

The FLUKA Code: Insight and features



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Last version:

FLUKA 2011.2.15, September 9th 2012 (last respin) FLAIR 1.0.0

News:

Fluka Release (10.08.2012)

FLUKA 2011.2.14 has been released.

A A A

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Jefferson Lab







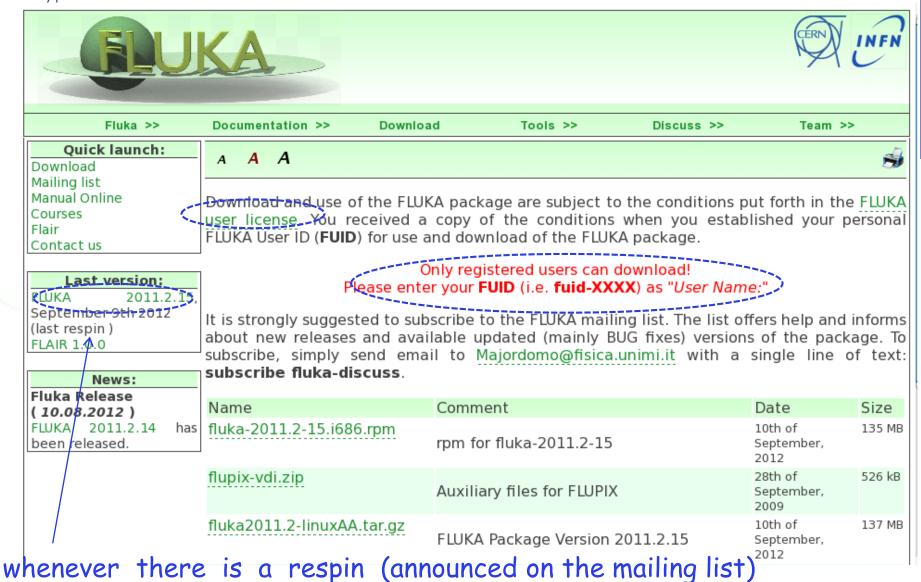








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please update your installation FLUKA Advanced Course

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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
 - > n 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
- Maintained and developed under CERN-INFN agreement and copyright 1989-2014
- More than 7000 registered users

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 this 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 course relies heavily on the experience of past advanced courses: feedback is welcome!!!

Release / Registration

- □ You received a USB stick with Fluka2014.5pre (pre-release/alpha version of Fluka2015), that is *not* yet publicly distributed. The public release will occur in 2015
- □ If you are not a registered user, PLEASE REGISTER NOW on the fluka web site
- This pre-release should not be used for scientific work, neither results obtained with this pre-release should be used for any project, publication or comparison. Its use is strictly limited at getting a flavour of the new features
- □ Please download the public fluka2015 version as soon as it will available on the web site sometimes next year
- Bugs/questions related to this pre-release version should be addressed to fluka-discuss@fluka.org only if strictly necessary, with the tag [fluka2014] in the subject

Important notice:

 PEANUT has been extended to cover the whole energy range since several years. The extended PEANUT is NOW THE DEFAULT at all energies, that is the default is now the equivalent of:

PHYSICS 100000. 100000. 100000. 100000. 100000. 100000. PEATHRESH

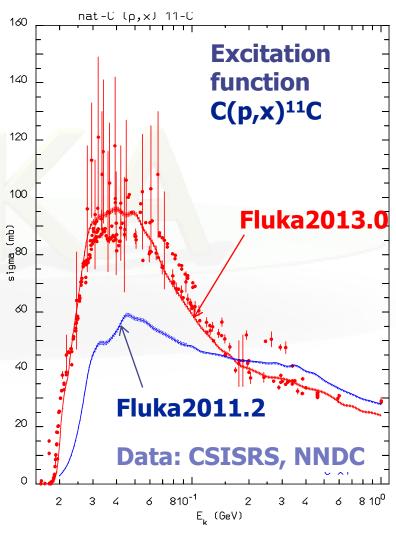
 Coalescence and heavy evaporation are still required to be activated explicitly for precise calculations (hopefully changed for the final release at least for coalescence):

PHYSICS 1. COALESCE

PHYSICS 3. EVAPORAT

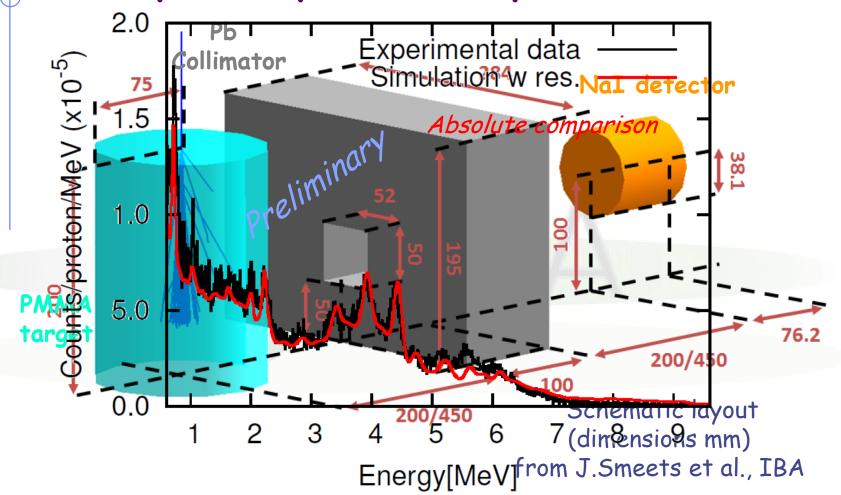
New features in low energy nuclear int.

- \blacktriangleright Direct (p, α) reactions introduced for light nuclei
- New model for "first interaction" deuteron production 140 for light nuclei
- General cleanup/retuning of PEANUT for p/n at low energies
 - Example: effect on the production of β^+ emitters, important for medical (PET on line) applications
- > De-excitation γ angular distribution according to multipolarity and spin orientation
- Example of prompt photon emission: see next slide





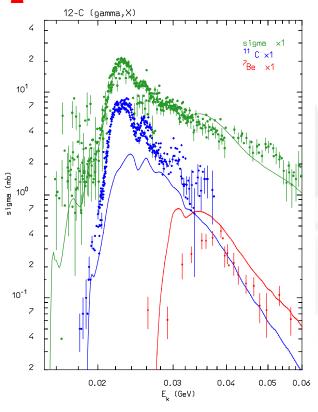
Photon yields by 160 MeV p in PMMA ENVISION



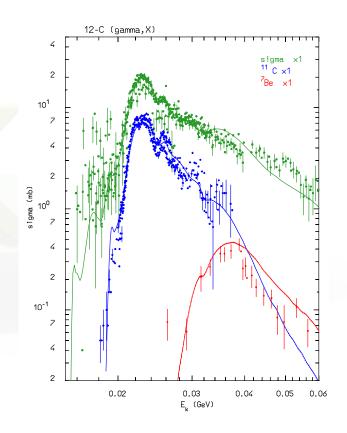
Energy spectrum of "photons" after background subtraction (collimator open collimator closed) for 160 MeV p on PMMA. FLUKA red line, data black line (J. Smeets et al., IBA, ENVISION WP3)
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New features in Fermi break-up

Account for initial spin and parity, when known, in Fermi break-up \rightarrow major improvement for (γ, x) reactions on light targets.



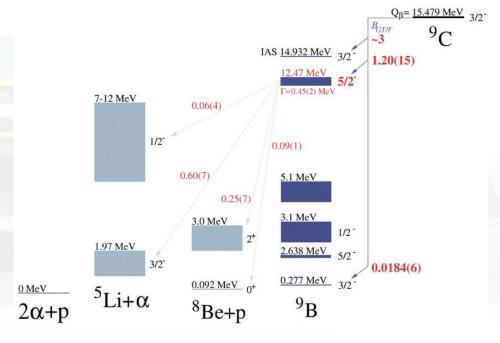
12C + γ in GDR \Rightarrow J $^{\pi}$ = 1 $^{-}$ \Rightarrow 3 α and α + 8 Be impossible in L=0 \Rightarrow Factor 3 on 11 C production



Broad 8-Be* 1st excited state now accounted for in Fermi break-up

New features in Decays etc

- ullet Emission of α particles in radioactive decays added
- Special decay model for 9-C



- New masses/half-lives/decays/radiations database
- Branchings for isomer production by neutrons below 20 MeV now based on JEFF activation file and no longer on a naive 50-50% assumption 3rd FLUKA Advanced Course

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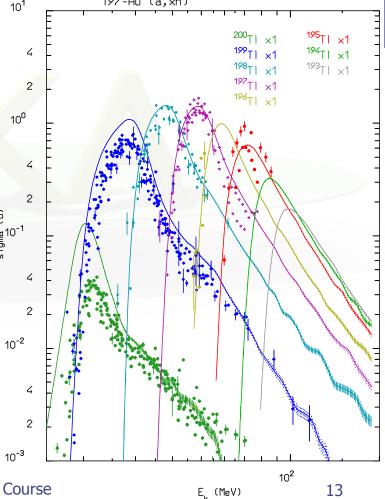
New features in ion-ion generators

 Nuclear discrete levels accounted for in BME, rQMD and DPMJET interactions when considering fragment excitation

(Initial) extension of BME to A=3 projectiles

 BME coupled with Peanut preequilibrium for configurations where the BME native preequilibrium is not available -> major improvement in the description of alpha (and not only) induced reactions

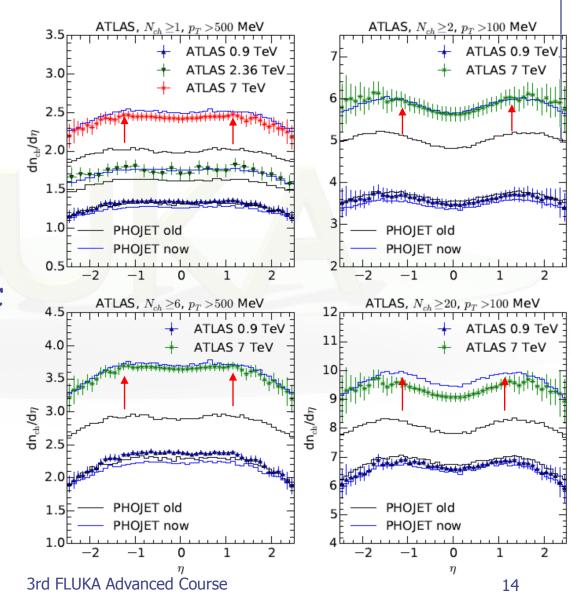
Excitation functions for the production of radioisotopes from α interactions on Au (left) and Pb (right) (Data: CSISRS, NNDC)



197-Au (a,xn)

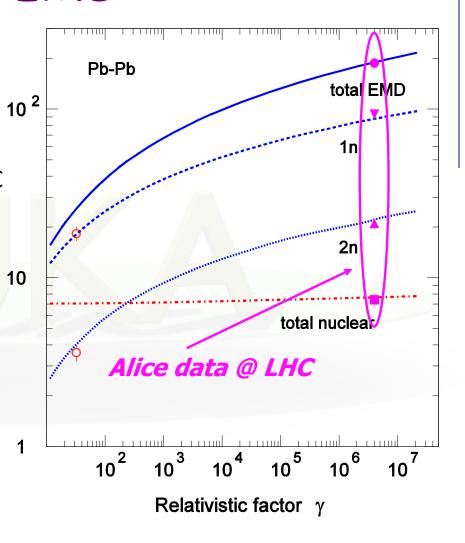
New features in Dpmjet-3 ATLAS - Charged particle pseudorapidity density.

- Dpmjet-3 used for heavy ion interactions above
 GeV/A, pp and hA above 20 TeV
- Major revision with significant improvement of agreement with LHC data
- New model for high energy p/pbar-p elastic and total cross sections and elastic scattering



New features in EMD

- General improvement of ElectroMagnetic Dissociation (EMD), now including the E2 multipolarity → important at low energies and for µ[±] and e[±]
- \triangleright EMD extended to μ^{\pm} below the γ -N threshold
- EMD extended to e[±] → electronuclear interactions now implemented (see exercise)
- Deuteron Coulomb dissociation (stripping). Please note nuclear stripping not yet implemented



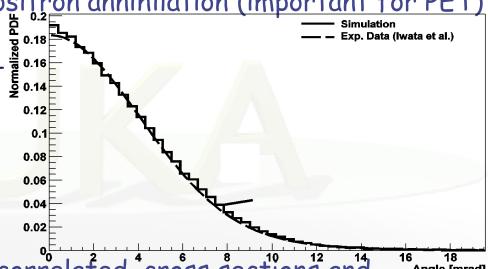
Cross section (b)

More new features...

 Improvement of the transition between the resonance and DPM models for Nucleon-Nucleon interactions

Acolinearity model for positron annihilation (important for PET)

Example: deviation from γ - γ co-linearity after positron annihilation in H_2O , FLUKA(line) vs data (histo)



- □ Neutron pointwise, fully correlated, cross sections and Angle [mrad] interactions for 2-H, 3-He and 4-He
- Synchrotron radiation generation through a new SPECSOUR option (see lecture on sources)
- Offset dipole and IGRF11 magnetic field tracking for cosmic ray module (see lecture on cosmic rays)

Technical improvements

- > Alternate material for radioactive decays extended to support whichever material, not only vacuum
- New DEFAULT: DAMAGE for DPA calculations
- > Revised DEFAULTS, towards better precision in general
- Possibility to assign numeric or character values to preprocessor codewords and then use them in the input file
- Extension of signed rotation indexes to lattices and geometry, even in preprocessor parameterized form
- Multiple DETECT estimators with arbitrary number of channels
- New generalized estimators for (rough) Single Event Upset estimates: HEHAD-EQ, THNEU-EQ

Technical improvements -II

- New generalized estimators: LGH-IONS, HVY-IONS, E+E-GAMM, DOSE-H2O, LOWENNEU, NTLOWENE, ALL-IONS
- > Blank common (initial) dynamic memory allocation now possible, and further run-time dynamic allocation for usrbins and voxels, obviously on the gfortran version only
- > Alarm set up to catch TERM signals and stop runs cleanly
- EMD cross sections for the projectile and all charged hadrons/leptons tabulated at initialization (improved speed)

Some reminders:

- □ The present version works with the g77 (32 bit) and gfortran compilers (64 bit). For 64 bit computers, if you wish to use the 32 bit, g77, version compatibility packages are required
- gfortran >= 4.6 required, to avoid mis-compilations
- On Windows, a virtual-machine package can be installed
- □ The code is in fortran, 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 script. There are two of them: DPMJET-3 (E/A > 5 GeV), rQMD (E/A > 100 MeV)
- □ The low energy ion interaction generator (BME) is 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):

```
*...+....5....+....6....+....7....+...4....+....5....+....6....+....7....+...
              1.E+04
                            0.0
                                      0.0
                                                0.0
                                                           0.0
BEAM
                                                                     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 <u>commands</u> also as: <u>cards</u>, <u>options</u>, <u>directives</u>, <u>definitions</u>
- We refer to <u>input parameters</u> as <u>WHAT's</u>
- 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
 - > 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	$^{3}\mathrm{He}$	Helium 3		Doginning
	TRITON (1)	-4	$^{\mathrm{s}}\mathrm{H}$	Triton	_	Beginning
	DEUTERON (1)	-3	$^{2}\mathrm{H}$	Deuteron	_	Of the list,
I	HEAVYION (1)	-2	_	Generic Heavy Ion		More follows
				(see command HI-PROPE)		More rollows
	OPTIPHOT	-1	_	Optical Photon	_	
I	RAY ⁽²⁾	0	_	Pseudoparticle	_	
I	PROTON	1	P	Proton	2212	
I	APROTON	2	$\bar{\mathbf{p}}$	Antiproton	-2212	
I	ELECTRON	3	e-	Electron	11	
I	POSITRON	4	e ⁺	Positron	-11	

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

Electron Neutrino

Electron Antineutrino

NEUTRIE

ANEUTRIE

ALL-NEGA	204	All negative particles				
ALL-POSI	205	All positive particles	DPA-SCO DOSE-EQ	239	Displacements per atoms Dose Equivalent (pSv) ⁽⁶⁾	
NUCLEONS	206	Protons and neutrons				
NUC&PI+-	207	Protons, neutrons and charged pions	240	Dose Equivalent (pov)		
ENERGY	208	8 For dose scoring: Deposited energy				
		For energy fluence բարարիան Alagorie energy	22			

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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 280 material/temperature combinations are available
- > The library handles also gamma generation, energy deposition by kerma factors, residual nuclei production (now including isomers), 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 yet 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

^{*}Except low-energy neutrons
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Events, statistics, normalization

- □ In a Monte Carlo 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.

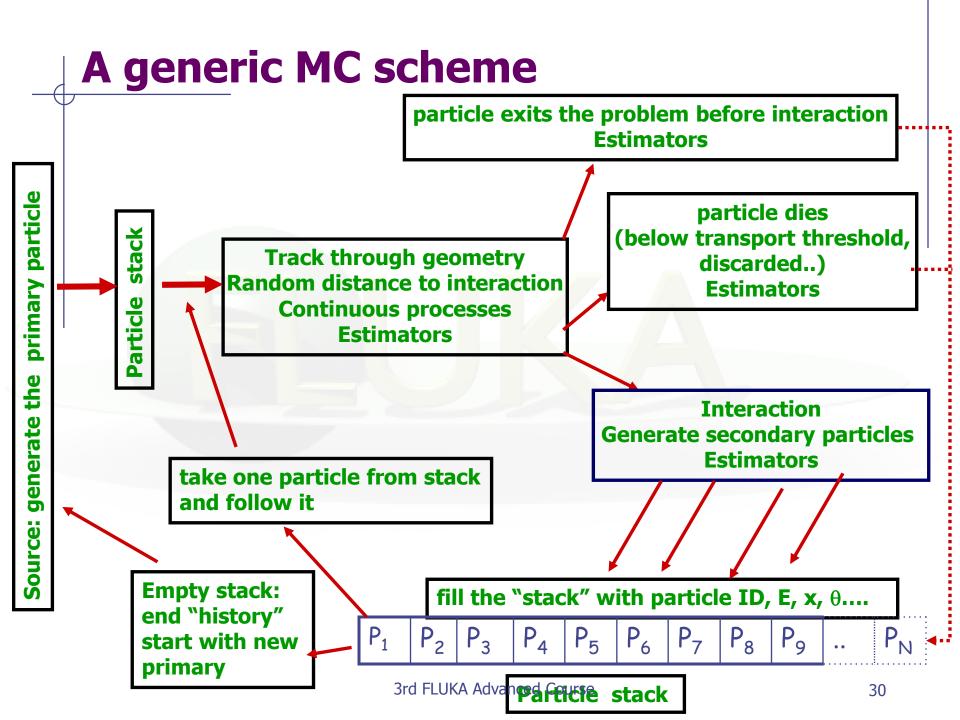
Consequences

- > The TOTAL amount of memory is limited. At present the blank common dimension is about 500 MB: 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

^{*} Most of the memory limitations disappeared in this (gfortran) pre-release where dynamic memory allocation is introduced with a maximum set a priori by the user, or automatically for scoring and geometry, with a global limit around 4 GB

Order of input cards parsing

- 1. DEFAULTS GLOBAL ROT-DEFI TITLE USRGCALL
- 2. BEAM BEAMAXES BEAMPOS BME DISCARD DPMJET EMF EVENTYPE GEOBEGIN IONTRANS 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
- USROCALL STOP



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 onto 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 it 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
 - Interaction probability (elastic, non-elastic, δ rays ...)
 - Decay probability

Discrete or continuous processes

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
- \triangleright **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 and inelastic reactions (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.

FLUKA provides a large variety of biasing techniques. A proper understanding of their use is essential for many shielding (and not only) problems!

End A