The FLUKA Code: Insight and new features


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News:
Courses Update (04.06.2009)
The 9th FLUKA Course will be held in Mumbai at the Bhabha Atomic Research Centre (India).
Registration is completed!
A A A
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For more info see for about page and manuals.
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FLUKA Description

- FLUKA is a general purpose tool for calculations of particle transport and interactions with matter, covering an extended range of applications: from proton and electron accelerator shielding to target design, calorimetry, activation, dosimetry, detector design, Accelerator Driven Systems, cosmic rays, neutrino physics, radiotherapy etc.
- 60 different particles + Heavy Ions
  - Hadron-hadron and hadron-nucleus interaction "0"-10000 TeV
  - Electromagnetic and μ interactions 1 keV – 10000 TeV
  - Nucleus-nucleus interaction up to 10000 TeV/n
  - Charged particle transport and energy loss
  - Neutron multi-group transport and interactions 0-20 MeV
  - ν interactions
  - Transport in magnetic field
  - Combinatorial (boolean) and Voxel geometries
  - Double capability to run either fully analogue and/or biased calculations
  - On-line evolution of induced radioactivity and dose
  - User-friendly GUI interface thanks to the Flair interface

Full mixed field capability

- Maintained and developed under CERN-INFN agreement and copyright 1989-2010
- More than 3000 users all over the world

http://www.fluka.org

Preliminary considerations:

What this course is not about:

This is an advanced course, no detailed instructions will be given on

- Installing and running the code
- Using the basic Flair features
- Writing/debugging a simple geometry
- Writing/debugging a simple input file
- Use the built-in scoring , and process the results

Moreover, there will be no lecture on the physics embedded in the code.

However, a few reminders / summaries will be provided

What is course is about:

- New features in fluka
- A bit of the internal structure of the code
- Advanced geometry issues
- Advanced biasing
- User routines, with examples
- And in general how to exploit at best the code

This is the first advanced course: please be patient and give feedback!!!

Release / Registration

- You received a USB stick with a pre-release of fluka2010.2. This is an alpha version prepared for this course, so that you can already profit from all the new features of fluka2010
- If you are not a registered user, PLEASE REGISTER NOW on the fluka web site
- The pre-release that you have is for your personal use only, and not intended for routine work and/or publication
- Please download the public fluka2010 version as soon as it is available on the web site
- Please report any crash/bug /whatever you may find in the pre-release to fluka-alpha@fluka.org , NOT to the fluka-discuss list (until next release of course), with [fluka2010] in the subject (include square brackets)

New features in Fluka2010

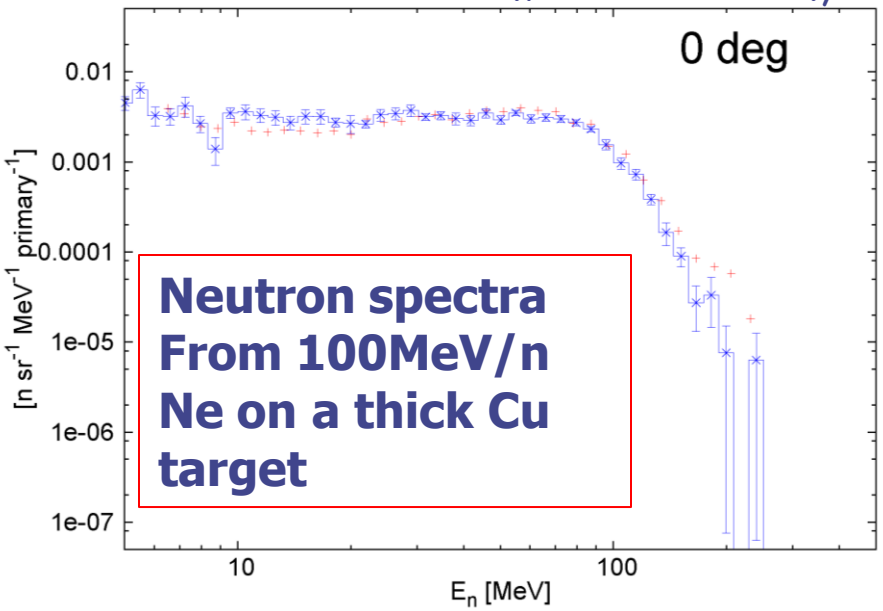
- The low energy ion interaction generator (BME) is now included
- The peripheral interaction part of BME has been deeply improved
- The detailed treatment of electron profiles in Compton scattering is now the default for all "precision" defaults
- The treatment of specific energy losses has been reworked, with the addition of Z^3 (Barkas) and Z^4 (Bloch) corrections, re-calculation of shell corrections and effective charges.
- The Landau-Pomeranchuk-Migdal (LPM) effect is now added to pair production (was already in bremsstrahlung)
- Radiation damage to materials can now be simulated, both as NIEL (non-ionizing energy losses) and DPA (displacements per atom)
- In addition to the standard beams, sources distributed in volumes are now available, as well as a colliding beams source.

New features in Fluka2010

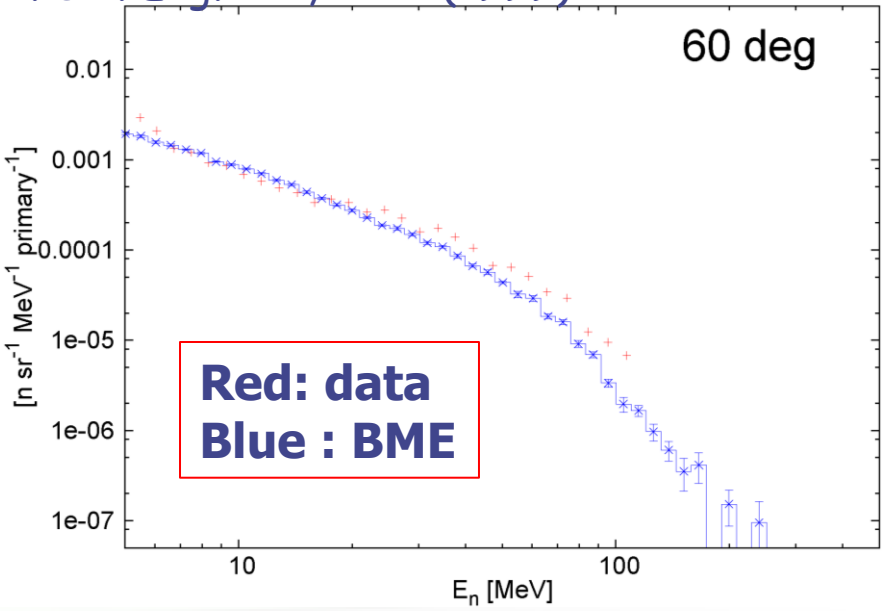
- A few compounds of dosimetric interest are now available as pre-defined materials
- The generic quadric body has been added in the geometry
- Tranformations (roto-translation and scaling) of bodies are now possible
- Scoring of net deposited charge has been introduced
- Scoring of arrival time is available in USRYIELD (for TOF)
- DOSEQLET : dose equivalent obtained folding with Q(LET) from ICRP60
- The #include directive is available for the input file
- A new FLUKA user license has been adopted, very similar to the previous one in the substance, please however read it.

New BME benchmarks

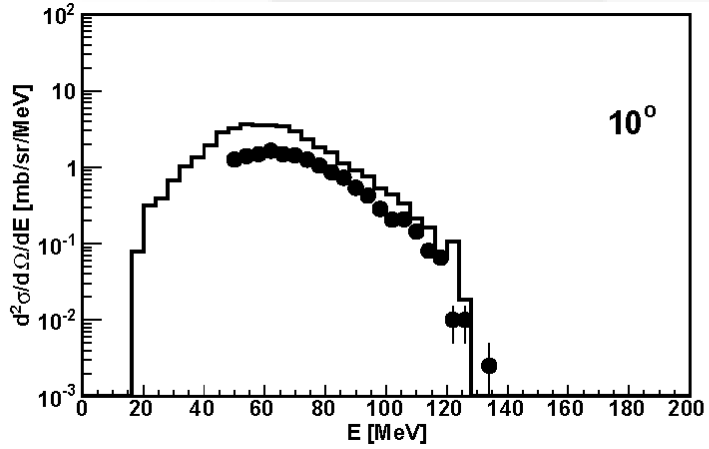
Data : T.Kurosawa et al., Nucl. Sci. Eng. 132,30-57(1999)

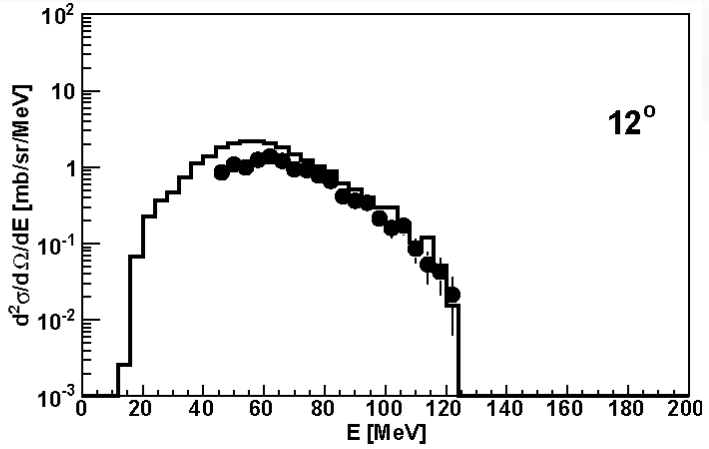


Neutron spectra From 100MeV/n Ne on a thick Cu target



Red: data Blue : BME





Double diff. F production from C+C at 13 MeV/n

Data (dots) : courtesy of S.Foertsch et al., iThemba labs, South Africa

Some reminders:

- The present version works only with the g77 compiler. For 64 bit computers, the 32 bit compatibility packages are required. The gfortran version will come with the release
- On Windows, a virtual-machine package can be installed
- The code is in fortran (mostly fortran 77), as well as all user routines.
- The high energy heavy ion interaction generators are external, if needed they have to be linked with the program using the ldpmqmd(bme) script. There are two of them, depending on the energy range: DPMJET (E/A >5 GeV), rQMD (E/A > 100 MeV)
- From the final release on, the low energy ion interaction generator (BME) will be part of the standard Fluka library (no need for specific linking)
- Units: ***GeV, g, cm, second, radian,*** with a few exceptions (for instance the Ionization potential is in eV, as well the DPA damage threshold)

Some reminder: the FLUKA input file jargon

The FLUKA input file is an ascii file containing the COMMANDS

Command:

One keyword, 6 floating point numbers, one keyword

Example (fixed format, FREE format is available as well):

```
*...+....1....+....2....+....3....+....4....+....5....+....6....+....7....+...
BEAM            1.E+04        0.0        0.0        0.0        0.0        0.0PROTON
*
*keyword     momentum mom.spread  diverg.   X-width   Y-width     flag  particle
*             WHAT(1)    WHAT(2)   WHAT(3)   WHAT(4)   WHAT(5)   WHAT(6)     SDUM
```

- **We refer to commands also as: cards, options, directives, definitions**
- **We refer to input parameters as WHAT's**
- **Command keywords must be in uppercase, fixed or free format**
- **Some commands require more than one "card"**
- **Generally, with few exceptions, the order of commands is irrelevant**
- **Most commands can be issued several times and each next commands adds information or overrides (in total or in part) the previous ones**
- **A line with a * character in column 1 is treated as a comment**
- **Nearly always there are default values for WHAT() values!**
- **Now most of the difficulties in building of the input file are managed by the FLAIR graphical interface**

Some reminders:

- The code works under IMPLICIT DOUBLE PRECISION for variables in the range (A-H,O-Z). ***Don't forget ..D+/-xx*** (eg 2.3D+00, 7.8D-03) in all numerical settings in user routines, and ***be careful in passing variables*** to/from Fluka or external packages (eg CERNLIB) routines
- Most mathematical and physical constants are predefined inside the (DBLPRC) include, ***use them whenever possible!***
- Compilation flags are already included in the fff script and should never be changed. The script should be used for user routines as well
- ***Floating point exceptions*** are enabled (hard-wired!!) and ***dump core*** size set to infinity at the start of each run
- If ***high precision input*** (> 10 digit) is required, FREE format can be invoked → no limit

Some reminder: the FLUKA particles

The list of particles transported by fluka is in the manual. Each particle is defined by a NAME and a NUMBER.
Only a few heavy ions have a predefined name and a number, the others are defined by A and Z

FLUKA name	FLUKA number	Symbol	Common name	Standard PDG number (Particle Data Group) [120]
4-HELIUM (1)	-6	α	Alpha	—
3-HELIUM (1)	-5	^{3}He	Helium 3	—
TRITON (1)	-4	^{3}H	Triton	—
DEUTERON (1)	-3	^{2}H	Deuteron	—
HEAVYION (1)	-2	—	Generic Heavy Ion (see command HI-PROPE)	—
OPTIPHOT	-1	—	Optical Photon	—
RAY (2)	0	—	Pseudoparticle	—
PROTON	1	p	Proton	2212
APROTON	2	$\bar{p}$	Antiproton	-2212
ELECTRON	3	e^-	Electron	11
POSITRON	4	e^+	Positron	-11
NEUTRIE	5	ν_e	Electron Neutrino	12
ANEUTRIE	6	$\bar{\nu}_e$	Electron Antineutrino	-12

Beginning Of the list, More follows

There exists also GENERALIZED particles, essentially used for scoring: ex

ALL-NEGA	204	All negative particles
ALL-POSI	205	All positive particles
NUCLEONS	206	Protons and neutrons
NUC&PI+-	207	Protons, neutrons and charged pions
ENERGY	208	For dose scoring: Deposited energy For energy fluence scoring: Kinetic energy
DPA-SCO	239	Displacements per atoms
DOSE-EQ	240	Dose Equivalent (pSv) (6)

Some reminders : neutrons

- Transport and interactions of neutrons with energies below 20 MeV are handled by a dedicated library
- Neutron interactions at higher energy are handled by FLUKA nuclear models
- In the FLUKA jargon neutrons below 20 MeV are called **low energy neutrons**
- The low energy neutron library uses a multigroup approach
- About 230 material/temperature combinations are available
- The library handles also gamma generation, energy deposition by kerma factors, residual nuclei production, secondary neutrons, fission neutrons, and NIEL
- For some isotopes/materials: self shielding, molecular binding, correlated gamma generation, point-wise transport

Reminder: radioactive isotopes

- In FLUKA, the production, build-up and decay of radioactive isotopes can be simulated within the same run
- Radioactive isotopes can also be used as source particles
- Caveat : the production of **metastable** states is not simulated by the Fluka nuclear models. When radioactive build-up/decay is requested, it is assumed that the initial isotope production is equally distributed (half-half) between the ground state and the (possible) metastable state. However, **metastable** states in the subsequent decay chain are populated and decayed according to the correct branching ratios

Events, statistics, normalization

- In a MonteCarlo code, the result is an estimator of the desired quantity, and is obtained as the average over many trials
- Mathematically, the MC treatment is based on the central limit theorem
- The higher the number of trials, the better the error on the estimator
- In particle transport MC, a trial is the full history following the primary event
- The primary event may be represented by a single particle in a beam (the most common situation), or by a more complex source event, like for instance the decay of a radioactive isotope or the products of an interaction. Therefore, a primary, or source, event may be composed by several particles.
- The estimators are obtained averaging over the number of primary events: therefore all results in FLUKA are given normalized per primary event.
- Nevertheless, event-by-event quantities are also available from the code and/or can be accessed through user routines. Event-by-event information is useful when correlations among estimators are required.

Reminder: biased and analogue

- Fluka can run both in fully analog and in biased mode
- BIASING techniques allow to improve the statistical convergence of results in a selected region of the problem phase space (see lecture)
- This is done using modified distributions, and associating corresponding weights to particles
- However, the statistical convergence usually worsens in other phase space regions
- BIASING does NOT reproduce correlations among different components of the same event
- BIASING may not reproduce fluctuations of physical quantities
- The type of calculation has to be chosen with care!

Initialization

- The input cards are parsed according to an optimized ordering different from the order in the input file.
- Names are converted to numbers for the internal use. The correspondence is kept and is accessible
- Geometry data are decoded and stored
- User scoring is decoded, checked, memory space is allocated
- External data files (cross sections etc) are read in and processed
- Neutron cross section sets are read in for used materials
- Tabulations of partial and total cross sections are generated for the materials in use: dE/dx, bremsstrahlung, pair production..
- The energy range and the granularity of these tabulations depend on the energy limits of the problem, essentially on the BEAM card definition and on the production thresholds
- All these quantities, including allocations for scoring, are stored in the Fluka BLANK COMMON. Pointers are kept to the different areas.

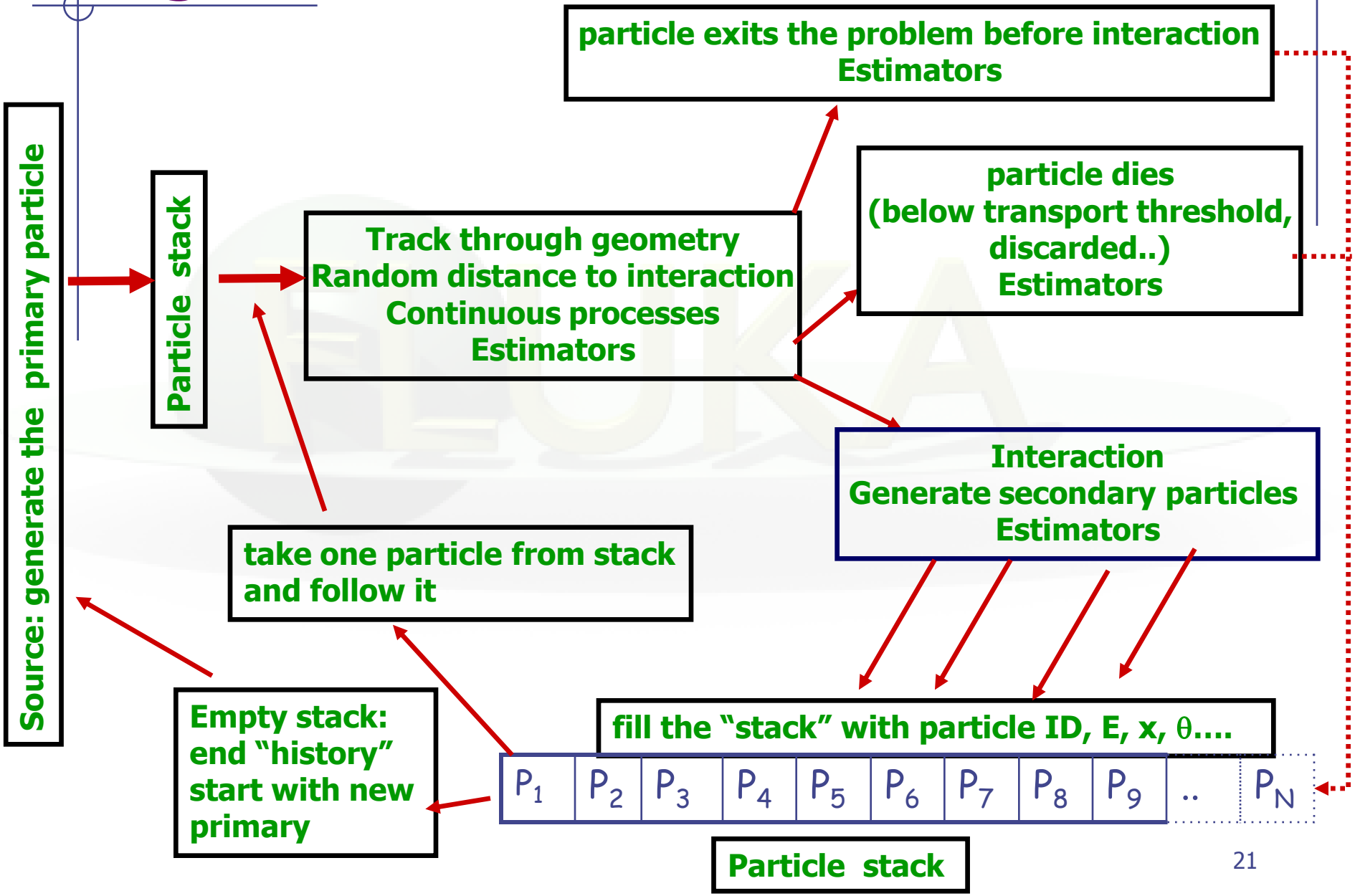
Consequences

- The TOTAL amount of memory is limited. At present the blank common dimension is about 400MB : to be kept in mind when asking for estimators
- The amount of information, thus of memory used, grows with the number of regions and materials used
- User settings have an impact on initialization of physical processes

Order of input cards parsing

1. DEFAULTS GLOBAL ROT-DEFI TITLE USRGCALL
2. BEAM BEAMAXES BEAMPOS BME DISCARD DPMJET EMF EVENTYPE GEOBEGIN HI-PROPE MATERIAL MCSTHRES PART-THR PHYSICS POLARIZAtion RQMD SOURCE SPECSOUR THRESHOLd
3. COMPOUND RADDECAY RANDOMIZe
4. DETECT WW-FACTO WW-PROFI WW-THRES ASSIGNMAt CORRFACT DCYTIMES DELTARAY ELCFIELD EMF-BIAS EMFCUT EMFFIX EMFFLUO EXPTRANS FLUKAFIX IONFLUCT IRRPROFI LAM-BIAS LOW-BIAS LOW-DOWN LOW-MAT MAT-PROP MGNFIELD MULSOPT MUPHOTON OPT-PROD OPT-PROP PAIRBREM PHOTONUC STERNHEI
5. EVENTBIN EVENTDAT RESNUCLEi SCORE TIME-CUT USERDUMP USERWEIG USRBDX USRBIN USRCOLL USRTRACK USRYIELD
6. AUXSCORE DCYSCORE ROTPRBIN TCQUENCH
7. PLOTGEOM START
8. USROCALL STOP

A generic MC scheme



The stack, secondary particles, tracks

- The properties of all the particles to be tracked are stored in the "stack": /flkstk/ in '(FLKSTK)'`
- NPFLKA counts the particles on stack
- The kaskad routine loops on NPFLKA until the stack is empty, going from bottom (npflka) to top (1)
- The "current particle" properties are copied from the stack to the TRACKR common, and updated during tracking
- At each interaction, secondaries are first stored in temporary stacks (GENSTK, FHEAVY..), then loaded on the main stack. The primary particle, if surviving, is loaded on the stack exactly like the others
- The particle on top of the stack is followed first, generally it is the less energetic, → avoid stack explosion
- The treatment of the stack for EM particles is slightly different, due to historical reasons EM secondaries are kept on the EMF particle stack , which is emptied before the normal stack

Consequences

- Steps related to the same particle track will (almost) always be non-consecutive in the program flow.
- Primary particles lose their identity as soon as an interaction occurs (this is physical!)
- Therefore, "follow a particle track" may be not straightforward
- However, a "track number" is associated to each "new" particle and is propagated to the stack and the TRACKR common (see dedicated lecture)
- Moreover, the generation level of each particle is recorded

Main loop

- The loop on events is controlled by the FEEDER routine.
  - It checks for run termination conditions (number of primaries)
  - calls the standard fluka source(s) or the user source,
  - May call the SODRAW, user routine
  - then gives the control to the KASKAD routine
- KASKAD keeps the control until the stack is empty. It handles directly the tracking of hadrons, ions and muons, while it dispatches
  - E.M particles to KASEMF,
  - Optical photons to KASOPH
  - Low energy neutrons to KASNEU
  - Heavy particles to KASHEA if approximate treatment is asked for
- Tracking is performed in steps , limited by
  - Maximum percentage energy loss in a step
  - Boundary crossing
  - Elastic and inelastic interaction probability
  - Decay probability

Discrete or continuous

- During, and at the end, of a step : discrete and continuous processes
- Continuous: Energy deposition by Ionization, bremsstrahlung, and pair production (below explicit production thresholds)
- Continuous: multiple scattering, deflection by magnetic field
- Discrete: interaction (including low energy neutron ones), particle decay, δ ray production, radioactive decay
- Discrete: track termination conditions, such as time cutoff, energy cutoff, escape in the black hole, boundary crossing
- Estimators can be activated for each of these processes, either built-in, or through user routines
- Tricky: energy deposition by recoil nuclei after elastic reactions (and after inelastic with some settings) and energy deposition by low-energy neutron reaction products (with exceptions..) are treated as discrete events.

Biasing

- At every interactions/boundary crossing/ step biasing is applied if required.
- If necessary, the particle weight is modified, and stored in TRACKR and propagated to the stack.
- Particle weights are automatically taken into account by built-in estimators
- User scoring routines must take care of proper weight handling.

end

kaskad

:stack: DO ! Stack possible secondaries and/or radioactive products

If(stack of secondaries not empty) Load secondaries on primary stack FLKSTK from GENSTK until empty

Else(stack of secondaries empty) load: radioactive residuals, optical photons, if any

If FLKSTK empty, exit :stack: DO ! return to FEEDER

Process the primaries

Download a particle from FLKSTK to TRACKR

If(heavy ion & not DPMJET) → *heavy fragment approximate transport*

If(e+e−*γ*) → *treatment of EM showers;*

If(n & E<20MeV) → *treatment of low E neutrons ;*

If(age > time cutoff) **→ *time-kill***

If(kinetic energy *< threshold)* → *particle below threshold*

:nextint: DO ! Selection of next interaction and transport

If(blackhole) → *escape; If(age > time cutoff)* → *time-kill*

If(kinetic energy *< threshold & not vacuum)* → *particle below threshold*

Select the next interaction point

Select the transport method:

If(Not Vacuum & Charged particle) → *Moli`ere multiple scattering + ionisation*

Else(Vacuum OR Neutral particle) → *Vacuum OR neutral particle*

Kaskad-II

→Molière multiple scattering + ionisation
If(age *> time cutoff)* → *time-kill;*
If(kinetic energy < threshold) → *particle below threshold*
:ustep: DO ! Ustep loop Compute max step size allowed,
accounting for Bethe, boundary proximity etc., or
distance to next single scattering
:mulscat: DO ! Multiple scattering loop
Check the geometry, with or without magnetic field:
Move particle by resulting step in resulting direction
Various possibilities: step too short, step back +
single scatt., global single scatt. requested,
no scattering etc.
If(new region) → *boundary crossing;*
If(age > time cutoff) → *time-kill*
If(kinetic energy *< threshold)* → *part. below thres.*
If(no interaction) cycle :ustep:
If(interaction),
random selection:
→ *inelastic interaction;* → *elastic interaction;*
→ *EM dissociation ;* → *radioactive decay;* → *delta ray;*
→ *high-energy pair production;* → *high e bremsst.*
END DO :mulscat:
END DO :ustep:

Kaskad-III

→ *Vacuum OR neutral particle*
:vacneu: DO ! Vacuum OR neutral particle
If(new region) → *boundary crossing;*
If(age > time cutoff) → *time-kill*
Random selection:
→ *inelastic interaction;*
→ *elastic interaction;* → *decay*
If(residual mfp *> 0) cycle :vacneu:*
END DO :vacneu:

→ *Boundary crossing*
If(new region is blackhole) → *escape;*
If(age > time cutoff) → *time-kill*
If(*γ or e± not in vacuum)* → *treatment of EM showers*
If(*γ or e± in vacuum) cycle :nextint:*
If(kinetic e *< threshold & not vacuum)* → *part. Bell. thresh*
If(kinetic energy *< threshold & vacuum) cycle :nextint:*
END DO :nextint:

end