

The FLUKA Code: Insight and features

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Mailing list Manual Online Courses Flair Contact us <u>Last version:</u> FLUKA 2011.2.15, September 9th 2012 (last respin) FLAIR 1.0.0	¹ Jefferson La <i>Contributing a</i> M.V.Garze	b, ² CERN, authors: G. Ili, M.Lantz	^{••} ¹ , A.Ferrari ² , ³ Siegen Unive Battistoni, F. C , A.Mairani, V.P rer, V.Vlachouc	rsity, ⁴ INFN M Cerutti, A.Empl, Patera, S.Roesl	lilan
News: Fluka Release (10.08.2012) FLUKA 2011.2.14 has			ed under an IN CERN and INF		ement
been released.					Ö



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71				-		
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Quick launch: Download Mailing list	A A A			3		
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(last respin) FLAIR 1.0.0	(last respin)					
News: Fluka Release	Subscribe naturalseass.					
(10.08.2012)	Name	Comment	D	ate Size		
FLUKA 2011.2.14 has been released.	fluka-2011.2-15.i686.rpm	rpm for fluka-2011.2-15	Se	Oth of 135 MB eptember, 012		
	flupix-vdi.zip	Auxiliary files for FLUPIX	Se	3th of 526 kB eptember, 009		
	fluka2011.2-linuxAA.tar.gz	FLUKA Package Version 201	.1.2.15 Se	Oth of 137 MB eptember, 012		
whenever there is a respin (announced on the mailing list) ²⁰¹²						
please update your installation of FLUKA Advanced Course 4						

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
 - v interactions
 - Transport in magnetic field
 - Combinatorial (boolean) and Voxel geometries
 - Kull mit eo relo coolini 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 1989-2012
- More than 5000 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 course relies heavily on the experience of the first advanced course: feedback is welcome!!!

Release / Registration

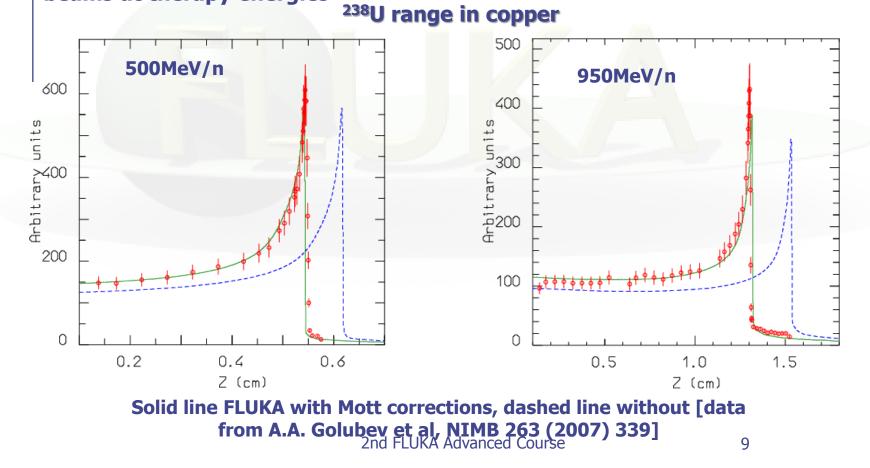
- You received a USB stick with the latest respin (15) of fluka2011.2. This is the current publicly distributed production version, a new major release will occur sometimes in 2013 (more info on the last day)
- If you are not a registered user, PLEASE REGISTER NOW on the **fluka** web site
- The copy you received is for the purpose of the course, unless you are a registered **fluka** user
- Please report as usual any crash/bug /whatever you may find in the production version to <u>fluka-discuss@fluka.org</u>

Some of the features in Fluka2011

- The low energy ion interaction generator (BME) is built-in (no longer any need to link it explicitly) in a vastly improved version
- The detailed treatment of electron profiles in Compton scattering is 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, and (big effect!) the inclusion of Mott corrections (see slide)
- The Landau-Pomeranchuk-Migdal (LPM) effect is 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 available, as well as a colliding beams source.

Higher order stopping power corrections

Barkas (Z³) and Bloch (Z⁴) corrections already implemented in the past. Novel approach (unique to FLUKA) for a fully self-consistent implementation of Mott corrections in the stopping power, in its fluctuations and in the delta spectrum (Parameterization of σ_{Mott} from Phys. Chem. 45 (1995) 235). Remarkable impact for high Z ion beams, effects still not negligible for C beams at therapy energies



Other physics news in FLUKA(2011.2)

- Inclusion of GCR model and tools for space radiation problems (see slides)
- ➤ New treatment of the fragmentation of low mass quark chains → improvements in neutrino interactions in the 0.5-5 GeV range, and hadron-nucleus particle production predictions in the 5-50 GeV range (see slides)
- Improvements in the AA reaction cross section, see slide
- Major improvements in the (prompt) photon emission modelling, see slides
- Extended database of known levels and transitions taken from RIPL-3 (IAEA)
- Discrete level treatment extended to evaporation stage

Galactic Cosmic Rays

Composition:

90% protons, 9% Helium, < 1% Ions *(particles)* 64% protons, 25% Helium, 11% Ions *(nucleons)* Spectrum:

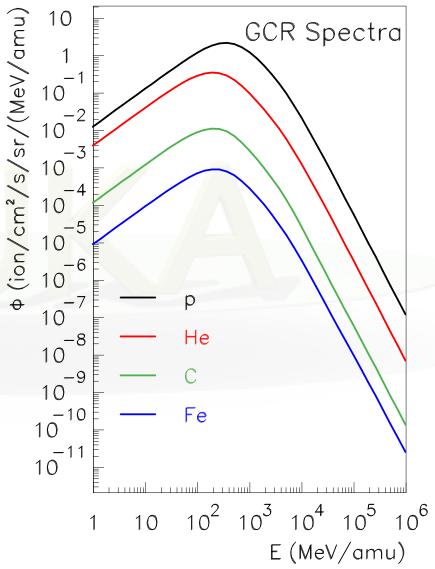
broad spectrum, peaks around 1 GeV/n

Intensity:

(E > 10 MeV/n) ~ 5 p/(cm² s) @ Solar Min.

Dose/Dose Equivalent:

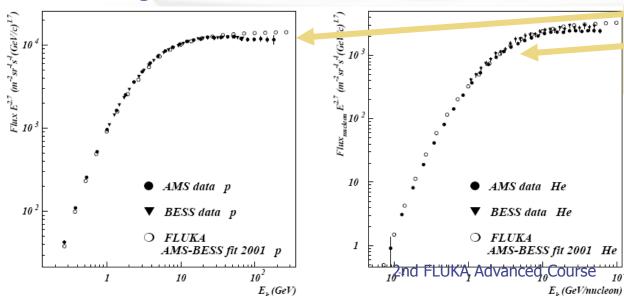
~ 0.4 mGy/d, 1 mSv/d (no geomagnetic cut off)

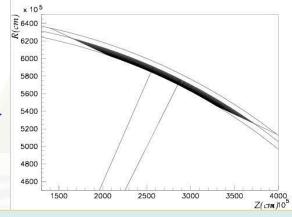


The FLUKA C.R. library

Dedicated FLUKA library + additional off-line packages including:

- Primary spectra from Z = 1 to Z = 28 (derived from NASA and updated to most recent measurements). Other primary flux choices can be added by the user (Agrawal-Stanev-Gaisser-Lipari flux. All nucleon spectrum).
- **\$olar Modulation model**
- (correlated to neutron monitors)
- Atmospheric model (MSIS Mass-Spectrometer-Incoherent-Scatter)
- 3D geometry of Earth + atmosphere
- Geomagnetic model



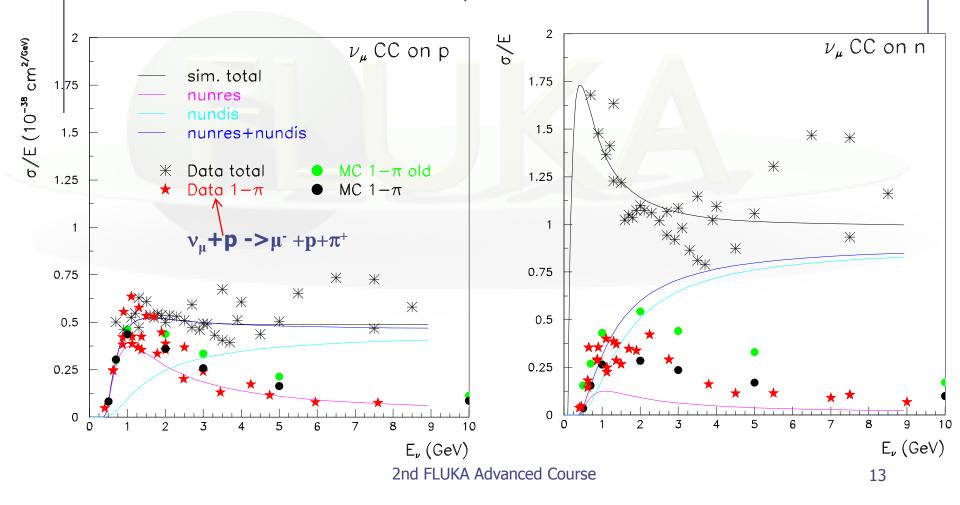


modulated for a given date, location according to geomag. model, solar modulation

FLUKA: superposition model \rightarrow nucleon-Air interaction **FLUKA+DPMJET:** full N-Air interactions

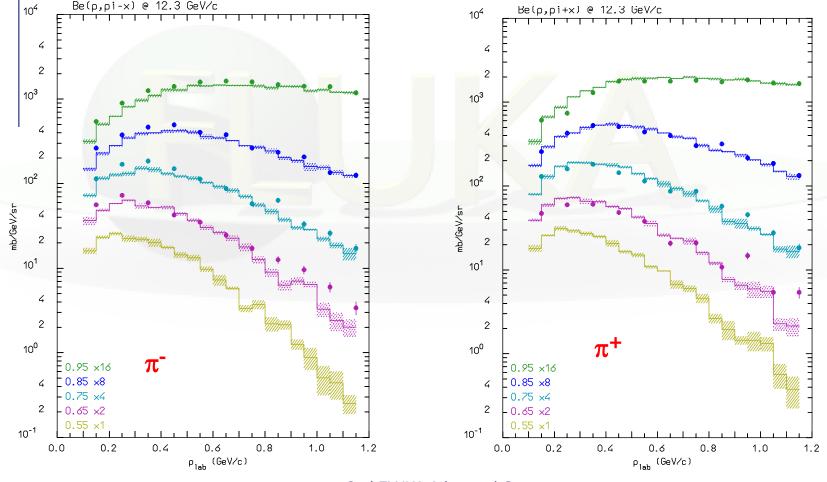
Neutrino interactions (ICARUS..):

Fluka has its own neutrino interaction generator, including QE, Resonance, DIS DIS uses the same chain hadronization as DPM Embedded in the FLUKA nuclear environment (PEANUT) New low-mass chain treatment-> improvements in the RES-DIS transition



Pion production close to DPM thr.

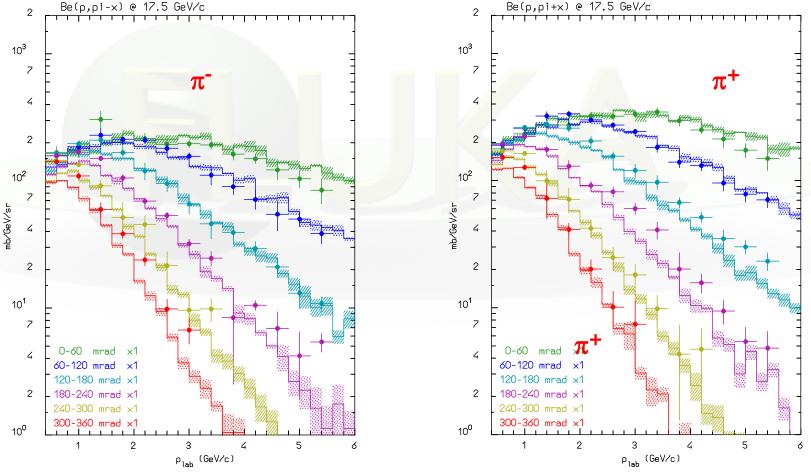
Pion production from proton interactions on Be at 12.3 GeV Emitted pion spectra at different angles in the range 30° - 60° Dots: data (BNL910 expt.), histograms : Fluka



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Pion production close to DPM thr. Pion production from proton interactions on Be at 17.5 GeV Emitted pion spectra at different angles in the range 0° - 20°

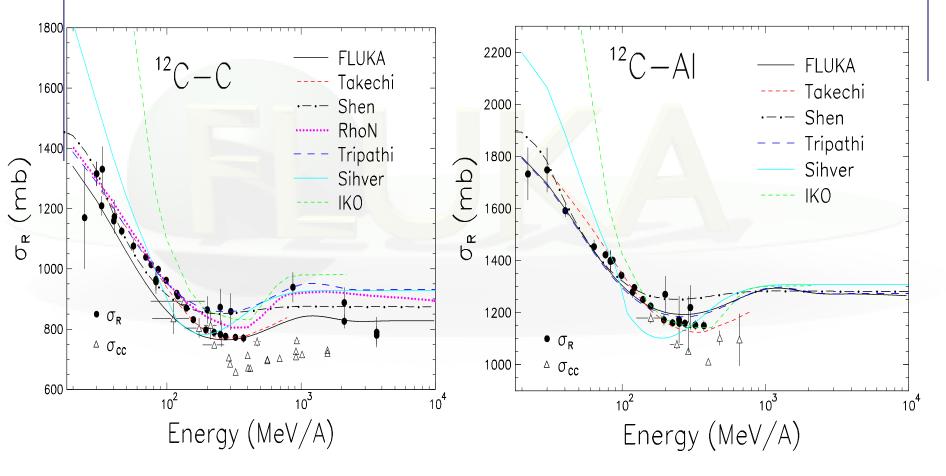
Dots: data (BNL910 expt.), histograms : Fluka



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AA reaction cross sections

Improvements in the AA reaction cross sections (finalized beginning 2011) and inter-comparison with other codes



[L. Sihver et al, Adv Space Res 49 812 (2012)]

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Gamma De-excitation in Fluka

- At the end of evaporation : cascade of γ transitions
- At high excitation: assume continuous level density and statistical emission:

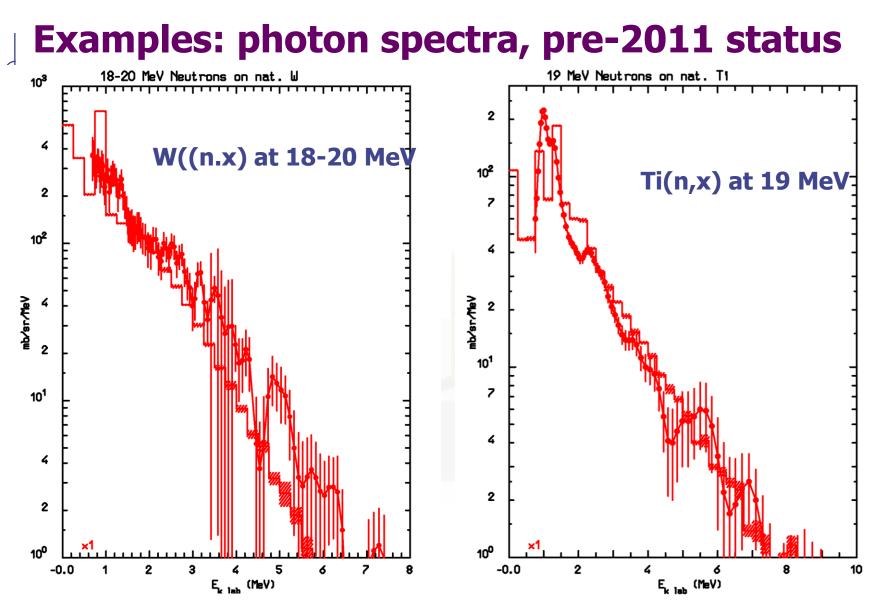
$$P(E_{\gamma})dE_{\gamma} = \frac{\rho_f(U_f)}{\rho_i(U_i)} \sum_L f(E_{\gamma}, L) \quad P = \frac{\rho_f(U_f)}{\rho_i(U_i)} \sum_L f(E_{\gamma}, L) \sum_L f(E_{\gamma},$$

L= multipole order p=level density at excitation energy. U

f = strength from single particle estimate (c)+ hindrance (F)

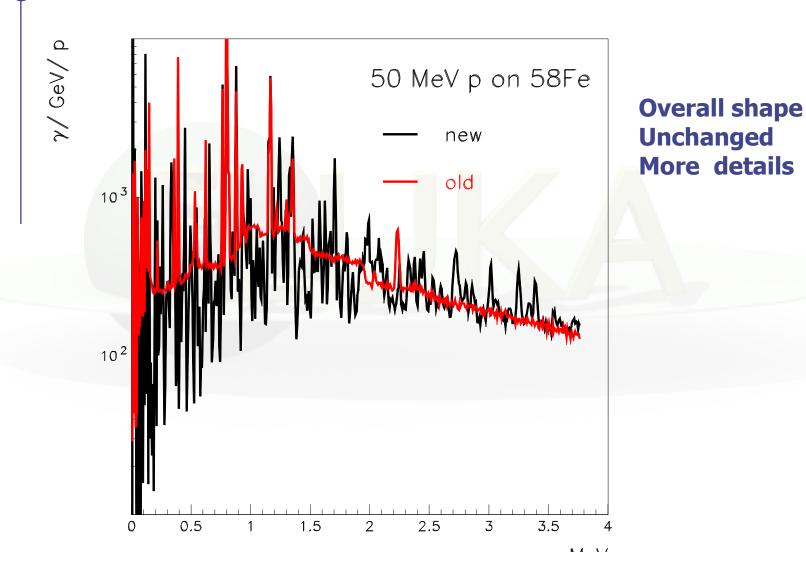
$$f(E_{\gamma},L) = c_L F_L(A) E_{\gamma}^{(2L+1)}$$

- At low excitation: through discrete levels
 - Tabulated experimental levels (partial coverage)
 - Rotational approximation outside tabulations
- See A. Ferrari et al., Z. Phys C 71, 75 (1996)



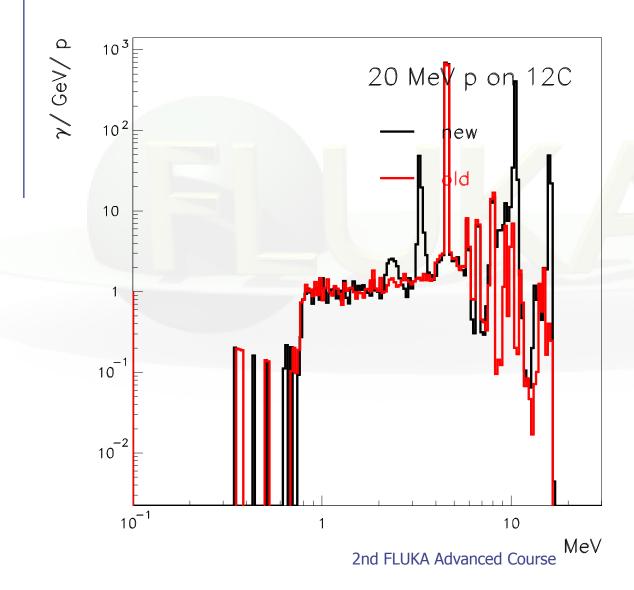
Histograms: FLUKA results with stat errors. Dots: expt data from Dickens et al. report ORNL-4847 (1973) and G.L.Morgan, report ORNL-2nd FLUKA Advanced Course 18

Improved model: example



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Improved model: example 2



Overall shape Unchanged More details are evident

Features in Fluka2011 cont.

- 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 revised FLUKA user license has been adopted, very similar to the previous one in the substance, please however read it.

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
- The gfortran version comes in two flavours due to idiosyncrasies among different gfortran versions (... kill the maintainers). The version working with gfortran-4.5 *will be soon abandoned* please move to a more recent version in case
- 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 script. There are two of them, depending on the energy range: DPMJET (E/A >5 GeV), rQMD (E/A > 100 MeV)
- The low energy ion interaction generator (BME) is now 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 <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 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 \rightarrow 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.

FLUKA name	Fluka number	Symbol	Common name	Standard PDG number (Particle Data Group) [120]	
4-HELIUM ⁽¹⁾	-6	α	Alpha		
3-HELIUM ⁽¹⁾	-5	$^{8}\mathrm{He}$	Helium 3	_	n · · ·
TRITON (1)	-4	$^{8}\mathrm{H}$	Triton	_	Beginning
DEUTERON (1)	-3	^{2}H	Deuteron	_	Of the list,
HEAVYION (1)	-2		Generic Heavy Ion		
			(see command HI-PROPE)		More follows
OPTIPHOT	-1		Optical Photon		/
RAY (2)	0		Pseudoparticle		
PROTON	1	р	Proton	2212	
APROTON	2	$\bar{\mathbf{p}}$	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	

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

ALL-NEGA	204	All negative particles				
ALL-POSI	205	All positive particles	DPA-SCO	239	Displacements per atoms	
NUCLEONS	206	Protons and neutrons	DOSE-EQ		Dose Equivalent (pSv) ⁽⁶⁾	
NUC&PI+-	207	Protons, neutrons and charged pions				
ENERGY	208	For dose scoring: Deposited energy				
		For energy fluence adoring Alara	ourse		25	

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, 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 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.

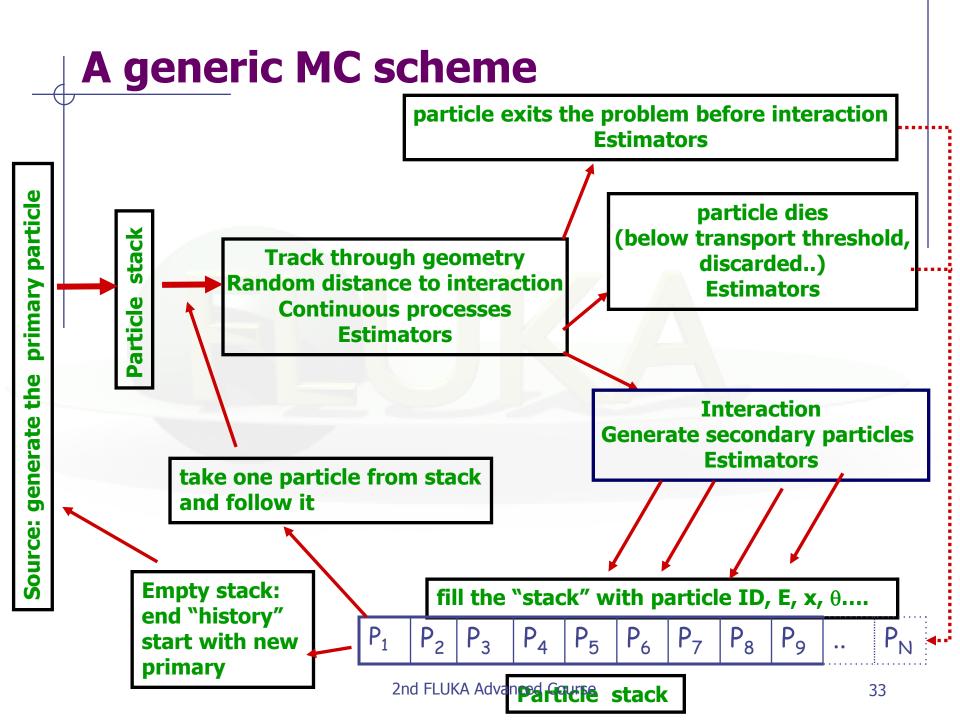
Consequences

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

* Most of the memory limitations will disappear in the next (gfortran) release where dynamic memory allocation will be introduced for scoring and geometry

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
- 8. 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, \rightarrow 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
 - Interaction probability (elastic, non-elastic, δ rays ...)
 - 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.

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





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)** \rightarrow *heavy fragment approximate transport* → treatment of EM showers; If (e+e-y)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) \rightarrow particle below threshold Select the next interaction point **Select the transport method:** If (Not Vacuum & Charged particle) \rightarrow *Moli* `*ere multiple* scattering + ionisation Else(Vacuum OR Neutral particle) -> Vacuum OR neutral particle 2nd FLUKA Advanced Course 40

Kaskad-II

 \rightarrow Molière multiple scattering + ionisation If(age > *time cutoff*) → *time-kill; If(kinetic energy < threshold)* \rightarrow *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;* \rightarrow EM dissociation ; \rightarrow radioactive decay; \rightarrow delta ray; \rightarrow high-energy pair production; \rightarrow high e bremsst. **END DO :mulscat:** END DO :ustep: 2nd FLUKA Advanced Course 41

Kaskad-III

 $\rightarrow \textit{Vacuum OR neutral particle} \\ \texttt{:vacneu: DO ! Vacuum OR neutral particle} \\ \texttt{If(new region)} \rightarrow \textit{boundary crossing;} \\ \texttt{If(age > time cutoff)} \rightarrow \textit{time-kill} \\ \\ \texttt{Random selection:} \\ \rightarrow \textit{inelastic interaction;} \\ \rightarrow \textit{elastic interaction;} \rightarrow \textit{decay} \\ \\ \texttt{If(residual mfp > 0) cycle :vacneu:} \\ \\ \texttt{END DO :vacneu:} \\ \end{aligned}$

→ Boundary crossing
If(new region is blackhole) → escape;
If(age > time cutoff) → time-kill
If(y or e± not in vacuum) → treatment of EM showers
If(y 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:</pre>

end

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