

User Programming in the FLUKA environment

FLUKA Advanced Course

Why user routines

- Fluka offers a rich choice of **built-in 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 needed information cannot be obtained through standard options

What is available for the users

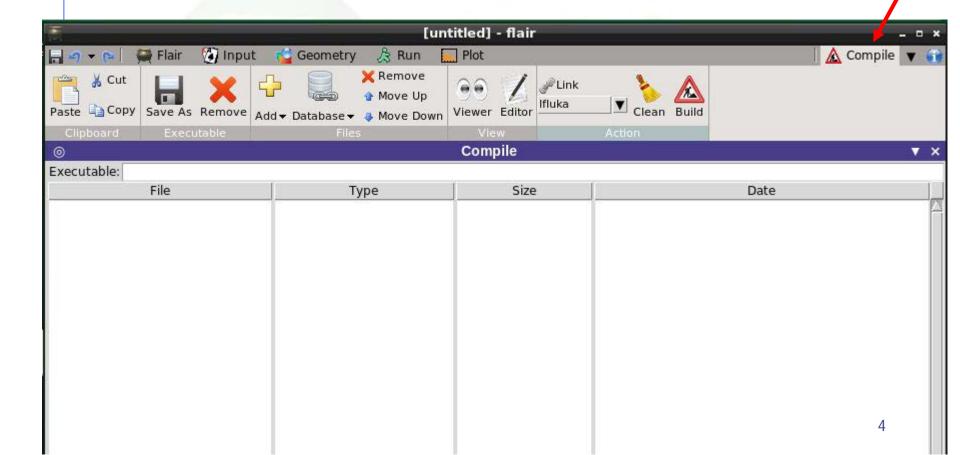
- A number of user routine templates are available in the \$FLUPRO/usermvax directory and can be modified/activated by the user in order to fulfill non-standard tasks
- The INCLUDE files containing the COMMON blocks are in the \$FLUPRO/flukapro directory
- An extended mathematical library can in principle be exploited by properly calling its members from inside an user routine
- The compiling and linking scripts are in the directory \$FLUPRO/flutil
- Most user routines need to be activated by input directives

Flair can be used to edit, compile and link user routines in order to build a user-specific FLUKA executable

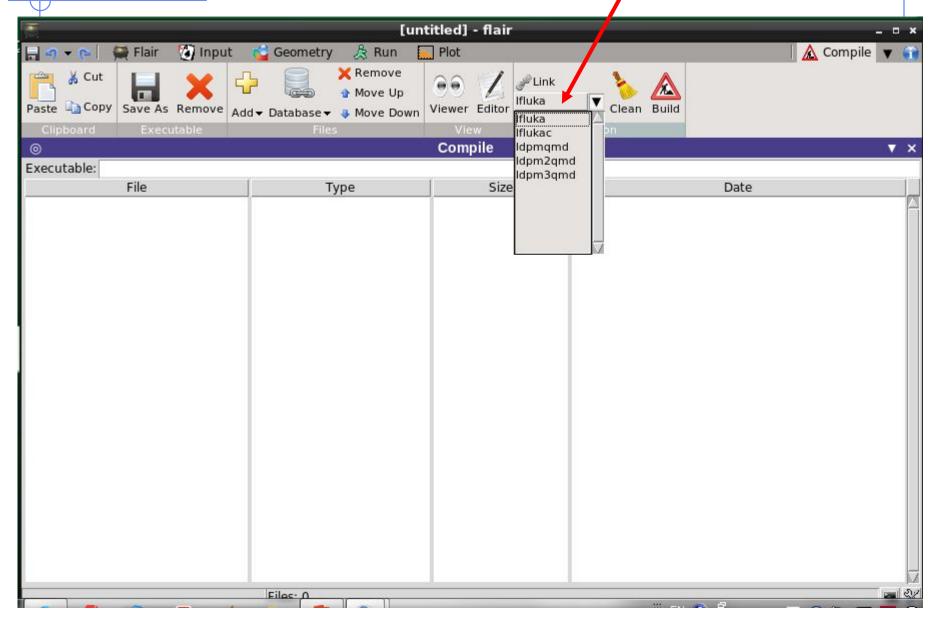
Flair interface (I)

Flair has a button in the Compile frame which scans the input file for possible cards that require a user routine

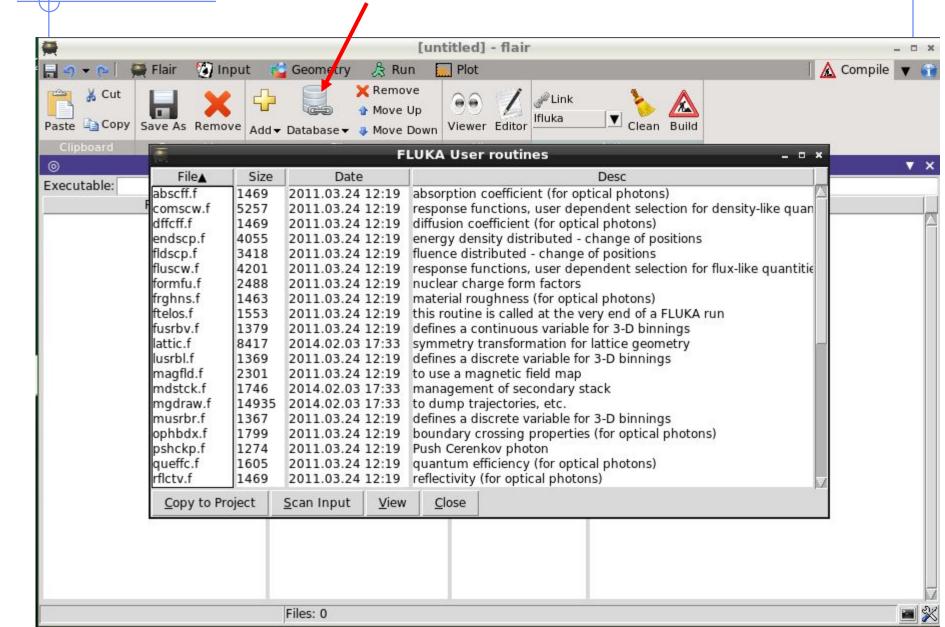
It allows to copy the template routine from \$FLUPRO/usermvax to the project directory



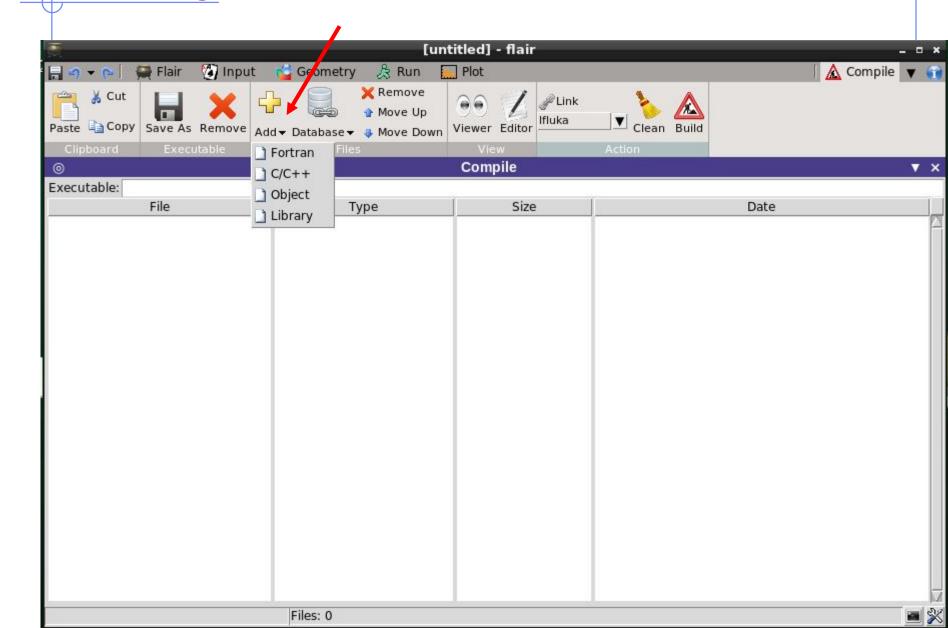
Choosing the builder



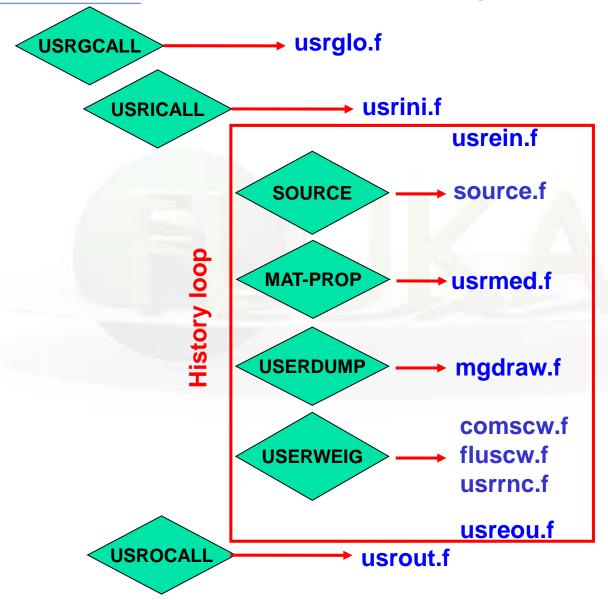
Parsing content of \$FLUPRO/usermvax



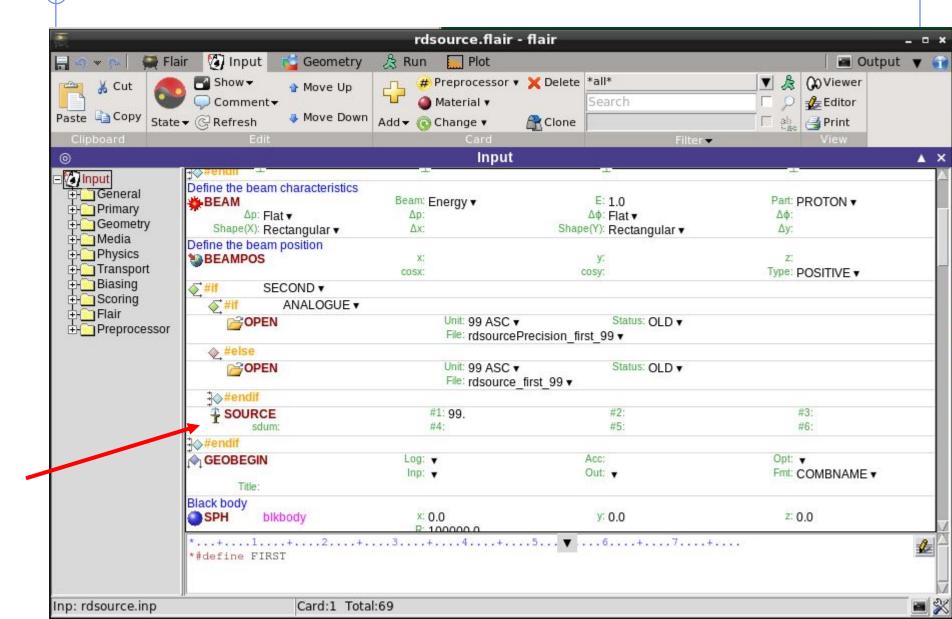
Adding routines from other directories



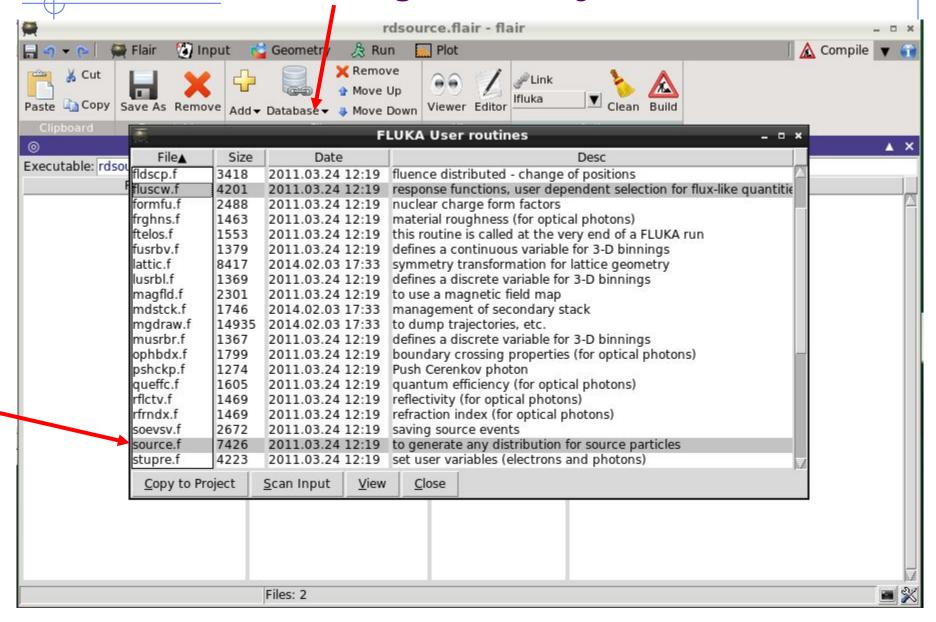
Card – user routine correspondence



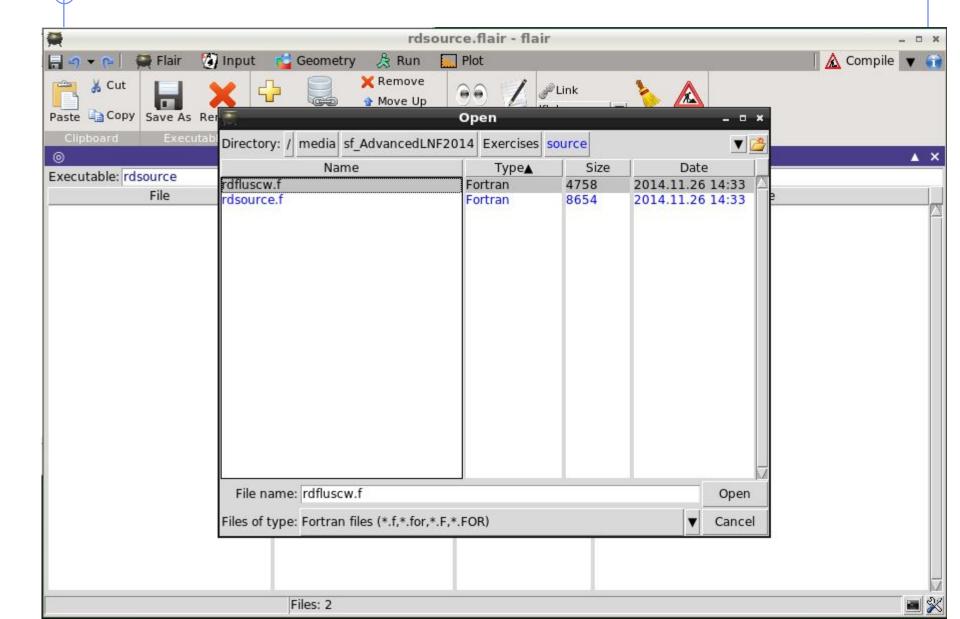
SOURCE card in the input



Automatic recognition by FLAIR



Manual insertion from a user directory



User routine scope (I)

SCORING

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

BIASING

- usbset.f
- usimbs.f
- udcdrl.f

LATTICE GEOMETRY

lattic.f

SOURCE GENERATION

- source.f
- (soevsv.f)

MAGNETIC FIELD

magfld.f

OPTICAL PHOTONS

- abscff.f
- dffcff.f
- frghns.f
- ophbdx.f
- queffc.f
- rflctv.f
- rfrndx.f

INITIALIZATION

- usrglo.f
- usrini.f
- usrein.f

OUTPUT

- usreou.f
- usrout.f

User routine scope (II)

accessing particle stack

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

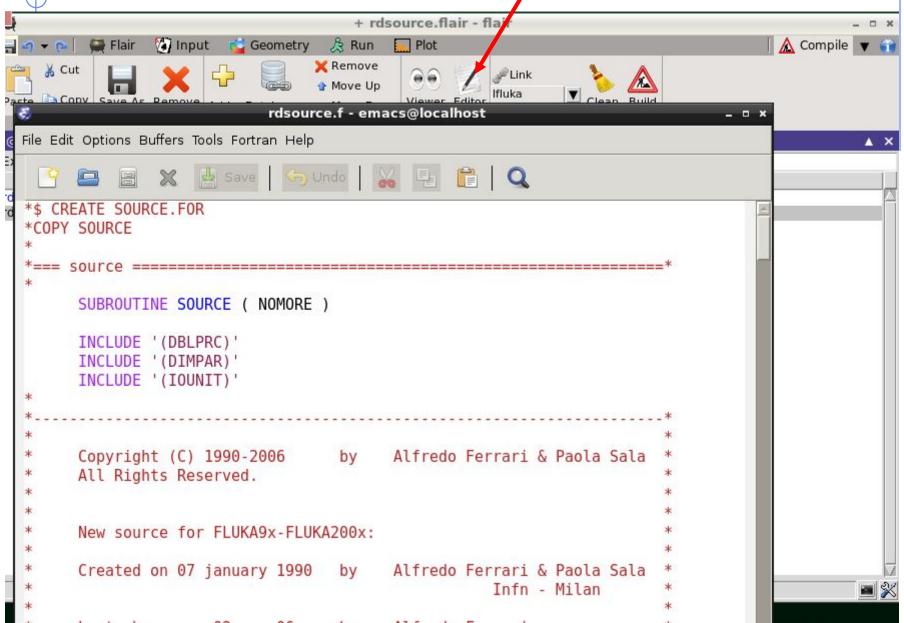
accessing (almost) everything

mgdraw.f

multipurpose

usrmed.f

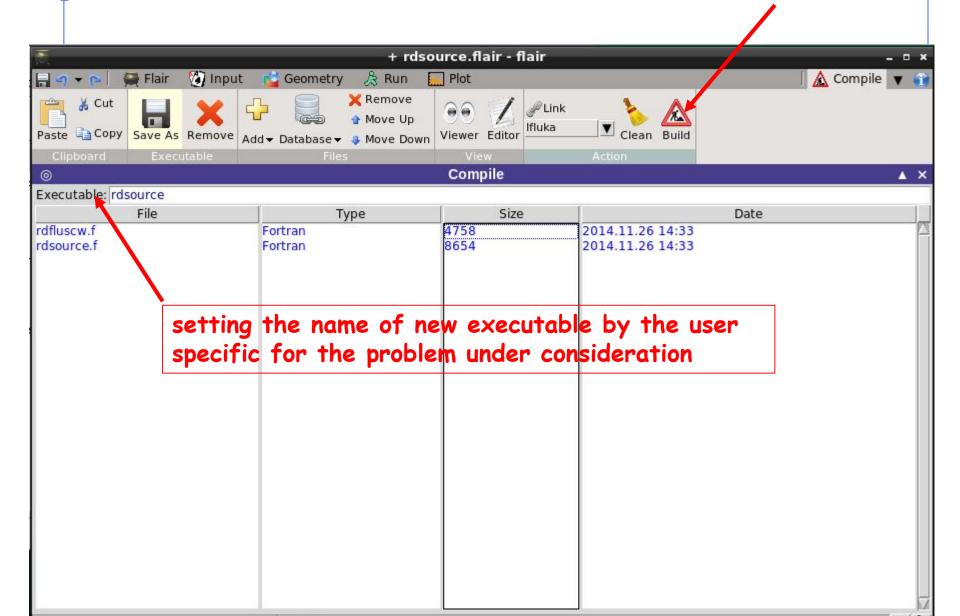
Editing routines



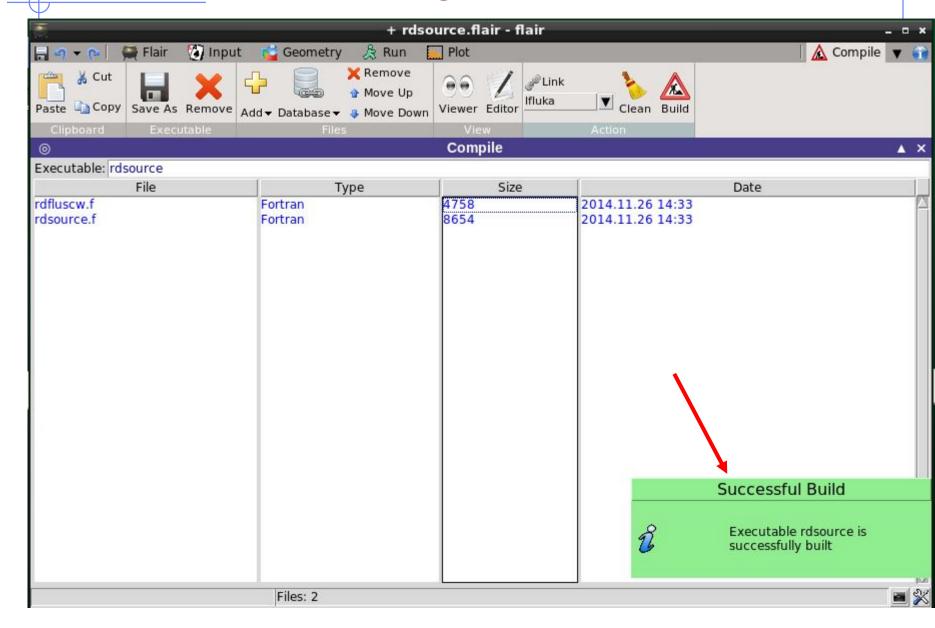
Compiling and linking

- A FLUKA executable with user routines is in general application specific. It must be named and kept separately from the standard FLUKA
- Everything can be managed today by FLAIR, however it is important to know the following details (managed automatically inside FLAIR):
 - Everything can be performed outside flair with terminal commands + editor
 - \$FLUPRO/flutil/fff is the compiling script with the proper path to the INCLUDE subdirectory and the required compiler (g77 or gfortran) 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

Compiling and linking (Build) by FLAIR



Successful building



FLUKA programming rules

- Language is Fortran 77 (C routines can be linked)
 - Note: when writing user-routines, bear in mind g77 and gfortrandon't always allow the same options
- Double Precision everywhere, except for integer variables beginning with a letter in the range [i-n]
- Common blocks are in \$FLUPRO/flukapro files and are loaded by the INCLUDE statement
- 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 other FLUKA commons as well as their own commons which may reside in different places

Numerical precision

Floating point representation

$$\pm d_0 d_1 d_2 \dots d_{p-1} \times \beta^e$$

where: β =base, *O.dddd*=significant

Represents the number

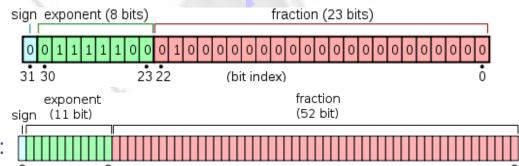
$$\pm (d_0 + d_1 \beta^{-1} + ... + d_{p-1} \beta^{-(p-1)}) \beta^e, \quad (0 \le d_i < \beta)$$

- Bits required: $\log_2(e_{max}-e_{min}+1) + \log_2(\beta^p) + 1$
- Real numbers might not be exactly represented as a floating-point number. Example: with β =2 the number 0.1 has an infinite representation and with p=24 will be represented as: 0.10000001490116119384765625

63

52

- IEEE representation:
 - Single precision (32bit):



Double precision (64bit):

Floating point: Accuracy

- Cancellation: subtraction of nearly equal operands may cause extreme loss of accuracy.
- Conversions to integer are not intuitive: converting (63.0/9.0) to integer yields 7, but converting (0.63/0.09) may yield 6.
 This is because conversions generally truncate rather than round.
- Limited exponent range: results might overflow yielding infinity, or underflow yielding a denormal value or zero. If a denormal number results, precision will be lost.
- Testing for safe division is problematic: Checking that the divisor is not zero does not guarantee that a division will not overflow and yield infinity.
- Equality test is problematic: Two computational sequences that are mathematically equal may well produce different floatingpoint values. Programmers often perform comparisons within some tolerance

Minimizing Accuracy Problems

- Use double precision whenever possible.
- <u>Small errors</u> in floating-point arithmetic can <u>grow</u> when mathematical algorithms perform operations an <u>enormous</u> <u>number of times</u>. e.g. matrix inversion, eigenvalues...
- Expectations from mathematics may not be realized in the field of floating-point computation. e.g. $\sin^2\theta + \cos^2\theta = 1$.
- Always replace the $x^2-y^2 = (x+y)(x-y)$
- <u>Equality test should be avoided</u>: replace with "fuzzy" comparisons (if (abs(x-y) < epsilon) ...)
- Adding a large number of numbers can lead to loss of significance, use <u>Kahan</u> algorithm instead
- For the quadratic formula use either

$$\frac{-b \pm \sqrt{b^2 - 4ac}}{2a} \quad \text{or} \quad \frac{2c}{-b \pm \sqrt{b^2 - 4ac}}$$

when $b^2 > 4ac$, then $\sqrt{(b^2-4ac)} \approx |b|$ therefore will introduce cancelation

Some COMMON blocks in short

BEAMCM: beam particle properties (from BEAM and BEAMPOS)

SOURCM: user variables and information for a user-written source

SOUEVT: recording of the source event

CASLIM: number of primary particles followed

FLKSTK: main particle stack of FLUKA

EMFSTK: particle stack for electrons and photons

GENSTK: properties of secondaries created in a hadronic event

FHEAVY: special stack for nuclear fragments

FLKMAT: material properties

LTCLCM: LaTtice CeLl CoMmon for lattice cell identification

TRACKR: properties of the particle currently transported

PAPROP: intrinsic particle properties (mass, charge, half live...)

SCOHLP: variables concerning the current estimator type

(DBLPRC) (I)

Included in all routines of Fluka, contains the declaration IMPLICIT DOUBLE PRECISION (A-H,O-Z) and sets many mathematical and physical constants.

Users are strongly encouraged to adhere to "Fluka style" by

- using systematically double precision (except for very good reasons such as calling external single precision scoring packages)
- and to use constants defined in this file for maximum accuracy.

(DBLPRC) (II)

```
*======= M A T H E M A T I C A L C O N S T A N T S ========*
* -----* Numerical constants (double precision): -----*
* Zerzer = 0 *
PARAMETER ( ZERZER = 0.D+00 )
* Oneone = 1 *
PARAMETER (ONEONE = 1.D+00)
* Twotwo = 2 *
PARAMETER ( TWOTWO = 2.D+00 )
* Pipipi = Circumference / diameter *
PARAMETER ( PIPIPI = 3.141592653589793238462643383279D+00 )
* Twopip = 2 x Pipipi *
PARAMETER (TWOPIP = 6.283185307179586476925286766559D+00)
* Eneper = "e", base of natural logarithm *
PARAMETER ( ENEPER = 2.718281828459045235360287471353D+00 )
* Sqrtwo = square root of 2 *
PARAMETER ( SQRTWO = 1.414213562373095048801688724210D+00 )
```

(DBLPRC) (III)

```
*====== P H Y S I C A L C O N S T A N T S ========*
* ----- Primary constants: ----- *
* Clight = speed of light in cm s^{-1} *
PARAMETER (CLIGHT = 2.99792458 D+10)
* Boltzm = k Boltzmann constant (J K<sup>-1</sup>) *
PARAMETER (BOLTZM = 1.380658 D-23)
* Amelgr = electron mass (g) *
PARAMETER (AMELGR = 9.1093897 D-28)
* Plckbr = reduced Planck constant (erg s) *
PARAMETER ( PLCKBR = 1.05457266 D-27 )
* ----- Perived constants: ----- *
*Alamb0 = Compton wavelength = 2 pi r0 / fsc , being r0 the classical electron radius *
* and fsc the fine structure constant *
PARAMETER ( ALAMBO = TWOTWO * PIPIPI * RCLSEL / ALPFSC )
* ----- Astronomical constants: ----- *
* Rearth = Earth equatorial radius (cm) *
PARAMETER ( REARTH = 6.378140 D+08 )
* ----- Conversion constants: ----- *
* GeVMeV = from GeV to MeV *
PARAMETER ( GEVMEV = 1.0 D+03 )
```

(IOUNIT)

Logical input and output unit numbers

The logical units up to 19 (included) are reserved for FLUKA

```
* lunin = standard input unit *
PARAMETER ( LUNIN = 5 )

* lunout = standard output unit *
PARAMETER ( LUNOUT = 11 )

* lunerr = standard error unit *
PARAMETER ( LUNERR = 15 )
...
```

Use the pre-defined output units when you need messages from your user routines:

```
WRITE (LUNOUT, *) ' My initialization is active' WRITE (LUNERR, *) ' MySource : warning, energy is 0'
```

(CASLIM)

Keeps preset number of histories and current number of histories

- * /caslim/ is needed to decide when to stop the run
- * Trnlim = if cpu-time-left<tlim the run will be ended
- * Tpmean = average time needed to follow one beam particle
- * Tprmax = i maximum time needed to follow one beam particle
- * Trntot = the cumulative time needed to follow the beam particles
- * Ncases = maximum number of beam particles to be followed
 * modulo 1,000,000,000)
- * Mcases = maximum number of beam particles to be followed
- * in excess of 1,000,000,000, divided by 1,000,000,000
- Ncase = current number of beam particles followed (modulo
- 1,000,000,000)
- * Mcase = current number of beam particles followed in excess
- * of 1,000,000,000, divided by 1,000,000,000

Useful to be included whenever the current event number is needed

(FLKSTK)

At each interaction/decay... etc new particles are feeding the stack

```
/Flkstk/ stack for the primaries
      Wtflk = particle statistical weight
      Pmoflk = particle (laboratory) momentum (GeV/c)
      Tkeflk = particle (laboratory) kinetic energy (GeV)
           = particle position x-coordinate
      Xflk
      Yflk = particle position y-coordinate
      Zflk = particle position z-coordinate
      Txflk = particle direction x-coordinate
      Tyflk = particle direction y-coordinate
      Tzflk = particle direction z-coordinate
      Txpol = x direction cosine of the particle polarization
      Typol = y direction cosine of the particle polarization
      Tzpol = z direction cosine of the particle polarization
*
      Dfnear = distance to the nearest boundary
      Agestk = age of the particle (seconds)
      Cmpath = cumulative path travelled by the particle since it was produced (cm) *
      Iloflk = particle identity (Paprop numbering)
      Igroup = energy group for low energy neutrons
      Loflk = particle generation
      Louse = user flag
      Nrgflk = particle region number
      Nlattc = particle lattice cell number
```

(TRACKR)

Transport of particles: particles are taken from the Stack and info for the particle during tracking are kept here

TRACK Recording

```
Ntrack = number of track segments
    Mtrack = number of energy deposition events along the track
0 < i < Ntrack
    Xtrack = end x-point of the ith track segment
    Ytrack = end y-point of the ith track segment
    Ztrack = end z-point of the ith track segment
1 < i < Ntrack
    Ttrack = length of the ith track segment
1 < j < Mtrack
    Dtrack = energy deposition of the jth deposition event
    Dptrck = momentum loss of the jth deposition event
    Ntrack > 0, Mtrack > 0 : energy loss distributed along the
                     track
    Ntrack > 0, Mtrack = 0: no energy loss along the track
    Ntrack = 0, Mtrack = 0: local energy deposition (the
                     value and the point are not re-
                     corded in Trackr)
 COMMON / TRACKR / XTRACK ( 0:MXTRCK ), YTRACK ( 0:MXTRCK ),
                       ZTRACK (0:MXTRCK), TTRACK (MXTRCK),
 &
                       DTRACK (MXTRCK), DPTRCK (3, MXTRCK),
 &
```

(TRACKR) : 2nd part

```
Jtrack = identity number of the particle: for recoils or
             kerma deposition it can be outside the allowed
            particle id range, assuming values like:
              208: "heavy" recoil
              211: EM below threshold
              308: low energy neutron kerma
            in those cases the id of the particle originating
            the interaction is saved inside JOtrck (which othe-
            rwise is zero)
      J0trck = see above
      Etrack = total energy of the particle
      Ptrack = momentum of the particle (not always defined, if
           < 0 must be obtained from Etrack)
   Cx,y,ztrck = direction cosines of the current particle
   Cx,y,ztrpl = polarization cosines of the current particle
      Wtrack = weight of the particle
      Wscrng = scoring weight: it can differ from Wtrack if some
             biasing techniques are used (for example inelastic
            interaction length biasing)
      Ctrack = total curved path
      Cmtrck = cumulative curved path since particle birth
```

(TRACKR) : 3rd part

&

```
Zfftrk = \langle Z eff \rangle of the particle
Zfrttk = actual Z_eff of the particle
Atrack = age of the particle
Wninou = neutron algebraic balance of interactions (both
      for "high" energy particles and "low" energy
      neutrons)
Wcinou = charge algebraic balance of interactions (for
      all interactions)
Spausr = user defined spare variables for the current
      particle
Ktrack = if > 0 neutron group of the particle (neutron)
Lt1trk = initial lattice cell of the current track
     (or lattice cell for a point energy deposition)
Lt2trk = final lattice cell of the current track
lprodc = flag for prompt(=1)/radioactive products(=2)
Ltrack = flag recording the generation number
Llouse = user defined flag for the current particle
Ispusr = user defined spare flags for the current particle
           SPAUSR(MKBMX1), STTRCK, SATRCK, TKNIEL, TKEDPA,
           WCINOU,
           IPRODC, ISPUSR(MKBMX2), LFSSSC, LPKILL
```

(FHEAVY)

```
npheav
                 = number of heavy secondaries
      kheavy(ip) = type of the secondary ip
              (3 = deuteron, 4 = 3-H, 5 = 3-He, 6 = 4-He,
               7-12 = "Heavy" fragment specified by Ibheav and Icheav ) *
      cxheav(ip) = direction cosine of the secondary ip with respect to x-axis *
      cyheav(ip) = direction cosine of the secondary ip with respect to y-axis *
      czheav(ip) = direction cosine of the secondary ip with respect to z-axis *
*
      tkheav(ip) = kinetic energy of secondary ip
      pheavy(ip) = momentum of the secondary ip
      wheavy(ip) = weight of the secondary ip
      agheav(ip) = "age" of the secondary ip with respect to the interaction time *
*
      amheav(kp) = atomic masses of the twelve types of evaporated *
               or fragmented or fissioned particles
      amnhea(kp) = nuclear masses of the twelve types of evaporated *
*
               or fragmented or fissioned particles
      anheav(kp) = name of the kp-type heavy particle
*
      icheav(kp) = charge of the kp-type heavy particle
*
      ibheav(kp) = mass number of the kp-type heavy particle
```

Note that kp = kheavy(ip) !!!

(PAPROP)

intrinsic PArticle PROPerties

```
* am (i) = i_th particle mass (GeV)
* ichrge(i) = electric charge of the i_th particle
* ibarch(i) = baryonic charge of the i_th particle
* ijdisc(i) = flag for discarding the i_th particle type
* tmnlf (i) = mean (not half!) life of the i_th particle (s)
* biasdc(i) = decay biasing factor for the i_th particle
* biasin(i) = inelastic interaction biasing factor for the i_th particle *
* lhadro(i) = True if the i_th particle type is a hadron
* jspinp(i) = i_th particle spin (in units of 1/2)
* iparty(i) = i_th particle parity (when meaningful)
*
```

(FLKMAT)

FLuKa MATerials

```
Amss(i) = Atomic weight (g/mole) of the i_th material
      Rho(i) = Density of the i_th material
      Ztar(i) = Atomic number of the i_th material
    AinIng(i) = Inelastic scattering length of the i_th material
             for beam particles at the average beam energy in cm *
    Aellng(i) = Elastic scattering length of the i_th material for
*
             beam particles at average beam energy in cm
*
     X0rad(i) = Radiation length of the i_th material in cm
    Dmgene(i) = Damage energy of the i_th material (GeV)
    Ainnth(i) = Inelastic scattering length of the i_th material
*
             for neutrons at threshold energy in cm
    Medium(k) = Material number of the k_th region
*
    Mssnum(i) = Mass number of the target nucleus for the i_th material *
*
*
             if =< 0 it means that it is in the natural isotopic composition *
    Libsnm(i) = flag whether inelastic interaction biasing must be done for this medium *
*
*
    Matnam(i) = Alphabetical name of the i_th material number
    Aocmbm(i) = Atomic density of the i_th material in barn^-1 cm^-1 *
*
             (Atoms Over Cm times Barn for Materials)
*
*
    Eocmbm(i) = Electron density of the i_th material in barn^-1cm^-1*
*
             (Atoms Over Cm times Barn for Materials)
```

(EVTFLG)

EVenT FLaGs:

Flags indicating the event interaction type:

```
LFLFVT = Flastic interaction
LINEVT = Inelastic interaction
LDECAY = Particle decay
LDLTRY = Delta ray production (Moller and Bhabha included)
LPAIRP = Pair production
LBRMSP = Bremsstrahlung
LANNRS = Annihilation at rest
LANNFL = Annihilation in flight
I PHOFI = Photoelectric effect
LCMPTN = Compton effect
LCOHSC = Rayleigh scattering
LLENSC = Low energy neutron scattering
LOPPSC = Optical photon scattering
LELDIS = Electromagnetic dissociation
LRDCAY = Radioactive decay
```

All LOGICAL variables!!!

stuprf.f and stupre.f (I)

SeT User PRoperties for Fluka <Emf> particles

These two functions are used to assign a value to one or more stack user variables when the corresponding particle is loaded onto one of the stacks (FLKSTK for hadrons/muons, and EMFSTK for electrons/positrons/photons). In each of these stacks the user has access to one integer variable, one integer array and one double precision array.

Each of them is copied to a correspondent variable or array in COMMON TRACKR at the beginning of transport:

Correspondence	FLKSTK	EMFSTK		TRACKR
integer variable:	LOUSE	LOUEMF	\longrightarrow	LLOUSE
integer array:	ISPARK	IESPAK	\longrightarrow	ISPUSR
double precision array:	SPAREK	ESPARK	\longrightarrow	SPAUSR

In this way, user variables can be PROPAGATED and KEPT in memory across tracking and interactions!

stuprf.f and stupre.f (II)

The user can access and modify user variables in TRACKR via subroutine MGDRAW and its entries ENDRAW, SODRAW and especially USDRAW.

STUPRF and STUPRE can be used to copy TRACKR user variables to those of the relevant stack.

Note that a stack OPPHST exists also for optical photons, containing similar user variables and arrays LOUOPP, ISPORK and SPAROK. They can be used in user routines, but they are not handled by STUPRE.

STUPRF is called before loading into stack hadrons, muons, neutrinos and low-energy neutrons. The default version copies to stack the user flags of the parent.

STUPRE is called before loading into stack electrons, positrons and photons. The default version does nothing (the user variables of the parent particle are already set equal to the original projectile by the various electromagnetic interaction routines). Also the region/position etc. are already set inside the stack arrays.

By default, the last place of the ISPARK array keeps the TRACK NUMBER of the current particle

Typical use of STUPRF/ STUPRE is to keep in memory the "history " of a particle

Stuprf: the default

IJ = ID of interacting particle MREG,XX,YY,ZZ: region and position of the interaction

SUBROUTINE STUPRF (IJ, MREG, XX, YY, ZZ, NPSECN, NPPRMR)

```
INCLUDE '(DBLPRC)'
INCLUDE '(DIMPAR)'
INCLUDE '(IOUNIT)'
INCLUDE '(EVTFLG)'
INCLUDE '(FLKSTK)'
INCLUDE '(TRACKR)'
```

END IF

RETURN

Suprf is called once for each particle in the stack of secondaries. NPSECN is the index of the current secondary, NPPRMR is the number of particles still flagged as "primary" (i.e. after elastic interaction

```
LOUSE (NPFLKA) = LLOUSE
DO 100 ISPR = 1, MKBMX1

SPAREK (ISPR,NPFLKA) = SPAUSR (ISPR)

100 CONTINUE
DO 200 ISPR = 1, MKBMX2

ISPARK (ISPR,NPFLKA) = ISPUSR (ISPR)

200 CONTINUE
```

This is the default: copy the TRACKR user variables to the stack.

* Increment the track number and put it into the last flag:
IF (NPSECN .GT. NPPRMR) THEN
IF (NTRCKS .EQ. 2000000000) NTRCKS = -2000000000
NTRCKS = NTRCKS + 1
ISPARK (MKBMX2,NPFLKA) = NTRCKS

By default: if this Particle is new, consider it as a new track.

Stuprf: an example (I)

The user need: keep the history of neutrino production from a proton beam The reaction scheme is: Proton on thick target-> mesons -> decay into leptons and neutrinos. reinteractions and multiple decay ($\pi \rightarrow \nu + \mu \rightarrow \nu + \nu + e$) Want to know: which particle decayed, and where, where was produced the meson that decayed and its initial mom.

```
* if decay : store father identity, energy , r,z
IF ( LDECAY ) THEN
SPAREK (1,NPFLKA) = ETRACK
SPAREK (2,NPFLKA) = SQRT ( XX**2 + YY**2 )
SPAREK (3,NPFLKA) = ZZ
ISPARK (1,NPFLKA) = IJ

* If inelastic interaction
ELSE IF ( LINEVT ) THEN
```

ISPARK (2, NPFLKA) = KPART (NPSECN)

ISPARK (3,NPFLKA) = MREG

SPAREK (4,NPFLKA) = XXSPAREK (5,NPFLKA) = YY LDECAY, LINEVT : from common EVTFLG

Store in the first users variables the energy and identity of the decaying particle, and the position

Use more variables to store the id and momentum of each particle from inelastic interaction

SPAREK (6,NPFLKA) = ZZ

SPAREK (7,NPFLKA) = PLR(NPSECN) * CXR (NPSECN)

SPAREK (8,NPFLKA) = PLR(NPSECN) * CYR (NPSECN)

SPAREK (9,NPFLKA) = PLR(NPSECN) * CZR (NPSECN)

Stuprf: an example (II)

In between interactions/decays, the user variables are copied WITHOUT CHANGES to the trackr common, and back to the stack. They are propagated to i.e. decay secondaries (neutrinos) by the default lines in the stuprf.f routine.

They are accessible from the TRACKR common at every moment. The user can dump them on disk from, for instance, the mgdraw.f routine (see lecture on scoring for details)

```
* if I am in detector and it is a neutrino
IF ( NEWREG = MYDETREG) THEN
IF ( JTRACK .EQ. 5 .OR. JTRACK .EQ. 6 .
```

Particle indeces of neutrinos

- & OR .JTRACK .EQ. 27 .OR. JTRACK .EQ. 28) THEN WRITE (MYDUMP , *) 'dump event ', NCASE
- & JTRACK, SNGL(ETRACK),
- & (ISPUSR(I), I=1,3),
- & (SNGL(SPAUSR(I)), I=1,9),
- & SNGL(WEE)

ENDIF ENDIF

Written: event number, neutrino ID, neutrino energy, ID of decaying particle, ID of ancestor from last inelastic int., Position of decay, position of last inel.int., momentum of the ancestor from the last inel. Int.

Recover the infos in the TRACKR user arrays and dump them

mdstck.f

MDSTCK is called after a nuclear interaction in which at least one secondary particle has been produced, before any biasing is applied, to decide which secondary will be loaded in the main stack for further transport.

The properties of the secondaries are stored in the secondary stack (COMMON GENSTK). With MDSTCK, users can analyse those secondaries, write them to a file, or even modify the content of GENSTK (for instance applying their own biasing).

In the latter case, however, it is their responsibility to make sure that energy is conserved, the various physical quantities are still consistent, etc.

usrmed.f (I)

USeR MEDium dependent directives

Argument list

IJ : particle type

EKSCO : particle kinetic energy (GeV)
PLA : particle momentum (GeV/c)

WEE : particle weight

MREG : previous region number NEWREG : current region number XX, YY, ZZ : particle position

TXX, TYY, TZZ : particle direction

Subroutine USRMED is activated by option MAT-PROP with SDUM = USERDIRE, for one or more materials indicated by the user. It is called every time a particle is going to be transported in one of the user-tagged materials.

usrmed.f (II)

Two cases are possible

- 1) MREG = NEWREG: the particle is going to move from a point inside the medium. The user is normally allowed to change only the particle weight. simulating *attenuation* of optical photons in an absorbing medium by reducing the photon weight
- 2) MREG # NEWREG: the particle is going to move from a point on a boundary between two regions. The user may change any of the following: particle weight, current region number, direction cosines.
- simulating *refraction*, by changing the direction cosines so that the particle is still inside the new region. To do this, one generally needs the direction cosines of the normal to the surface: TXNOR(NPFLKA), TYNOR(NPFLKA), TZNOR(NPFLKA) (COMMON FLKSTK must be included) simulating *reflection* (albedo) at a boundary. The direction cosines must be modified according to some reflection law or albedo angular distribution, and NEWREG must be set = MREG In both cases the weight can also be reduced to account for surface reflectivity
- But ... one can also kill the particle by putting WEE=ZERZER (note that its energy will be lost and not deposited)
- and particle coordinates and energy can be altered as well !!

a big power implies a big responsibility

Mathematical library

FLUKA contains many mathematical routines of general utility, so in general it should not be necessary to call external mathematical libraries (many taken from SLATEC):

flgaus: Gaussian adaptive integration

erffun: Error function

expin1: E1 exponential function

besi0d: Bessel function I0 (also I1, J0, J1, K0, K1)

dawsni: Dawson function

gamfun: Gamma function

radcub: Real solutions of 3rd order algebraic equation

flgndr: Legendre polynomials

yinter, d..intp: 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.

A few examples (I)

EXTERNAL FINTEG
DOUBLE PRECISION FUNCTION **FLGAUS** (FINTEG, XA, XB, EPSEPS, IOPT, NXEXP)

* Adaptive Gaussian quadrature routine

It gives the integral over the (XA,XB) interval of the product between X**NXEXP and the FINTEG function, to be coded by the user as a separate DOUBLE PRECISION FUNCTION FINTEG (X)

SUBROUTINE RADCUB (AAO, AA1, AA2, AA3, X, X0, NRAD)

* Real solutions of 3rd order algebric equation

It computes real solutions of the equation:

$$A0*X^3++A1*X^2+A2*X+A3=0$$

The solutions are put in the array X; if there is only one real solution it is put into X(1), while X(2) and X(3) are set to 1.d32. If A0=0 the routine computes standard solutions of a second or first degree equation. If it doesn't exist any real solution the whole array X is set to 1.d32. It is possible to compute solutions with a scale factor X0, to avoid loss of significancy with very large or very small numbers. The flag NRAD records the number of real solutions found.

A few examples (II)

DOUBLE PRECISION FUNCTION GAMFUN (X)

It calculates the double precision complete **Gamma function** for double precision argument X

SUBROUTINE RORDIN (RVECT, ICORR, LEN)

It rearranges a real array in increasing order

SUBROUTINE RORDDE (RVECT, ICORR, LEN)

It rearranges a real array in decreasing order

DOUBLE PRECISION FUNCTION FLGNDR (X, LMAX, PLGNDR)

* Function for **LeGeNDRe polynomials**

It computes P_{lmax} (x) and stores all values P_i (x) for $i\!=\!0$, lmax into the PLGNDR array