

The FLUKA User Routines: how to tailor FLUKA to specific user's needs.

User programming in the FLUKA environment

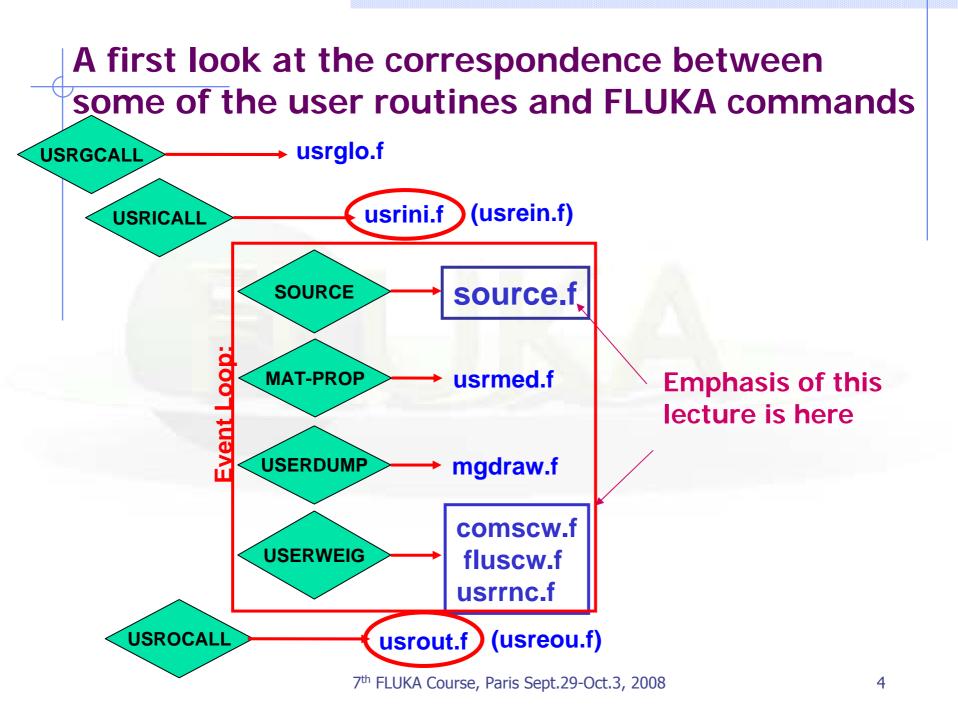
7th FLUKA Course NEA Paris, Sept.29-Oct.3, 2008

Why User Routines

- Fluka offers a rich choice of options for scoring most quantities and for applying variance reduction techniques, without requiring the users to write a single line of code.
- However there are special cases where "ad-hoc" routines are unavoidable, because the information cannot be obtained through standard options.
- A number of template of user routines (available in the usermvax directory) can be modified/activated by the user allow to fulfill non-standard tasks

What is available for the users

- The templates of all user routines are in the directory \$FLUPRO/usermvax
- The include files containing the COMMON blocks are in the directory \$FLUPRO/flukapro (see later)
- The compiling and linking scripts which are in the directory \$FLUPRO/flutil
- Flair can be used to edit, compile and link user routines in order to build a user-specific FLUKA executable



A possible classification in terms of their use (1)

User run control

- usrini.f
- usrein.f
- usrout.f
- usreou.f

Event generation, physics, kinematics

- source.f
- soevsv.f
- udcdrl.f
- formfu.f

Properties of medium User

magfld.f

<u>User global settings</u>usrglo.f

usrmed.f

A possible classification in terms of their use (2)

in association to FLUKA output

- comscw.f
- fluscw.f
- endscp.f
- fldscp.f
- musrbr.f
- Iusrbl.f
- fusrbv.f
- usrrnc.f

Intercepting particle stack

- mdstck.f
- stupre.f
- stuprf.f

Biasing

- usbset.f
- usimbs.f

A possible classification in terms of their use (3)

To drive optical photon transport

- abscff.f
- odffcff.f
- frghns.f
- ophbdx.f
- queffc.f
- orflctv.f
- rfrndx.f

<u>To manage lattice geometry</u>lattic.f

To access (almost) everything

mgdraw.f

See the relevant chap. of manual

Compiling and linking FLUKA user routines

• A FLUKA executable with user routines is in general application specific. It must be named and kept separately from the standard FLUKA

• Everything is managed today by FLAIR, however it is important to know the following details (managed automatically inside FLAIR):

• **\$FLUPRO/flutil/fff** is the compiling script with the proper path to the INCLUDE subdirectory and the required compiler (g77) options

Example: \$FLUPRO/flutil/fff usrini.f generates usrini.o

then \$FLUPRO/flutil/lfluka -m fluka -o flukamy usrini.o will perform the

proper linking generating the executable here called **flukamy**

• <u>Tip</u>: \$FLUPRO/flutil/lfluka –m fluka –o flukamy usrini.f will automatically call \$FLUPRO/flutil/fff

Help by FLAIR

- FLAIR has a button in the Compile frame which allows to scan the input file for possible cards that require the use of user routines
- It allows to copy the template routine from \$FLUPRO/usermvax to the project directory

Comp	ile Executab	le	
File	Size	Date	4
Link: Ifluka 💽 Exe:	🛃 Main:		
Options:	_	💷 D Line 👅 Bound Check	
		<u>Build</u> <u>Compile</u>	an

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Basics about FLUKA routines/functions

- Written in Fortran 77
- Double Precision everywhere, except for variables beginning with a letter within (i-n)
- Common blocks are in files which are loaded by INCLUDE statement
- All include files are in **\$FLUPRO/flukapro**
- Each routine must start with the following includes/common blocks:

INCLUDE '(DBLPRC)' INCLUDE '(DIMPAR)' INCLUDE '(IOUNIT)'

Note the parentheses which are an integral part of the Fluka INCLUDE file names
Users may add their own common(s) which may reside in different places

Basic FLUKA Include Files

DBLPRC: included in all routines of Fluka, contains (as PARAMETERS) the most common physical and mathematical constants and the declaration IMPLICIT DOUBLE PRECISION (A-H,O-Z)

DIMPAR: dimensions of the most important arrays

IOUNIT: logical input and output unit numbers (FLUKA uses those from 1 to 19, *they must be considered as reserved*)

• Users are encouraged to adhere to the "Fluka style" by <u>using</u> <u>systematically double precision</u> (except for calling external single precision scoring packages), and to use constants defined in this file for maximum accuracy and consistency

• Important: take some time to study the content of DBLPRC

Some important COMMON blocks in short (1)

- **BEAMCM:** beam properties of primary (BEAM and BEAMPOS)
- CASLIM: number of primary particles followed
- **EMFSTK:** particle stack for electrons and photons
- SOURCM: user variables and information for a user-written source
- FHEAVY: stack of heavy secondaries created in nuclear evaporation
- GENSTK: properties of each secondary created in a hadronic event
- LTCLCM: LaTtice CeLl CoMmon (needed when writing symmetry transformations for Lattice Geometry)
- FLKMAT: material properties
- FLKSTK: main Fluka particle stack
- SOUEVT: variables describing the source event
- TRACKR:variables concerning the properties of transportedparticle (track) at run time
- PAPROP: particle properties (masses, charges, mean lives...)
- SCOHLP: variables concerning the current estimator type

Converting Names↔**Number** FLUKA converts all <u>Names</u> given in the input file to <u>Numbers</u>: all the arguments that you will find in user routines are numeric To get the number starting from a region name CALL GEON2R (REGNAM, NREG, IERR) Input variable: * Regnam = region name (CHAR*8) * Similar routines * for lattice geometry * **Output variables:** * Nreg = region number * Ierr = error code (0 on success, 1 on failure)

To get the name of a region when you know the number: CALL GEOR2N (NREG, REGNAM, IERR)

- * Input variable:
- * Nreg = region number
- *
- * Output variables:
- * Regname = region name (CHAR*8)
- * Ierr = error code (0 on success, 1 on failure)

source (user written source: generation of initial kinematics)

Argument list

NOMORE : if set = 1, no more calls will occur (the run will be terminated after exhausting the primary particles loaded onto stack in the present call). The history number limit set with option START will be overridden

Subroutine SOURCE is probably the most frequently used user routine. It is activated by option SOURCE and is used to sample primary particle properties from distributions (in space, energy, time, direction or mixture of particles) which cannot be described with the BEAM, BEAMPOS and BEAMAXES cards. At each call, one (or more) particle(s) must be loaded onto COMMON FLKSTK (particle bank) before returning control. These values can be read from a file, generated by some sampling algorithm, or just assigned.

Using source

Option SOURCE allows the user to input up to 18 numerical values (WHASOU(1),(2). . . (18)) and one 8-character string (SDUSOU) which can be accessed by the subroutine by including the following line: INCLUDE '(SOURCM)'

The user can insert any first time initialization within the following IF block:

```
* +----*
* | First call initialisations:
    IF ( LFIRST ) THEN
* | *** The following 3 cards are mandatory ***
    TKESUM = ZERZER
    LFIRST = .FALSE.
    LUSSRC = .TRUE.
* | *** User initialisation ***
    END IF
* |
```

Using source (continues...)

The user can load onto the FLKSTK stack one or more particles at each call: for each particle loaded the pointer must be increased by 1

```
NPFLKA = NPFLKA + 1 | increases the pointer
```

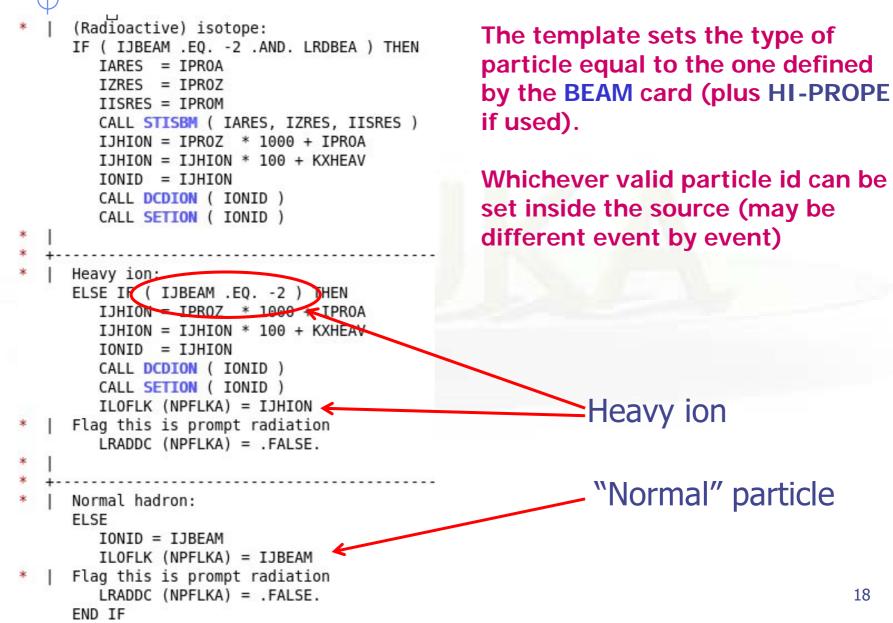
weight of the particle (values different from $1 \rightarrow$ biased source, advanced users)

WTFLK (NPFLKA) = ONEONE

update the total weight of the primaries (don't change):

```
WEIPRI = WEIPRI + WTFLK (NPFLKA)
```

Using source: setting the particle id



```
Using source: assigning momentum energy
     In the template routine, the momentum is taken from the BEAM option
       (PBEAM, in COMMON BEAMCM, which contains all values defined by
                        options BEAM and BEAMPOS)
      PMOFLK (NPFLKA) = PBEAM
* Kinetic energy of the particle (GeV)
     TKEFLK (NPFLKA) = SQRT ( PBEAM**2 + AM (IONID)**2 ) - AM (IONID)
     The user can select a momentum from a spectrum or a file
     Alternatively the user can sample/assign the kinetic energy and derive
     the momentum. Be coherent!
      TKEFLK (NPFLKA) = ENSAMP
      PMOFLK (NPFLKA) = SQRT ( TKEFLK (NPFLKA) * ( TKEFLK (NPFLKA)
     8
                              + TWOTWO * AM (IONID) ) )
```

Even when using SOURCE, <u>the BEAM card remains mandatory</u>. The momenta (or energies) assigned in SOURCE can never be larger than the momentum/energy set in BEAM (it is the one used during initialization)!!

Using source: setting position and direction

Direction cosines assignment:

TXFLK (MPFLKA) = UBEAM	! Assumed here to be the same as	
$\mathbf{TYFLK} (\mathbf{MPFLKA}) = \mathbf{VBEAM}$! defined by option BEAMPOS. UBEAM,	,
TZFLK (BFFLKA) = WBEAM	! VBEAN, WBEAN are some among the b	
	nroperties in COMMON REAMCM	

It is also possible to assign a polarization:

TXPOL (NPFLKA) = -TWOTWOTYPOL (NPFLKA) = +ZERZERTZPOL (NPFLKA) = +ZERZER ! -2 is a flag for "no polarisation"

Finally, initial space coordinate assigned/read/sampled:

XFLK	(NPFLKA) = XBEAM	1	Assumed here to be the same as
YFLK	(NPFLKA) = YBEAM	!	defined by option BEAMPOS. XBEAM,
ZFLK	(NPFLKA) = ZBEAM	!	YBEAM, ZBEAM are also in COMMON BEAMCM

Be careful to ensure the cosine proper normalization within machine accuracy!!! Ie...

TNORM = SQRT (TXFLK(NPFLKA)**2 + TYFLK(NPFLKA)**2 + TZFLK(NPFLKA) **2) TXFLK (NPFLKA) = TXFLK(NPFLKA) / TNORM TYFLK (NPFLKA) = TYFLK(NPFLKA) / TNORM TZFLK (NPFLKA) = TZFLK(NPFLKA) / TNORM 7th FLUKA Course, Paris Sept.29-Oct.3, 2008 20

Using source (continues...)

The following lines can remain as they are

AGESTE (NPFLEA) = $+ZERZER$ AENSHR (NPFLEA) = $-TWOTWO$	Particle age is zero by default Resets the Kshort component of
IGROUP (NPFLKA) = 0	! K0/K0bar. Usually not to be changed. ! Group number for low-energy ! neutrons: if set to 0, the program
Don't change the lines below:	! derives it from the kinetic emergy
* From this point	
LOFLK (NPFLKA) = 1 LOUSE (NPFLKA) = 0	! Generation is 1 for source particles ! User variables: the user can set
DO 100 ISPR = 1, MKBMX1	! different values in the STUPRF or
DFNEAR (NPFLKA) = +ZERZER	! Resetting the distance to the ! nearest boundary
* to this point: don't change a	nything

At the end, source makes a copy into SOEVSV of the generated particles in case this info is required by some user routine at scoring stage

Using the FLUKA Random Number Generator in user routines

Fundamental for SOURCE!!! No other external random generators must be used, otherwise the history reproducibility will be lost

• ... = FLRNDM (XDUMMY)

returns a 64-bit random number [0-1)

CALL FLNRRN (RGAUSS)

returns a normally distributed random number RGAUSS

CALL FLNRR2 (RGAUS1, RGAUS2)

returns an uncorrelated pair of normally distributed random numbers: RGAUS1 and RGAUS2

• CALL SFECFE (SINT,COST)

returns SINT and COST, sine and cosine of a random azimuthal angle SINT**2 + COST**2 = 1.D+00

• CALL RACO (TXX, TYY, TZZ)

returns a random 3D direction (TXX, TYY, TZZ) such that:

 $TXX^{**2} + TYY^{**2} + TZZ^{**2} = 1.D+00$

Useful routines

CALL OAUXFI ('file', LUN, 'CHOPT', IERR)

to open an auxiliary file (to read data or parameters) looking automatically for the file in some default locations (temporary directory, working directory, **\$FLUPRO**, **\$HOME**)

CALL FLABRT ('name','message')

this allows to force a FLUKA abort on user request: it might be useful to perform a debugging (using gdb for instance)

CALL SFLOOD (XXX, YYY, ZZZ, UXXX, VYYY, WZZZ)

returns in XXX, YYY, ZZZ a random position ON the surface of a sphere of radius 1 and centre 0 (multiply XXX, YYY, ZZZ by the actual radius and add the centre coordinates) and UXXX, VYYY, WZZZ are random cosines distributed so as to generate a uniform and isotropic fluence inside the sphere numerically given by $1/(\pi R^2)$

R being the sphere radius.

comscw (weighting energy deposition or star production)

Argument list (all variables are input only)IJ: particle type (1 = proton, 8 = neutron, etc.: see code in 5.1)XA,YA,ZA: current particle positionMREG: current geometry regionRULL: amount to be deposited (unweighted)LLO: particle generationICALL: internal code calling flag (not for general use)

Activated by option USERWEIG with WHAT(6) > 0.0. Energy and stars obtained via SCORE, USRBIN and EVENTBIN, and production of residual nuclei obtained via RESNUCLEi are multiplied by the value returned by this function. The user can implement any desired logic according to the argument list (particle type, position, region, amount deposited, particle generation), or information available in COMMON SCOHLP (binning number, type of scored quantity). The scored quantity is given by the flag ISCRNG (in SCOHLP):

 $\frac{\text{ISCRNG} = 1 \rightarrow \text{Energy density binning}}{\text{ISCRNG} = 3 \rightarrow \text{Residual nuclei scoring}}$

ISCRNG = $2 \rightarrow$ Star density binning

comscw (continues...)

The binning/detector number is given by JSCRNG (in SCOHLP) and is printed in output between the estimator type and the detector name.

Note that a detector of residual nuclei can have the same JSCRNG number as a binning (use the value of ISCRNG to discriminate).

Further information can be obtained including COMMON TRACKR (for instance particle's total energy, direction cosines, age). TRACKR contains also special user variables (both integer and in double precision) which can be used to save information about particles which have undergone some particular event.

If data concerning the current material are needed, it can be accessed as MEDIUM(MREG) if file (FLKMAT) is included.

usrini (USeR INItialization)

Argument list

WHAT(1),(2),(3),(4),(5),(6) : user-provided numerical parameters SDUM : user-provided character string (8 characters)

Subroutine USRINI is called every time a USRICALL card is read in the input stream, before particle showering starts. Useful for initialisation: ie reading and manipulating data from one or more files, calling other private routines, etc.

The calling parameters can be used by the user to pass variables/flags to the routine.

usrein (USeR Event INitialization)

Subroutine USREIN is called just before the start of an event. An event is the full history of a group of related particles and their descendants.

If primaries are loaded into stack by the input option BEAM, there is only one source particle per event; there can be more if the user routine SOURCE is used to load particles into stack. USREIN is always called: the default version of USREIN does nothing.

usrout (USeR OUTput)

Argument list

WHAT(1),(2),(3),(4),(5),(6) : user-given numerical parameters
SDUM : user-given character string (8 characters)

Subroutine USROUT is called every time a USROCALL card is read in the input stream. It is used for user-written output in addition to the standard one provided by default. The calling parameters can be used by the user to pass variables/flags to the routine.

usreou (USeR Event OUtput)

Subroutine USREOU is called at the end of each event, namely after all event primary particles and their descendants have been transported.

USREOU is always called: the default version of USREOU does nothing. The user can plug in any kind of event analysis, output, etc.

Mathematical library in FLUKA

• FLUKA contains many mathematical routines of general utility, so in general it should not be necessary to call external mathematical libraries:

flgaus:	Gaussian adaptative integration
simpsn:	Simpson integration
gamfun:	Gamma fuction
radcub:	Real solutions of 3 rd order algebric equation
flgndr:	Legendre polinomials
yinter, finter,	
dintp:	interpolation routines
rordin, rordde:	Sorting of vector values

Also: expansion in Laguerre and Chebyshev polynomials, Bezier fit, and many others...

For users who access the FLUKA source: they are in mathmvax directory At some time it will be possible to have a short-writeup for their use.

fluscw (weighting fluence, current and yield)

Argument list (all variables are input only)
IJ : particle type
PLA : particle momentum (if > 0.0)
or $-PLA = \text{kinetic energy}$ (if < 0.0)
TXX, TYY, TZZ : particle current direction cosines
WEE : particle weight
XX, YY, ZZ : particle position
NRGFLK : current region (after boundary crossing)
IOLREG : previous region (before boundary crossing). Useful only with
boundary crossing estimators (for other estimators it has no meaning)
LLO : particle generation
NSURF : internal code calling flag (not for general use)

Similar to COMSCW. Function FLUSCW is activated by option USERWEIG, with WHAT(3) > 0.0. Yields obtained via USRYIELD, fluences calculated with USRBDX, USRTRACK, USRCOLL, USRBIN, and currents calculated with USRBDX are multiplied by the value returned by this function.

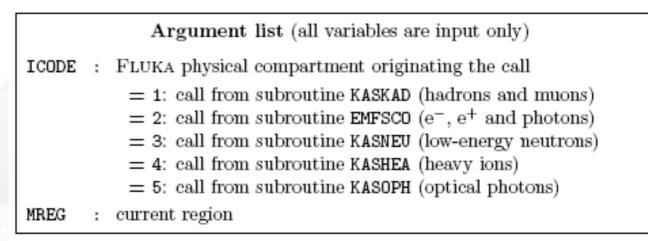
fluscw (continues...)

The user can implement any desired logic according to the argument list (particle type, energy, direction, weight, position, region, boundary, particle generation), or information available in COMMON SCOHLP (binning or detector number, estimator type). The estimator type is given by the flag ISCRNG (in COMMON SCOHLP):

A very special user routine: mgdraw.f

mgdraw (general event interface)

The most general interface to FLUKA content (if you know how to use it...)



Subroutine MGDRAW, activated by option USERDUMP with $WHAT(1) \ge 100.0$, usually writes a "collision tape", i.e., a file where all or selected transport events are recorded. The default version (unmodified by the user) offers several possibilities, selected by WHAT(3) in USERDUMP.

mgdraw (continues...)

The different **ENTRY** points of **MGDRAW**

Additional flexibility is offered by a user entry USDRAW, interfaced with the most important physical events happening during particle transport.

The user can modify of course also any other entry of this subroutine:

BXDRAW called at boundary crossings,

EEDRAW called at event end,

MGDRAW called at each step, for trajectory drawing and dE/dx energy deposition events,

ENDRAW for recording of point energy deposition events, SODRAW for recording of source events

mgdraw (continues...)

The format of the output file can be changed, and different combinations of events can be written to file.

But the most interesting aspect of the routine is that the six entries (all of which, if desired, can be activated at the same time by setting USERDUMP with WHAT(3) = 0.0 and WHAT(4) \geq 1.0) constitute a complete interface to the whole Fluka transport. Therefore, MGDRAW can be used not only to write a collision tape, but to do any kind of complex analysis. Typical: event by event output (common for HEP applications).

mgdraw: the MGDRAW entry

MTRACK: JTRACK:	number of energy deposition events along the track type of particle
ETRACK:	total energy of the particle
WTRACK:	weight of the particle
NTRACK:	values of XTRACK, YTRACK, ZTRACK: end of each track
	segment
MTRACK:	values of DTRACK: energy deposited at each deposition
	event
CTRACK:	total length of the curved path

Other variables are available in TRACKR (but not written by MGDRAW unless the latter is modified by the user: particle momentum, direction cosines, cosines of the polarisation vector, age, generation, etc. see a full list in the comment in the INCLUDE file).

mgdraw: the BXDRAW entry

Called at Boundary Crossings

Argument list (all variables are input only)

ICODE : physical compartment originating the call, as in the MGDRAW entry
MREG : region from which the particle is exiting
NEWREG : region the particle is entering
XSCO, YSCO, ZSCO : point where the boundary crossing occurs



Argument list (all variables are input only)

ICODE : physical compartment originating the call, as in the MGDRAW entry

mgdraw: the ENDRAW entry

Called at pointlike Energy Deposition dumps (for example: ICODE = 1 ICODE = 1 = 2 ICODE = 3 I

stopping particles, photoelectric eff., etc.)

Argument list (all variables are input only) **ICODE** : type of event originating energy deposition ICODE = 1x: call from subroutine KASKAD (hadrons and muons); = 10: elastic interaction recoil = 11: inelastic interaction recoil = 12: stopping particle = 14: particle escaping (energy deposited in blackhole) ICODE = 2x: call from subroutine EMFSCO (electrons, positrons and photons) = 20: local energy deposition (i.e. photoelectric) = 21 or 22: particle below threshold = 23: particle escaping (energy deposited in blackhole) ICODE = 3x: call from subroutine KASNEU (low-energy neutrons) = 30: target recoil = 31: neutron below threshold = 32: neutron escaping (energy deposited in blackhole) ICODE = 4x: call from subroutine KASHEA (heavy ions) = 40: ion escaping (energy deposited in blackhole) ICODE = 5x: call from subroutine KASOPH (optical photons) = 50: optical photon absorption = 51: optical photon escaping (energy deposited in blackhole) : current region MREG RULL : energy amount deposited XSCO, YSCO, ZSCO : point where energy is deposited

mgdraw: the SODRAW entry

Argument list

No arguments

SODRAW writes by default, for each source or beam particle:

NCASE: (in COMMON CASLIM, with a minus sign to identify SODRAW output) number of primaries followed so far (in COMMON FLKSTK) stack pointer NPFLKA: (in COMMON FLKSTK) highest value of the stack **NSTMAX:** pointer encountered so far (in COMMON SOURCM) total kinetic energy of the TKESUM: primaries of a user written source, if applicable. Otherwise = 0.0WEIPRI: (in COMMON SUMCOU) total weight of the primaries handled so far type of source particle NPFLKA times: ILOFLK: total particle energy (kinetic+mass) (all variables in TKEFLK + AM: COMMON FLKSTK) source particle weight WTFLK: source particle position XFLK, YFLK, ZFLK: TXFLK, TYFLK, TZFLK: source particle direction cosines

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mgdraw: the USDRAW entry

USDRAW is called <u>after each</u> <u>particle interaction</u> (requested by the user with option USERDUMP, WHAT(4) \geq 1.0)

Argument list (all variables are input only) ICODE : type of event ICODE = 10x: call from subroutine KASKAD (hadron and muon interactions); = 100: elastic interaction secondaries = 101: inelastic interaction secondaries = 102: particle decay secondaries = 103: delta ray generation secondaries = 104: pair production secondaries = 105: bremsstrahlung secondaries ICODE = 20x: call from subroutine EMFSCO (electron, positron and photon interactions) = 208: bremsstrahlung secondaries = 210: Møller secondaries = 212: Bhabha secondaries = 214: in-flight annihilation secondaries = 215: annihilation at rest secondaries = 217: pair production secondaries = 219: Compton scattering secondaries = 221: photoelectric secondaries = 225: Rayleigh scattering secondaries ICODE = 30x: call from subroutine KASNEU (low-energy neutron interactions) = 300: neutron interaction secondaries ICODE = 40x: call from subroutine KASHEA (heavy ion interactions) = 400: delta ray generation secondaries MREG : current region XSCO, YSCO, ZSCO : interaction point

When mgdraw should better not be used

When biasing is requested

 Whenever low-energy neutrons (E<20 MeV) are used, unless one has a deep knowledge of the peculiarities of their transport (ie kerma, etc)

(or at least one has to be a very experienced user to manage these cases without making mistakes...)

