FLUKA: New features and a general overview

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Abstract

FLUKA is a general purpose Monte Carlo code, capable of handling all radiation components from thermal energies (for neutrons), or 1 keV (for all other particles) till cosmic ray energies. The code is a joint CERN-INFN project, and is continuously undergoing development and benchmarking. It is the standard tool used at CERN for the radioprotection and beam-machine interaction calculations.

Several improvements and additions to the code capabilities will be presented, in particular:

- *new radioactive inventory evolution algorithm, which allows to compute inventories and residual dose rates for arbitrary irradiation profiles and cooling times;*
- *improved evaporation/fragmentation model, which allows to produce up to 600 different fragments;*
- *new fission model;*
- *the nucleus-nucleus models (interfaces to DPMJET-III, rQMD-2.4, and the newly developed BME and QMD models);*
- *improvements and additions to the geometry and user interface.*

Introduction

FLUKA [1-4] is a multipurpose transport Monte Carlo code, for calculations of particle transport and interactions with matter, covering an extended range of applications spanning from proton and electron accelerator shielding to target design, calorimetry, activation, dosimetry, detector design, accelerator-driven systems, cosmic rays, neutrino physics, radiotherapy etc. Presently is maintained and supported as a joint CERN-INFN project, which is continuously undergoing development and benchmarking. FLUKA is able to transport 60 different elementary particles and whichever heavy ions and can perform hadron-hadron, hadron-nucleus, neutrino, electromagnetic, and μ interactions from 1 keV up to 10 000 TeV/n. It is able to perform charged particle transport both in magnetic and electric field (currently under development) including all relevant processes [1]. About nucleus-nucleus collisions, since ion-ion nuclear interactions were not yet treated in FLUKA, past results have been obtained in the superposition model approximation, where primary nuclei (0-10 000 TeV/A) were split into nucleons before interacting. With the integration of ion interactions codes (DPMJET, rQMD, BME) and the suitable cross-sections package, this approximation is now obsolete. FLUKA features a combinatorial geometry which was recently enhanced with the use of parenthesis expansions and geometrical optimisations, while for the tracking it has a double capability to run either fully analogue and/or biased calculations.

Code design

FLUKA is based, as far as possible, on original and well tested microscopic models. Due to this "microscopic" approach to hadronic interaction modelling (Figures 1, 2), each step is self-consistent and has solid physical bases. Performances are optimised comparing with particle production data at single interaction level: *"theory driven, benchmarked with data"*. No tuning whatsoever is performed on "*integral*" data, such as calorimeter resolutions, thick target yields, etc. Therefore, final predictions are obtained with a minimal set of free parameters, fixed for all energies and for all target/projectile combinations. Results in complex cases as well as scaling laws and properties come forth naturally from the underlying physical models and the basic conservation laws which are fulfilled *a priori*, therefore the code provides predictive capabilities where no experimental data are directly available.

The philosophy of the FLUKA authors was not to provide a toolkit for particle physics simulations, but rather a code that provides the best physics available. For this reason all physical models in FLUKA are fully integrated in the code and the user has limited means of tweaking them. All correlations are fully preserved within interactions and among shower components. The authors continues to make a huge effort to ensure self-consistency with full cross-talk between all components (hadronic, electromagnetic, neutrons, muons, heavy ions), and to achieve the same level of accuracy for each component and for all energies. For example, the transport and interactions of electromagnetic particles are fully coupled to the hadronic sector, allowing to follow in the same event secondary hadrons from photon nuclear interactions and γ rays from nuclear de-excitation.

Interface improvement

Since the official release of 2005.6 the FLUKA code went a major reworking, in view of the public release of the source code. The code now is even more robust, it is continually enhanced with modern and sound physics, and more users friendly. The major features of the latest release 2006.3 are the following:

- PEMF preprocessor eliminated. Now, electron and photon cross-sections are generated during initialisation time. Photon cross-sections have been rebased on EPDL-97. There is a small penalty in time for the initialisation, but it removes completely the hassle of creating the cross-sections with an external program, as well all the problems that could appear from miss-synchronisation of the pemf files and what is described in the input file.
- Input file now is fully name based, including all materials, geometry bodies and regions, particles and scoring cards. This allows a more flexible way of writing input files as well sharing resources among various input files.

Figure 1: Thin target example of angle-integrated ^{90}Zr(p,xn) at 80.5 MeV

The various lines show the total in blue, intranuclear cascade in green, pre-equilibrium in cyan and evaporation magenta contributions. The experimental data are the red points and extracted from Ref. [5].

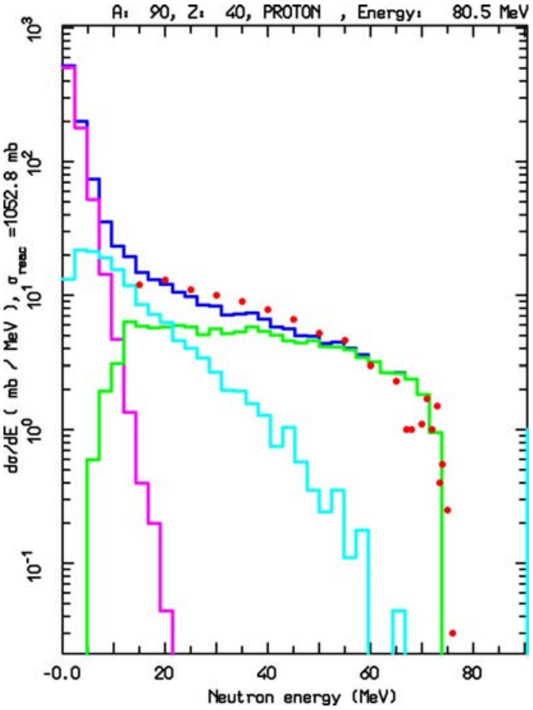
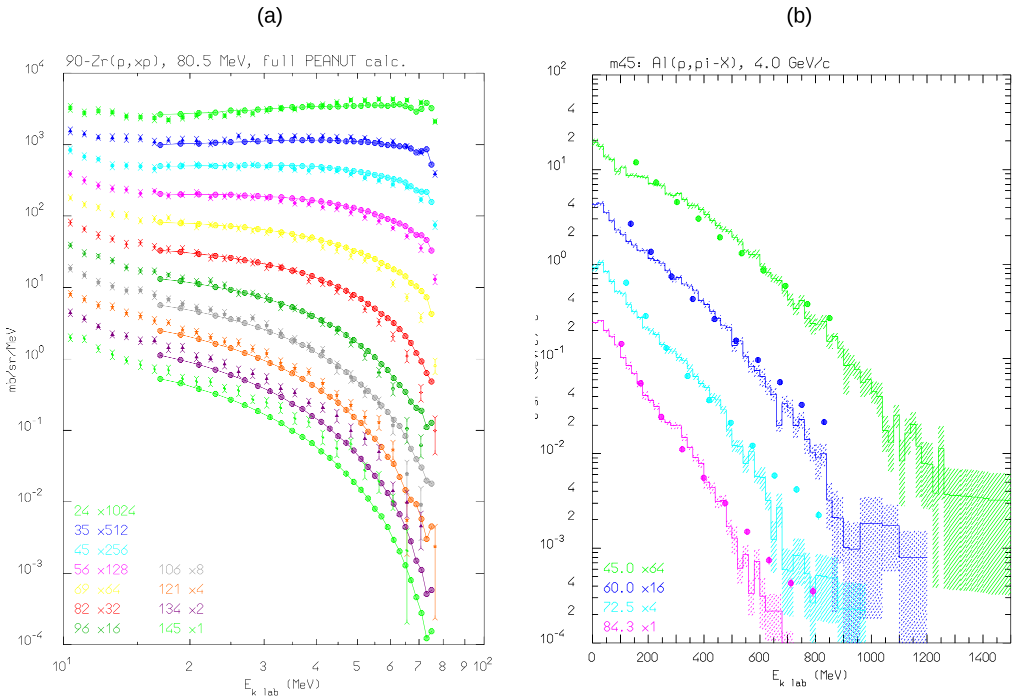


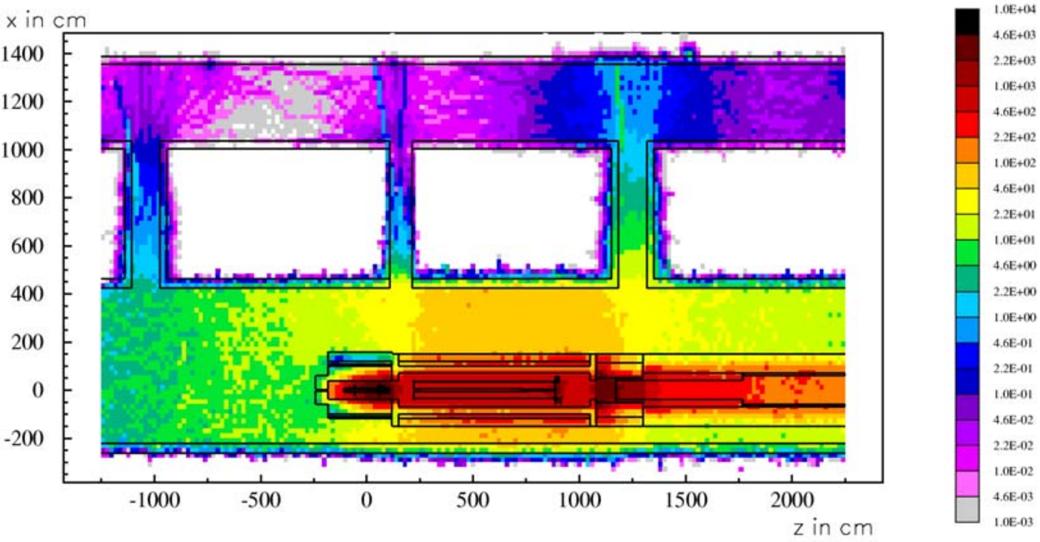
Figure 2: Double differential of a thin target example
(a) p + ^{90}Zr → p + X (80 MeV) [5] and (b) p + Al → π^- + X (4 GeV/c)


(a)

(b)

- The input file is initially treated by the FLUKA preprocessor. A C/C++ like preprocessor that accepts definition of variables and conditional inclusion of input code. This a powerful mechanism if treated correctly by the user, that allows a more structured input file. The user can treat the input file in different ways by simply enabling or disabling some preprocessor defines.
- There are several enhancements in the voxel geometry which are quite important for comparing using of FLUKA in a way similar to the treatment planning systems usually found in radiotherapy centres. Namely: *i)* Voxel-by-voxel density correction factors, *ii*) water equivalence factors for atomic processes (dE/dx, δ ray) while at the same time keeping the real material for the nuclear processes.
- The geometry can now handle more complicated combinatorial geometry objects including parenthesis expansion and both algebraic and geometrical optimisations, for the minimisation of the number of produced zones in a region.
- The code is now able to follow on-line the decay radiation from unstable residual nuclei together with an exact analytical calculation of activity evolution during irradiation and cooling down. Decay, β, γ are produced and transported "*on line*", with time evolution of induced radioactivity calculated analytically using the Bateman equations. As a consequence, results for production of residuals and their effects as a function of time can now be obtained in the same run.
- The user is now able to score results for activity, energy deposition, particle fluence etc, calculated for custom irradiation/cooling down profile, as well the new scoring type activity maps (Bq/cm^3) (Figure 3).

Figure 3: Residual Dose Equivalent Rate (mSv/h) at the CNGS (CERN) target after 200 days irradiation with 8 10^{12} p$^+$/s and 1 day of cooling



Equilibrium particle emission

The latest updates in the evaporation, fission, fragmentation and Fermi break-up made an impressive improvement in the residual nuclei prediction especially in the low mass region. This is a crucial point for many safety calculations. As an example in Figures 4 and 5 are shown the predicted mass distribution for the residual nuclei produced by Pb ions on proton target at 1 GeV/n using inverse kinematics, and Ag on proton target at 300 GeV and 800 GeV, where is evident the improved FLUKA predictions with the new fragmentation model, especially in the low mass region. A discussion of the recent improvements in these models is discussed in the following paragraphs.

Evaporation, fragmentation and Fermi break-up

Evaporation, the latest stage of the nuclear reaction chain, is essential for the prediction of residual nuclei distribution. Therefore, it is a crucial ingredient in activation and residual dose rate simulations, but also in the exact determination of the fragment spectra following nucleus-nucleus interaction.

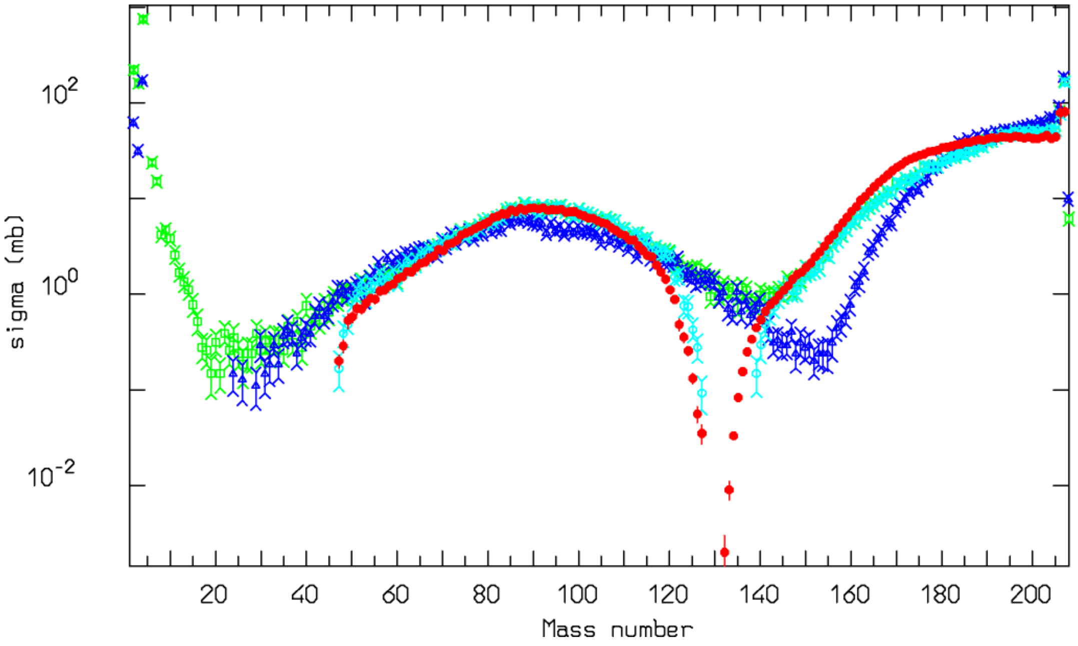
The FLUKA evaporation model, which is based on the Weisskopf-Ewing approach, has been continuously updated along the years, with the inclusion, for instance, of sub-barrier emission, full level density formula, and analytic solution of the emission widths. The latest upgrade is the extension to the evaporation of nuclear fragments up to $A \leq 24$, with impressive improvements in the low mass region of residual nuclei distributions. This, coupled to the exact energy and momentum balance in all reaction steps, allows to predict the mass and energy distribution of fragments, including very low energy, almost non-ionising ones, whose biological effects are not precisely known.

The new evaporation model how is able to handle about 600 possible emitted particle/states with an extended evaporation/fragmentation formalism. It is using the full level density formula with level density parameters and excitation dependent. The inverse cross-section is calculated with proper sub-barrier, while there is analytic solution for the emission widths, neglecting the level density parameter dependence on excitation energy which is taken into account by rejection. For the Fermi break-up for $A < 18$ nuclei, the code is taking into account up to 6 ejectiles resulting ~50 000 possible combinations.

FLUKA is now using new energy dependent and self-consistent, evaporation level densities as well as new pairing energies, according to the IEAE working group recommendations RIPL-2 [6]. The isotopes mass table has been updated with both experimental and calculated values till $A = 330$. The use of masses calculated offline done with high reliability complex models, it allows: *i)* to extend to larger isotope masses A than those experimentally accessible; *ii)* to minimise resorting to empirical mass formulae which often generates artifacts. The shell corrections have been reworked also to be coherent with the new masses.

Figure 4: Cross-section for the production of residual nuclei from the 1 GeV/n ^{208}Pb + p reactions

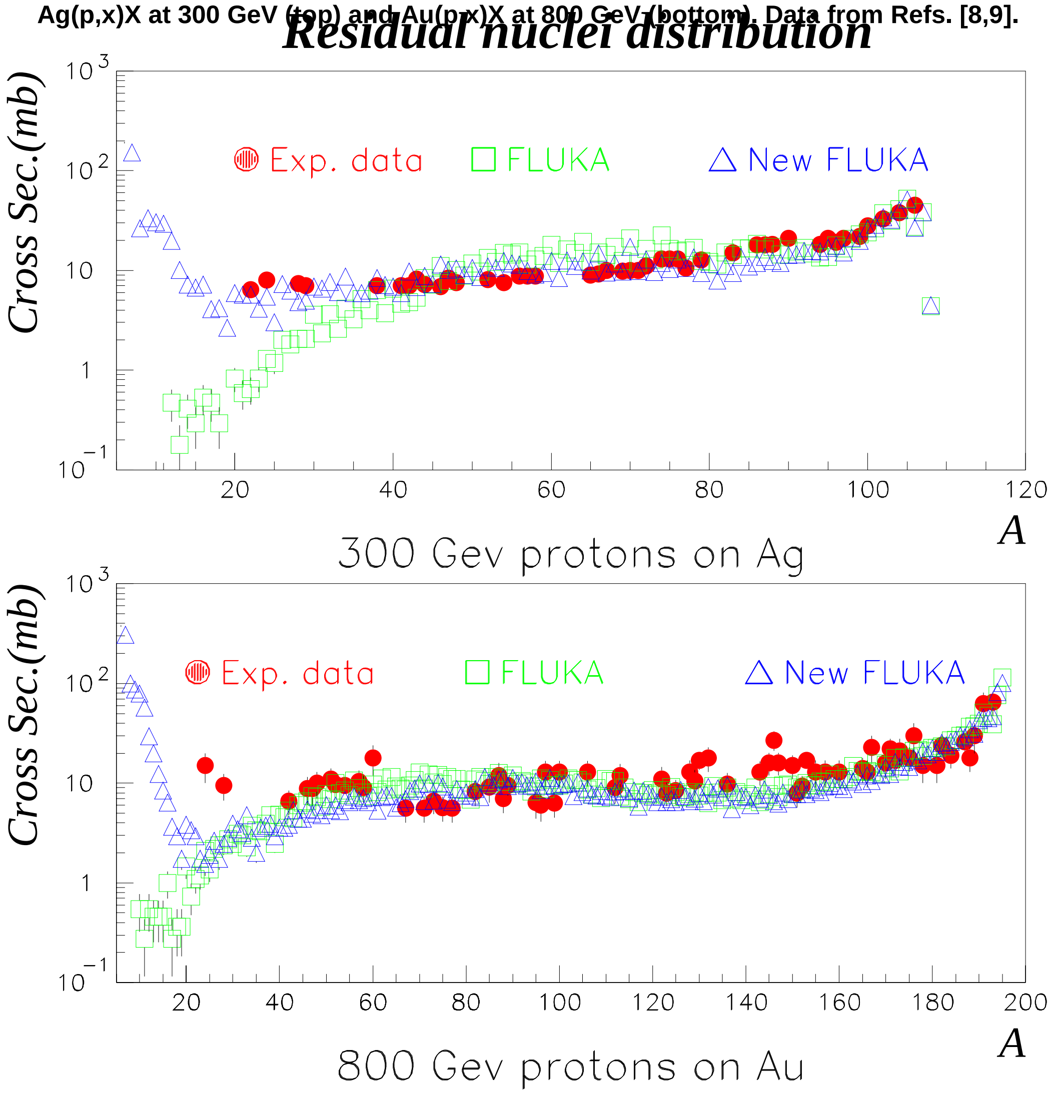
Red dots are experimental data, blue the old FLUKA prediction, green the new FLUKA prediction and cyan the new FLUKA prediction limited to the isotopes where experimental data are available [7]



New fission model

The new fission model is no longer an enhanced version of the Atchison algorithm. Fission is now done on first principles and is also in full competition with evaporation. Actinide fission is done on first principles and no longer using parameterised $\Gamma_{fiss}/\Gamma_{neu}$. The fission barrier calculations follow the most recent suggestions by Myers and Swiatecki. An enhanced fission level density is used at saddle point, which is no longer independent from the excitation energy but now is washing out with excitation in agreement with the most recent studies. Fission product widths and asymmetric versus symmetric probabilities are better parameterised according to the most recent data/approaches.

Figure 5: Experimental and computed residual nuclei mass distribution for Ag(p,x)X at 300 GeV (top) and Au(p,x)X at 800 GeV (bottom). Data from Refs. [8,9].



Heavy ion interaction models

Ion-ion interactions are of great interest both for therapeutic beams, and for space radiation assessment. FLUKA has the necessary interfaces to couple with the DPMJET-III, rQMD and BME models.

FLUKA implements DPMJET-III [10,11] as event generator to simulate nucleus-nucleus interactions for energies in excess of 5 GeV/n up to the highest cosmic ray energies (10^{18}-10^{20} eV). DPMJET is based on the two components Dual Parton Model in connection with the Glauber formalism.

FLUKA also has an interface to rQMD-2.4 [12,13], a relativistic QMD model which has been applied successfully to relativistic A-A particle production over a wide energy range from 0.1 GeV/n up to several hundred of GeV/n. Several important modifications have been implemented in the rQMD code, in order to ensure energy-momentum conservation taking into account experimental binding energies, and to provide meaningful excitation energies for the residual fragments. A thorough discussion of the FLUKA implementation, as well as some results of this modified model can be found in [9].

FLUKA has a preliminary implementation of the BME (Boltzmann Master Equation) model [14] for lower energies ions E < 100 MeV/n, which is presently under testing for A < 17.

For all generators, de-excitation and evaporation of the excited residual nuclei is performed by calling the standard FLUKA evaporation/fission/fragmentation module described above.

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