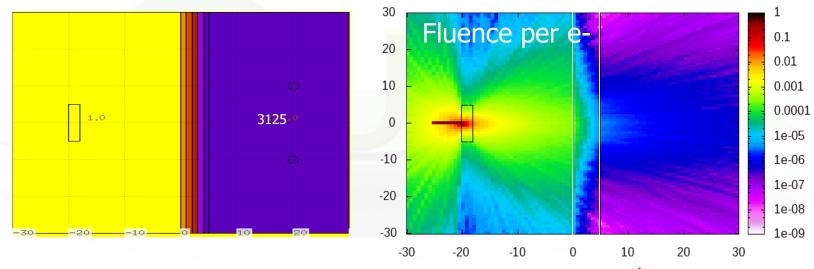
Importance biasing - 7

```
2.0
                             0.0
                                      10.0
                                                  7.0
                                                                       2.0
BIASING
                                                            11.0
                  2.0
                             0.0
                                      15.0
                                                  8.0
                                                             9.0
                                                                       0.0
BIASING
                 -1.0
                             0.0
                                       3.0
                                                  4.0
                                                             0.0
                                                                       0.0
BIASING
```

```
If WHAT (1) < 0.0:
       WHAT(1): flag indicating that all region importances shall be
               modified by a particle-dependent factor
     WHAT(2) >= 0.0 : modifying factor M
             < 0.0 : M is reset to the default value 1.0
     WHAT(3) = lower bound of the particle indices/names (Default: = 1.0)
     WHAT (4) = upper bound of the particle indices/names
                (Default: = WHAT(3) if WHAT(3) > 0, all particles otherwise)
     WHAT (5) = step length in assigning particle indices (Default: 1.0)
     WHAT(6) = not used
                            importance biasing is applied also to primaries
     SDUM
             = PRIMARY :
                            importance biasing is applied only to secondaries
               NOPRIMARy :
            Default = PRIMARY
```

Importance Biasing – Example

- (same example as in slide <u>8</u>)
- The 5 cm tungsten wall is segmented in 5 x 1-cm slabs
- Importance is set to 1 to the left of the wall, then increased by x5 in each layer of the wall

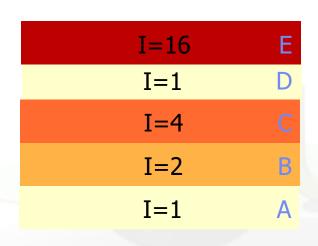


- Analogue: N = 1E6; t = 217s; $FOM \approx 4E-10$; $\sigma/\mu \approx 60\%$
- IB: N = 2E5; t = 232s; FOM = 5.4E-12; $\sigma/\mu = 7\%$

 $4E-10/1.3E-11 \approx 75 \text{ times "faster"}$

Importance Biasing – 8: Problems 1

 In complex geometries, it may be hard to keep track of all importances in every region



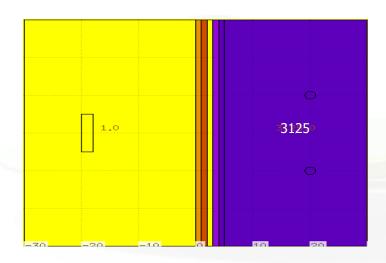
When going from C to D 75 % of the particles are killed!! – waste of previous tracking effort (then the remaining particles entering E are split in an average of max(16/1,5) = 5 copies)

Backscattered particles going from D to C will be split into 4 copies! – unnecessary!

 To avoid such 'cold spots', it is helpful to plot importances. This can be performed with Flair>Geoviewer

Importance Biasing – Example (2)

- (continuation of slide 21)
- Cold spot in importance biasing



Max(1/25, 1/5) = 0.2

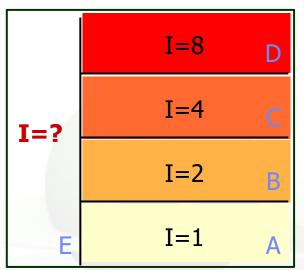
→ 80% of the population is killed when moving from the 2nd to the 3rd layer of the wall

- Analogue: N = 1E6; t = 217s; $FOM \approx 4E-10$; $\sigma/\mu \approx 60\%$
- IB: N = 3E5; t = 232s; FOM = 5.4E-12; $\sigma/\mu = 7\%$
- IB (cold spot): N = 1E6; t = 292s; FOM = 5.1E-11; $\sigma/\mu = 21\%$

≈ **10** times "slower"

Importance Biasing – 8 : Problems 2

 Although important biasing is relatively easy and safe to use, there are a few cases where caution is recommended



Which importance shall we give to region E? Whatever value we choose we will get an inefficient splitting/RR at some of the boundaries.

- Another case is that of splitting in vacuum (or air). Splitting daughters are strongly correlated. It must be made sure that their further histories are differentiated enough to forget their correlation.
- The above applies in part also to muons (the differentiation provided by multiple scattering and by Landau *dE/dx* fluctuations is not always sufficient).

usimbs.f: User Defined Importance Biasing

- Typical problem: Spend a lot of time to write the problem input, geometry and on the first runs you realize that statistics are not good
- First method (and safest) is to introduce region importance biasing. In FLUKA you can introduce it with two ways:
 - 1st Manually slice the geometry and increase the number of regions.
 Modifying an existing geometry to introduce biasing can be a very cumbersome process
 - 2nd Introduce the "importance biasing" information with a user fortran routine independent of the regions defined in the geometry
- Routine: usimbs.f

USer defined IMportance BiaSing

Allows to implement any importance biasing scheme based on region number and/or phase space coordinates

usimbs.f: User Defined Importance Biasing

- Enable the call to USIMBS routine with the BIASING card:
 - WHAT(1) Particles to be biased
 - WHAT(2) and WHAT(3) \neq 1.0

- (Any value \neq 1.0)
- WHAT(4) Lower bound of region
- WHAT(5) Upper bound of region
- WHAT(6) Step
- SDUM = USER



Remember:

- If WHAT(3)=1 for a region, the routine will not be called during tracking of particles inside that region
- Cannot have both normal importance BIASING with cards and the routine at the same time

usimbs.f - Routine

The routine is called on every particle step! WARNING: can slow down the execution speed! Use with caution.

Input:

- Region information at the beginning and end of the step
- X,Y,Z coordinates through the TRACKR dommon.

X, Y, Ztrack(0) X, Y, Ztrack(Ntrack) Beginning:

End:

Particle type and Energy could be used for even more advanced biasing schemes

Output:

The routine must return the importance ratio to the new position (end/beginning) in the variable FIMP < 5.0

Entry: USIMST

Split the particles step between interactions in half (or any other user defined value)

```
SUBROUTINE USIMBS ( MREG, NEWREG, FIMP )
     INCLUDE '(DBLPRC)'
     INCLUDE '(DIMPAR)'
     INCLUDE '(IOUNIT)'
     USer defined Importance BiaSing:
                  02 july 2001
     Created on
                                         Alfredo Ferrari & Paola Sala
                                                     Infn - Milan
     Last change on 09-jul-01
                                         Alfredo Ferrari
                                   by
     Input variables:
                 Mreg = region at the beginning of the step
              Newreg = region at the end of the step
     (thru common TRACKR):
               Jtrack = particle id. (Paprop numbering)
               Etrack = particle total energy (GeV)
       X,Y,Ztrack(0) = position at the beginning of the step
  X,Y,Ztrack(Ntrack) = position at the end of the step
    Output variable:
                 Fimp = importance ratio (new position/original one)
     INCLUDE '(TRACKR)'
     FIMP
            = ONEONE
     RETURN
     Entry USIMST:
     Input variables:
                 Mreg = region at the beginning of the step
                 Step = length of the particle next step
    Output variable:
                     = possibly reduced step suggested by the user
     ENTRY USIMST ( MREG, STEP )
     IF ( STEP .GT. ONEONE ) STEP = HLFHLF * STEP
     RETURN
*=== End of subroutine Usimbs
                                                          26
     END
```

usimbs.f – Important Notes

- The routine has only a relative effect on the weight of the particle
 ⇒ Beam particles can have any weight.
- Importance ratio will be limited by WW-THRESh card
- The Russian Roulette / Splitting will take place at the middle (defined by the ENTRY) of the step, and not on a fixed region boundary.
- The biasing position will be a little fuzzy depending on the particle step. This has a visible effect when it is applied to low density materials (i.e. air)
- Results will be similar, but not the same as with the manual region biasing.
- It is a great time saver for complex geometries, as well different biasing schemes
- Combined with the particle type and energy could become very powerful

usimbs.f: Simple Example

 Biasing a factor of 2 every 50 cm on the Z direction from 100 cm to 500 cm

```
Initial position
  ZSTART = ZTRACK(0)
   IF (ZSTART .LT. 100.0D0) THEN
        FSTART = ONEONE
   ELSE IF (ZSTART .GT. 500.0D0) THEN
        FSTART = TWOTWO ** NINT((500.0D0-100.0D0)/50.0D0)
   FI SF
        FSTART = TWOTWO ** NINT((ZSTART-100.0D0)/50.0D0)
   ENDIF
                                     Final position
   * Similarly calculate the FEND from ZEND
                                   Importance Ratio
  FIMP = FEND / FSTART \leftarrow
```

usimbs.f: Function example

• Introduce an importance biasing assuming an exponential law of attenuation in the R direction $exp(-\lambda \times R)$, for R>1cm

```
RSTART = SQRT(XTRACK(0)**2 + YTRACK(0)**2 + ZTRACK(0)**2)
REND = SQRT(XTRACK(NTRACK)**2 + YTRACK(NTRACK)**2 +
     ZTRACK(NTRACK)**2)
IF (RSTART .LT. ONEONE) THEN
     FSTART = ONEONE
ELSE
     FSTART = EXP(-ALAMBDA * RSTART)
FNDIF
IF (REND .LT. ONEONE) THEN
     FEND = ONEONE
ELSE
     FEND = EXP(-ALAMBDA * REND)
ENDIF
FIMP = FSTART / FEND
```

Card: EMF-BIAS

N-step method

2-step method explained in sources lecture

- Events from one run are dumped in a file (mgdraw.f)
 and used as starting particles through source.f routine
- This method is similar to importance biasing, as (selected) particles crossing a given interphase are sampled many times in the next step, which is equivalent to splitting them

Card: EMF-BIAS

Leading Particle Biasing - 1

- Leading Particle Biasing is available only for e+, e- and photons
- It is generally used to avoid the geometrical increase with energy of the number of particles in the electromagnetic shower
- It is a characteristic of EM interactions that
 2 particles are present in the final state
- if LPB is activated only one is randomly retained and its weight is adjusted so as to conserve weight × probability
- The most energetic of the two particles is kept with higher probability (as it is the one which is more efficient in propagating the shower)
- LPB is reducing t, but increases σ by introducing large weight fluctuations. Therefore is should nearly always be backed up by WW
- Very useful for shielding calculations at both electron and proton accelerators

Leading Particle Biasing - 2

```
1022.
                               0.
                                       5.E-4
                                                    16.
                                                                20.
EMF-BIAS
                                                                            2.LPBEMF
Type: LPBEMF ▼
                                              Ethr e-e+:
                                                                        Ethr y:
                                              Pair Prod.: off ▼
Old bremss.: off ▼
                  Bremsstrahlung: off ▼
                                                                   e+ ann @rest: off ▼
                   Bhabha&Moller: off ▼
                                           Photo-electric: off ▼
  Compton: off ▼
                                                                  e+ ann @flight: off ▼
                           Reg: 🔻
                                                to Reg: 🔻
                                                                         Step:
For SDUM = LPBEMF (default):
      WHAT(1) > 0.0: leading particle biasing (LPB) is activated
                WHAT (1) = 2^{0} \times b0 + 2^{1} \times b1 + 2^{2} \times b2 + 2^{3} \times b3 + 2^{4} \times b4 +
                             2^{5} \times b5 + 2^{6} \times b6 + 2^{7} \times b7
                   (b0 = 1 : LPB for bremsstrahlung and pair production)
                    b1 = 1 : LPB for bremsstrahlung
                    b2 = 1 : LPB for pair production
                    b3 = 1 : LPB for positron annihilation at rest
                    b4 = 1 : LPB for Compton scattering
                    b5 = 1 : LPB for Bhabha & Moller scattering
                    b6 = 1 : LPB for photoelectric effect
                    b7 = 1 : LPB for positron annihilation in flight
                   Note: WHAT(1) = 1022 activates LPB for all physical effects
                    (values larger than 1022 are converted to 1022)
                    (FLAIR uses 254)
```

Leading Particle Biasing - 3

```
1022.
                             0.
                                    5.E-4
                                                 16.
                                                           20.
EMF-BIAS
                                                                       2.LPBEMF
                        Type: LPBEMF ▼
Ethr e-e+:
                                                                    Ethr γ:
                                           Pair Prod.: off ▼
Old bremss.: off ▼
                 Bremsstrahlung: off ▼
                                                               e+ ann @rest: off ▼
                                        Photo-electric: off ▼
 Compton: off ▼
                 Bhabha&Moller: off ▼
                                                              e+ ann @ flight: off ▼
                         Reg: 🔻
                                             to Reg: 🔻
                                                                     Step:
     WHAT(2) > 0.0: energy threshold below which LPB is played for
                       electrons and positrons
                        electrons: kinetic energy
                        positrons: total energy plus rest mass energy
              < 0.0: resets any previously defined threshold to infinity
                       (i.e., LPB is played at all energies, Default)
               = 0.0: ignored
       WHAT(3) > 0.0: energy threshold below which LPB is played for photons
               < 0.0: resets any previously defined threshold to infinity
                       (i.e., LPB is played at all energies, Default)
               = 0.0: ignored
     WHAT (4) = lower bound of the region indices/names (Default = 2.0)
     WHAT (5) = upper bound of the region indices/names (Default = WHAT(4))
                                                                                    33
     WHAT (6) = step length in assigning indices/names (Default = 1.0)
```

Multiplicity tuning - 1

- Multiplicity tuning is meant to be for hadrons what Leading Particle Biasing is for electrons and photons.
- A hadronic nuclear interaction at LHC energies can end in hundreds of secondaries. Thus, to simulate a whole hadronic cascade in bulk matter may take a lot of CPU time.
- Except for the leading particle, many secondaries are of the same type and have similar energies and other characteristics.
- Therefore, it is possible to discard a predetermined average fraction of them, provided the weight of those which are kept and transported be adjusted so that the total weight is conserved (but the leading particle is never discarded).
- The user can tune the average multiplicity in different regions of space by setting a region-dependent reduction factor (in fact, it can even be > 1! But this possibility is seldom used).

Multiplicity tuning - 2

SDUM

1.0 1.0 18. 0.7 8. 1. BIASING BIASING Type: All particles ▼ RR: 1.0 Imp: 0.000189 to Reg: Sphere ▼ Step: 1.0 Opt: 🔻 Reg: Box ▼ WHAT(1) specifies the particles to be biased with WHAT(3) (see before) = 0.0 : all particles = 1.0 : hadrons and muons = 2.0 : electrons, positrons and photons WHAT(2) = RR (or splitting) factor by which the average number of secondaries produced in a collision should be reduced (or increased). (Default = 1.0) – No RR if less than 3 secondaries WHAT(3) = (see importance biasing)WHAT (4) = lower bound of the region indices/names (Default = 2.0) WHAT (5) = upper bound of the region indices/names (Default = WHAT(4)) WHAT (6) = step length in assigning indices/names (Default = 1.0)

= RRPRONLY: multiplicity biasing for primary particles only

= (blank): ignored (Default)

Cards: LAM-BIAS

Biasing mean free paths - 1

Decay lengths:

- The mean life/average decay length of unstable particles can be artificially shortened.
- It is also possible to increase the generation rate of decay products without the parent particle actually disappearing.
- Typically used to enhance statistics of muon or neutrino production.
- The kinematics of the decay can also be biased (decay angle).

Biasing mean free paths - 2

 LAM-BIAS
 Type: GDECAY ▼
 × <λ>:
 × λ inelastic:

 Mat: ▼
 Part: ▼
 to Part: ▼
 Step:

for SDUM = GDECAY:

- WHAT(1): mean decay length (cm) of the particle in the laboratory frame is set = |WHAT(1)| if smaller than the physical decay length (otherwise it is left unchanged).
 - < 0.0 : At the decay point Russian Roulette (i.e. random choice) decides whether the particle actually will survive or not after creation of the decay products. The latter are created in any case and their weight adjusted taking into account the ratio between biased and physical survival probability.</p>
 - > 0.0 : Let P_u = unbiased probability and P_b = biased probability: at the decay point **the particle always survives with a reduced** weight $W=(1-P_u/P_b)$. Its daughters are given a weight $W=P_u/P_b$ (as in case WHAT(1) < 0.0).

Biasing mean free paths - 3

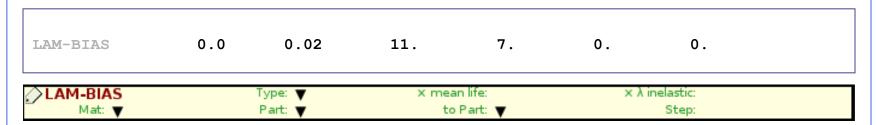
```
1.
                                                         16.
                 -0.5
                                      1.
                                               13.
                                                                    0.
 LAM-BIAS
 LAM-BIAS
                        Type: ▼
                                        × mean life:
                                                              × λ inelastic:
      Mat: 🔻
                        Part: 🔻
                                           to Part: 🔻
                                                                  Step:
for SDUM = blank:
    WHAT(1): the mean life of the particle in its rest frame is reduced
                by a factor |WHAT(1)| (must be \leq 1.0)
                   < 0.0 : (as for SDUM=GDECAY) Russian Roulette
                   > 0.0 : (as for SDUM=GDECAY) the particle always survives
                                                   with a reduced weight
for SDUM = blank or GDECAY
     WHAT (2) and WHAT (3) : (see interaction length biasing)
     WHAT (4) = lower bound of the particle index (Default = 1.0)
     WHAT(5) = upper bound of the particle index
                 (Default = WHAT(4) if WHAT(4) > 0, 46 otherwise)
     WHAT (6) = step length in assigning indices (Default = 1.0)
                                                                                 38
```

Biasing mean free paths - 4

Interaction lengths:

- In a similar way, the hadron or photon mean free path for nonelastic nuclear interactions can be artificially decreased by a predefined particle or material-dependent factor.
- This option is useful for instance to increase the probability for beam interaction in a very thin target or in a material of very low density.
- It is also necessary to simulate photonuclear reactions with acceptable statistics, the photonuclear cross section being much smaller than that for EM processes.

Biasing mean free paths - 5



WHAT(1): (see decay length biasing)

WHAT(2): biasing factor for hadronic inelastic interactions

The hadronic inelastic interaction length of the particle is reduced by a factor |WHAT(2)| (must be ≤ 1.0)

- < 0. : At the interaction point Russian Roulette (i.e. random choice) decides whether the particle actually will survive or not after creation of the secondaries products. The latter are created in any case and their weight adjusted taking into account the ratio between biased and physical survival probability.</p>
- > 0. : At the interaction point **the particle always survives with a reduced weight.** The secondaries are created in any case and their weight adjusted taking into account the ratio between biased and physical survival probability.

Biasing mean free paths - 6

```
0.
                                                                      0.
                 0.0
                          0.02
                                      11.
                                                 7.
LAM-BIAS
 LAM-BIAS
                                         × mean life:
                                                               × λ inelastic:
                        Type: 🔻
    Mat: 🔻
                        Part: 🔻
                                            to Part: 🔻
                                                                    Step:
     WHAT (3): If > 2.0: number of the material to which the inelastic
                                biasing factor has to be applied.
                     < 0.0 : resets to the default a prev. assigned value
                     = 0.0 : ignored if a value has been previously assigned to a specific
                                material, otherwise all materials
                 0.0 < WHAT(3) = < 2.0 : all materials
                 (Default = 0.0)
     WHAT (4) = lower bound of the particle indices/names (Default = 1.0)
     WHAT(5) = upper bound of the particle indices/names
                 (Default = WHAT(4) if WHAT(4) > 0, 46 otherwise)
     WHAT (6) = step length in assigning indices (Default = 1.0)
```

Biasing can be applied to photons and muons if **PHOTONUC** and **MUPHOTON** cards are included.

Weight Windows - 1

- The WW technique is a combination of splitting and RR, but it is based on the absolute value of the weight of each individual particle, rather than on relative region importance
- The user sets an upper and a lower weight limit, generally as a function of region, energy and particle
- Particles having a weight larger than the upper limit are split, those with weight smaller than the lower limit are submitted to RR ⇒ killed or put back "inside the window"
- WW is a more powerful biasing tool than Importance Biasing, but it requires also more experience and patience to set it up correctly
 - "It is more an art than a science" (From MCNP Manual)
- Use of the WW is essential whenever other biasing techniques generate large weight fluctuations in a given phase space region.
- For Low Energy neutrons the energy range should be defined through WW-PROFILe (instead of WW-THRESh)

Weight Windows - 2

Killing a particle with a very low weight (with respect to the average for a given phase space region) decreases t but has very little effect on the score (and therefore on σ)

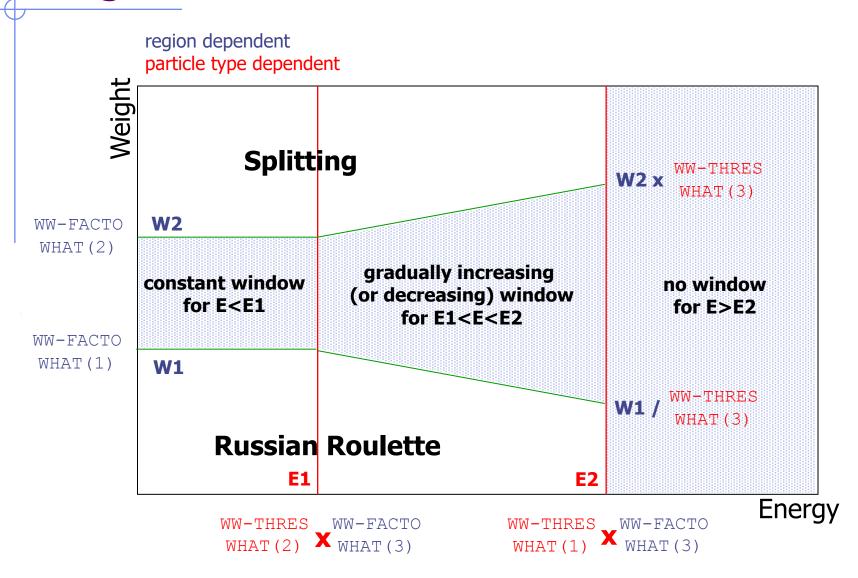
Splitting a particle with a large weight *increases* t (in proportion to the number of additional particles to be followed) but at the same time reduces σ by avoiding large fluctuations in the contributions to scoring.



The global effect is to reduce ott

A too wide window is of course ineffective, but also too narrow windows should be avoided. Otherwise, too much CPU time would be spent in repeated splitting / Russian Roulette. A typical ratio between the upper and the lower edge of the window is about 10. It is also possible to do Russian Roulette without splitting (setting the upper window edge to infinity) or splitting without Russian Roulette (setting the lower edge to zero)

Weight Windows - 3



Card: WW-FACTO

Weight Windows - 4

 WW-FACTO
 13.0
 120.0
 1.5
 27.0
 31.0
 2.0

 WW-FACTO
 RR:
 Split:
 mult f:

 LowE n:
 ▼
 Reg:
 ▼
 Step:

Defines Weight Windows in selected regions

Weight below which *Russian Roulette* is played at the lower energy threshold (set by WW-THRES).

Weight above which *Splitting* is applied at the lower energy threshold (set by WW-THRES).

```
WHAT(3) > 0.0 : Multiplicative factor (Default: 1.0)
= 0.0 : ignored
< 0.0 : resets to 1.0</pre>
```

Factor to be applied to the two energy thresholds for Russian Roulette / Splitting (set by WW-THRES)

Card: WW-FACTO

Weight Windows - 5

< 0.0: resets to 1.0

```
1.5
                13.0
                         120.0
                                               27.0
                                                         31.0
                                                                     2.0
WW-FACTO
                                             Split:
 WW-FACTO
                                                                   mult f:
  LowE n: ▼
                        Reg: 🔻
                                            to Reg: ▼
                                                                   Step:
     WHAT (4) = lower bound of the region indices/names (Default = 2.0)
     WHAT (5) = upper bound of the region indices/names (Default = WHAT(4))
     WHAT (6) = step length in assigning indices/names (Default = 1.0)
               : a number from 1.0 to 5.0 in any position, indicating the low-energy neutron
     SDUM
           weight-window profile to be applied in the regions selected
                  (see WW-PROFI). (Default = 1.0)
              = blank, zero or non numerical: ignored
```

Attention: Option WW-FACTO alone is not sufficient to define a weight window.

One or more WW-THRES cards are also necessary in order to activate the window.

Card: WW-THRES

Weight Windows - 6

2.0 0.05 2.4 3.0 7.0 0.0 WW-THRES WW-THRES E lower: amp f: E upper: Opt: 🔻 Part: 🔻 to Part: 🔻 Step: WHAT(1) > 0.0: upper kinetic energy threshold (GeV) Low-energy neutrons: lower group number (included) = 0.0: ignored < 0.0: any previously selected threshold is cancelled WHAT (2) >= 0.0 and < WHAT (1): lower kinetic energy threshold (GeV) Low-energy neutrons: upper group number (included) < 0.0 or > WHAT(1): WHAT(2) is set = WHAT(1)WHAT (3) > 0.0: amplification factor to define the weight window width at the higher energy threshold represented by WHAT(1). The weight window at the higher energy threshold is obtained by multiplying by WHAT(3) the upper weight limit and by dividing by the same factor the lower

weight limit. (Default = 10.0)

< 0.0: |WHAT(3)| multiplication factor for the lower and upper
weight limits for the particles selected by WHAT(4-6)
(Default = 1.0)</pre>

Card: WW-THRES

Weight Windows - 7

2.0 0.05 2.4 3.0 7.0 0.0 WW-THRES WW-THRES E upper: E lower: amp f: Opt: 🔻 Part: 1 to Part: 🔻 Step: WHAT (4) = lower bound of the particle indices (Default = 1.0) Note that particle index 40 indicates low-energy neutrons (for this purpose only!). Particle index 8 indicates neutrons with energy > 19.6 MeV. WHAT(5) = upper bound of the particle indices (Default = WHAT(4) if WHAT(4) > 0, all particles otherwise) WHAT(6) = step length in assigning indices (Default = 1.0) SDUM = PRIMARY: the weight window applies also to primary particles (default) = NOPRIMARy: the weight window doesn't apply to primaries

0.0 0.0 4.64 8. 18. 2.PRINT BIASING BIASING Type: ▼ RR: Imp: 0.000189 Opt: PRINT V to Reg: ▼ Reg: ▼ Step: FLUKA output file: Hadron importance RR/Splitting counters Reg. # N. of RR <Wt> in <Wt> kil Reg. # N. of RR <Wt> in <Wt> kil Reg. # N. of RR <Wt> in <Wt> kil 1 0.00E+00 0.00E+00 0.00E+00 2 0.00E+00 0.00E+00 0.00E+00 3 1.15E+05 9.31E-01 4.70E-02 Reg. # N. of Sp <Wt> in <Wt> out Reg. # N. of Sp <Wt> in <Wt> out Reg. # N. of Sp <Wt> in <Wt> out 1 0.00E+00 0.00E+00 0.00E+00 2 0.00E+00 0.00E+00 0.00E+00 3 0.00E+00 0.00E+00 0.00E+00 Req. # N. of RR <Wt> in <Wt> kil Req. # N. of RR <Wt> in <Wt> kil Req. # N. of RR <Wt> in <Wt> kil 4 1.36E+04 4.66E-01 1.47E-01 5 8.97E+03 3.22E-01 1.06E-01 6 6.03E+03 2.16E-01 7.10E-02 Reg. # N. of Sp <Wt> in <Wt> out Reg. # N. of Sp <Wt> in <Wt> out Reg. # N. of Sp <Wt> in <Wt> out 5 9.25E+04 6.80E-01 5.23E-01 6 8.24E+04 4.65E-01 3.55E-01 4 1.01E+05 9.99E-01 7.64E-01 "N. of RR" --> Number of FLUKA particles entering a region and which are not split (i.e., particles undergoing Russian Roulette as well as neither Russian Roulette nor splitting) "<\table t> in" --> Average weight of these particles "<Wt> kil" --> Average weight of particles killed after being submitted to Russian Roulette "N. of Sp" --> Number of FLUKA particles entering the region and which are split "<\table t> in" --> Average weight of these particles "<Wt> out" --> Average weight of particles after being submitted to splitting

where

- B/A = average weight of the particles entering the region
- Note -1: RR and splitting arising from Weight-Window biasing (options WW-FACTOR, WW-THRESh, WW-PROFI) or from multiplicity biasing (WHAT(2) in option BIASING) are not accounted for in the counters.
- Note 2: Separate counters are printed for hadrons/muons, electrons/photons and low-energy neutrons (referring to importance biasing requested by BIASING, respectively, with WHAT(1) = 1.0, 2.0 and 3.0, or = 0.0 for all).

Strategy:

1. run without any biasing and print counter, e.g.,

BIASING 0.0 1.0 1.0 9. PRINT

2. analyze counter and adjust region importance biasing, *e.g.*, according to the inverse of the attenuation in shielding, add other biasing, *e.g.*, leading particle biasing run and print counter again

```
0.0
                     1.0
                               1.0
                                                  9.
BIASING
                                                            PRINT
            0.0
                     1.0
                              1.47
BIASING
            0.0
                     1.0 2.15
BIASING
                     1.0
            0.0
                             3.16
BIASING
BIASING
            0.0
                     1.0
                            4.64
            0.0
                     1.0
                              4.64
BIASING
```

3. analyze counter, select Weight Windows (WW-THRES, WW-FACTO) around average weights and perform final (high-statistics) run

Alternative Strategy:

1. Include USERDUMP card in input file to activate call to mgdraw.f

```
USERDUMP 100.0 25.0 4.0 1.
```

2. Edit mgdraw.f (bxdraw) to print energy and weight of particles (filter by particle if wanted) entering specific areas of the geometry, e.g.

```
IF ( .NOT. LFCOPE) THEN
    LFCOPE = .TRUE.
    OPEN (UNIT = 86, FILE = "tuneWW.dat", STATUS = "UNKNOWN")
END IF
. . .
IF (MRGNAM.eq."OLDCELL".and.NRGNAM.eq."NEWCELL".and.jtrack.eq.3) THEN
    write(86,*)wtrack, etrack
END IF
```

- 3. Produce scatter plot weight(E) by loading file "tuneWW.dat" in gnuplot gnuplot> plot 'tuneWW.dat' using 2:1
- 3. Tune WW accordingly

Cards: LOW-BIAS

Non analogue absorption

- Implemented in most low-energy neutron transport codes, where at each neutron collision the neutron always survives with its weight multiplied by the physical survival probability σ_s/σ_τ
- In FLUKA there is an additional choice: the user can force the neutron absorption probability to take an arbitrary value, preassigned on a region-by-region basis as a function of energy. The neutron weight is properly normalized by the code accordingly.

When and How

- A smaller survival probability is often assigned to thermal neutrons to limit the number of scatterings in non-absorbing media
- Also very useful in materials with unusual scattering properties (e.g. Iron)
- Survival probabilities too small with respect to the physical one σ_s/σ_τ may introduce large weight fluctuations due to the very different number of collisions suffered by individual neutrons. In these cases a WW should be applied.
- Also called survival biasing

Card: RADDECAY [1/2]

```
* 1) request radioactive decays
RADDECAY
                       1.0
                                                  3.0
                                                                   0000099999
                                                                                             0
RADDECAY
                                 Decays: Active ▼
                                                                                                       3.0
                                                             Patch Isom:
                                                                         Ŧ
                                                                                              Replicas:
    h/u Int: ignore ▼
                                 h/µ LPB: ignore ▼
                                                                        ignore ▼
                                                                                                       ignore ▼
                                                               h/u WW:
                                                                                              e-e+ Int:
                                e-e+ WW: ignore ▼
  e-e+ LPB: ignore ▼
                                                                        ignore ▼
                                                                                                       ignore ▼
                                                             Low-n Bias:
                                                                                           Low-n WW:
                                decay cut: 0.0
                                                                        99999.0
                                                                                          Coulomb corr:
                                                             prompt cut:
```

WHAT(1)
Decays:

= 1 Active radioactive decays activated for requested cooling times

"activation study case": time evolution calculated analytically for <u>fixed</u> (cooling) times. Daughter nuclei as well as associated radiation is considered at these (fixed) times

> 1 Semi-Analogue radioactive decays activated in semi-analogue mode each radioactive nucleus is treated like all other unstable particles (random decay time, daughters and radiation), all secondary

particles/nuclei carry time stamp ("age")

WHAT(2) > 0
Patch Isom: On

isomer "production" activated

WHAT(3)

number of "replicas" of the decay of each individual nucleus

Replicas: #

Card: RADDECAY [2/2]

RADDECAY

h/µ Int: ignore ▼ e-e+ LPB: ignore ▼ Decays: Active ▼
h/µ LPB: ignore ▼
e-e+ WW: ignore ▼
decay cut: 0.0

Patch Isom: ▼
h/µ WW: ignore ▼
Low-n Bias: ignore ▼
prompt cut: 99999.0

Replicas: 3.0
e-e+ Int: ignore ▼
Low-n WW: ignore ▼
Coulomb corr: ▼

WHAT(4)

h/m Int .. Low-n WW

switch for applying various biasing features only to prompt radiation or only to particles from radioactive decays

9 digits, each responsible for a different biasing Example:

5th digit, e+/e-/gamma leading particle biasing applied 000010000 to prompt radiation only 000020000 to decay radiation only 000030000 to both

Default: 111111111 (or blank as above)

WHAT(5)

decay cut: #
prompt cut: #

multiplication factors to be applied to transport cutoffs

10 digits, first five for decay radiation, second five for prompt radiation (see manual)

Special cases:

0000099999 kill EM cascade for prompt radiation 9999900000 kill EM cascade for residual radiation

Source.f: Biasing distribution of primaries

- Low occurrence primaries may have important consequences on the final response, e.g. high energy tail of synchrotron radiation can generate neutrons (i.e. activation)
- Actual distributions, e.g. f(E), can be biased (i.e. distorted) by a function, e.g. b(E) = c*E

$$\rightarrow$$
 g(E) = f(E)*b(E)

- Whether g(E) is sampled through inverse transform or through rejection, starting weights of particles WTFLK(NPFLKA) should then be adjusted by *1/fb
- Use with moderation/care...this can introduce strong weight dispersion → weigh-windows to split highweight particles...

udcdrl.f: Neutrino Decay Biasing

 There is a special routine udcdrl.f where one can bias the direction of the emitted neutrino in decays.

DOUBLE PRECISION **FUNCTION** UDCDRL(IJ, KPB, NDCY, UDCDRB, VDCDRB, WDCDRB)

Input variables:

IJ decaying particle

KPB outgoing neutrino

Output variables:

U,V,W DCDRB preferential outgoing direction for the neutrino

UDCDRL Lambda for direction biasing $(1-\cos(\theta))$

The biasing expression is of the form:

$$e^{-(1-\cos\theta/\lambda)}$$

- Useful for neutrino applications like CNGS, Beta Beams...
- For a fixed direction the LAM-BIAS card with SDUM=DCY-DIRE could be used instead
- NOTE: angular biasing is only available (and mostly only makes sense) for neutrinos due to their low interaction cross-sections

udcdrl.f: Example (n_TOF)

• Bias the direction of the neutrino in the pion decay so the daughter muon to be directed to the exp. area @(-120,0,18500). The direction is given in the lab-frame, and in this example the energies we are dealing are small, so safely we can assume that also in the lab-frame, the neutrino and muon go in opposite directions. The lambda is ¼ wide enough to cover the whole exp area.

```
INCLUDE '(TRACKR)'

UDCDRB = XTRACK (NTRACK) + 120.D+00

VDCDRB = YTRACK (NTRACK) - ZERZER

WDCDRB = ZTRACK (NTRACK) - 18500.D+00

HLPHLP = SQRT ( UDCDRB**2 + VDCDRB**2 + WDCDRB**2 )

UDCDRB = UDCDRB / HLPHLP

VDCDRB = VDCDRB / HLPHLP

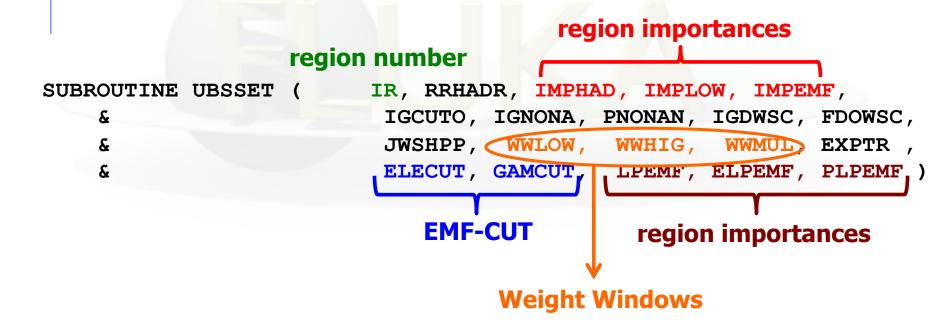
WDCDRB = WDCDRB / HLPHLP

UDCDRL = ONEFOU

Width [1-cos(θ)]
```

usbset.f: User BiaSing SETting

- called after reading in the input file and before the first event
- allows to alter almost any biasing weight on a region-dependent basis



Raising EMF thresholds (EMF-CUT)...

- in regions far from the scoring area or deep into the shielding
- in heavy materials (at least 100-200 keV, unless in single scattering mode)
- to GDR threshold (5-15 MeV) for neutron-dominated problems
- to muon production threshold (>~100 MeV) for muon-dominated problems

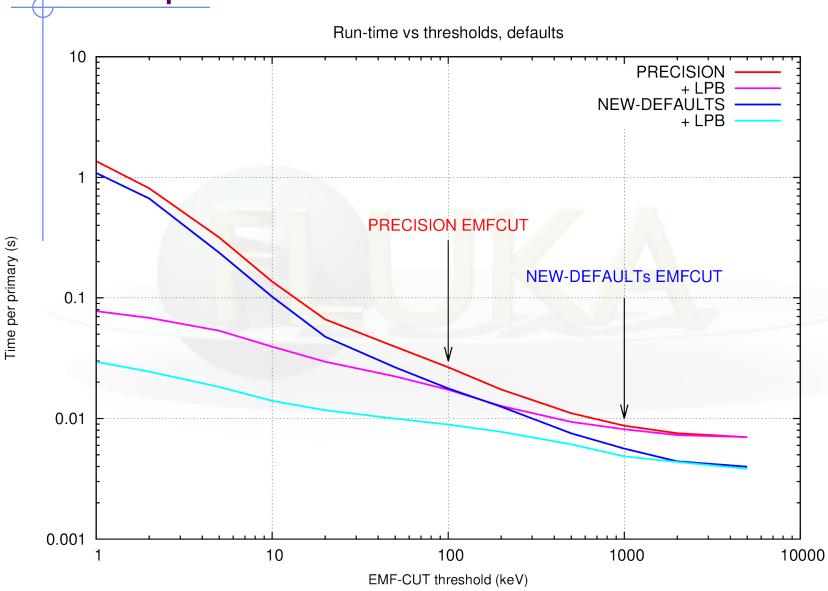
Notes:

- These techniques will help get a faster estimate with relatively good accuracy
- The sensitivity of results to EMF-CUT changes should be tested to assess biasing effect on results
- In many cases further simulations with lower thresholds are not needed

WARNING:

 Rather than optimization, raising thresholds is OFTEN a user mistake as done irrespectively of the relevant physical processes

Example: CPU vs Thresholds and LPB



- Data initialization in user routines: Avoid unnecessary repetition of global initialization steps at each call of a user routine
 - Use one-time check with logical variable, e.g.

```
IF (LFIRST) THEN
...
LFIRST = .FALSE.
END IF
```

- Example 1: number to name conversion: generate conversion table, save and use thereafter
- Example 2: preliminary mathematical transformations before sampling in source routine
- Move instructions that are not updated in loops out of those

• Using symmetries for mesh scoring, e.g. |x|, |y|, |z|, |r|, r-phi-z, r-phi-|z|, r-z, r-|z|

Notes:

- For example a symmetry over one plane saves 40% CPU time
- Symmetry can also be forced through usrmed.f (activated by option MAT-PROP with SDUM USERDIRE).
- Rebinning 1-D and 2-D to coarser mesh
- Data writing: dumping or writing large amount of data can considerably slow down calculations.
 - In large input files, and inherited setups, deactivate unnecessary legacy scoring, especially fine grid 3D histograms (e.g. USRBIN)
 - Avoid using 3D histograms (large size scoring), use instead 2D histograms (scoring in a plane) or 3D histograms with a coarse grid in one of the axis
 - Limit tape writing to necessary. Optimize the mathematical expressions in mgdraw.f
 - Tune-up scoring cards with short runs (good practice for several aspects) to optimize scoring scales

Geometry optimization

- Adjust NAZ in region definition to make it equal or slightly larger than the number of neighboring regions. Check for for "GEOMETRY SEARCH ARRAY" warnings in output
- If a region has too many neighboring cells, subdivide it in zones or regions to lower number of neighboring cells per zone
- If there are components (with sub-structure) that are repeated many times in the geometry use LATTICE capabilities to reduce number of regions
- More: Biasing impurities in compounds, number of replica in activation/decay...
- Other checks: these are not ON by default, so check only if you are recycling an input file or you are using it for a different application and CPU is an issue:
 - Make sure single EMF scattering (MULSOPT) is not ON unless needed (low energy, thin geometry)
 - If not looking at activation, heavy ion evaporation does not need to be switched ON (WHAT(2) of PHYSICS card with SDUM EVAPORAT)

Warnings...

- BIASING focuses the CPU onto a phase-space area of the problem, sacrificing other areas
- Reducing simulation time does not necessarily mean the simulation has been optimized
- Similarly, reducing variance does not necessarily mean the simulation has been optimized
- Small statistical error does not mean the error is actually low. This is specially true if splitting / two step methods, etc. are used. Correlations may be hidden.
- Biasing may reduce the error in the estimation of the average of a variable, but the higher momenta of that variable will not be obtained (e.g. the variance of the PDF distribution for that variable cannot be estimated).
- Simulation optimization may safe CPU time, but it can cost considerable manpower





Biasing

Beginners' FLUKA Course

usimbs.f: Sampling from array [1/4]

 Create a concentric cylindrical biasing with the weights sample from an array with various radii

Define the variables:

```
PARAMETER (NBIAS=5)
PARAMETER (Xcenter=ZERZER)
PARAMETER (Ycenter=ZERZER)
DOUBLE PRECISION BIASR(NBIAS), BIASF(NBIAS)
* Radius
DATA BIASR / 200.0, 250.0, 300.0, 400.0, 500.0 /
* Biasing factor
DATA BIASF / NBIAS * 2.0 /

LOGICAL LFIRST
DATA LFIRST / .TRUE. /
SAVE LFIRST, BIASR, BIASF
```

usimbs.f: Sampling from array [2/4]

Initialization – build the cumulative importance factor

```
IF (LFIRST) THEN
      WRITE(LUNOUT,*) "*** User defined biasing ***"
      PREVBIAS = 1.0
      DO N=1,NBIAS
            PREVBIAS = PREVBIAS * BIASF(N)
            BIASF(N) = PREVBIAS
            WRITE(LUNOUT,*) "Bias cylinder: ",N, BIASR(N), BIASF(N)
            convert the radius to square to avoid sqrt
            BIASR(N) = BIASR(N)**2
      ENDDO
      LFIRST = .FALSE.
 ENDIF
```

usimbs.f: Sampling from array [3/4]

Calculate the importance biasing * Find square of radius for starting/ending position Rold = (Xtrack(0)-Xcenter)**2 + (Ytrack(0)-Ycenter)**2Rnew = (Xtrack(Ntrack)-Xcenter)**2 + (Ytrack(Ntrack)-Ycenter)**2 * Search index of the starting position Nold = NBinSearch(Rold, NBIAS, BIASR) IF (Nold.EQ.0) THEN BIASOLD = 1.0**ELSE** BIASOLD = BIASF(Nold)**ENDIF** * Search index of the new position Nnew = NBinSearch(Rnew, NBIAS, BIASR) IF (Nnew.EQ.0) THEN BIASNEW = 1.0**ELSE** BIASNEW = BIASF(Nnew) **ENDIF**

FIMP = BIASNEW / BIASOLD

usimbs.f: Sampling from array [4/4]

```
INTEGER FUNCTION NBinSearch(x, N, VEC)
   INCLUDE '(DBLPRC)'
   DOUBLE PRECISION VEC(N)
   NLOW = 1
   NHIGH = N
   NBinSearch = 0
   IF (X.GE.VEC(NLOW) .AND. X.LE.VEC(NHIGH)) THEN
          CONTINUE
10
                    MID = (NLOW + NHIGH)/2
                   IF (MID.EQ.NLOW) THEN
                              NBinSearch = MID
                              RETURN
                    ELSEIF (X .GT. VEC(MID)) THEN
                              NLOW = MID
                    ELSEIF (X .LT. VEC(MID)) THEN
                              HIGH = MID
                    ELSE
                              NBinSearch = MID
                              RETURN
                    ENDIF
         GOTO 10
```

END IF

END

Perform a binary search Converge in log₂(N) steps