Benchmarking nuclear reaction models of the FLUKA Monte Carlo code for heavy ion collisions

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Abstract

In this report, I summarize the work conducted during my eight weeks as a summer student in the EN-STI-FLU department of CERN. The work focused on the benchmarking of FLUKA double differential cross sections of secondary fragments produced in fixed-target heavy ion collisions in the beam energy range between 10 MeV/nucleon and 1 GeV/nucleon. Specifically, the accuracy of FLUKA models for nucleus-nucleus interactions, namely the Boltzmann Master Equation (BME) and the Relativistic Quantum Molecular Dynamics (rQMD) models, were analyzed. Furthermore, we compared the FLUKA production version 2011.2x.6 with the FLUKA development version 2018.2 and found that the latter is a considerable improvement to the former. Nevertheless, further improvements are required to better reproduce the experimental data. The major refinements needed are presented and discussed in this report.

Introduction

During the last century, nuclear physics and its subfields have enabled remarkable progress in many areas of science and technology. A wide range of applications is found in medical physics and space research, in which the study of heavy ion collisions with energies on the order of 10^1-10^3 MeV/nucleon are of particular importance. Indeed, when calculating the impact of space radiation on satellites and astronauts as well as the effects of hadronic therapy on patients, it is crucial to have a precise understanding of the physical mechanisms involved and their consequences. The FLUKA Monte Carlo code [1][2] allows predictions of particle transport and interactions by means of embedded nuclear physics models developed following a microscopic approach. In this project, we benchmark FLUKA simulations against an extensive list of experimental data in order to assess the accuracy of the physics models and identify the factors that need refinements. In particular, the Boltzmann Master Equation (BME) [3] and the Relativistic Quantum Molecular Dynamics (rQMD) [4] models were tested against experimental data from heavy ion collisions with beam energies ranging between 15 MeV/nucleon and 1050 MeV/nucleon. Traditionally, the energy range around 125 MeV/nucleon sits intermediate between the regions where the two models are known to be effective. Thus, by studying these energies, we illuminate the nature of the transition from one domain to the other. In addition, two versions of the FLUKA code will be compared in order to compare the progress of its continuous improvement. Hence, this work contributes to the further development of the nuclear models in FLUKA.

Particle Transport and Monte Carlo Simulations

The problem we are concerned with is that of predicting the double differential cross sections (with respect to energy and laboratory emission angle) of the creation of secondary fragments from the interaction between a particle beam and a monoatomic, rectangular fixed target. In the FLUKA simulations, the beam, which is assumed to be perfectly perpendicular to the flat target surface, is allowed a cross-sectional extent. Virtual detectors are placed behind the cards, by means of FLUKA scoring cards, to measure the secondary fragment yields. The entire configuration is enclosed by a large box dividing space into the inside and outside regions. The space inside is filled with vacuum (apart from target, beam and fragments), and the outside is filled with an artificial material that has an infinite cross section (a *black hole*), such as to stop the simulation of any particles that exit the box. A sketch of the geometry of the configuration can be found on figure 1 below.

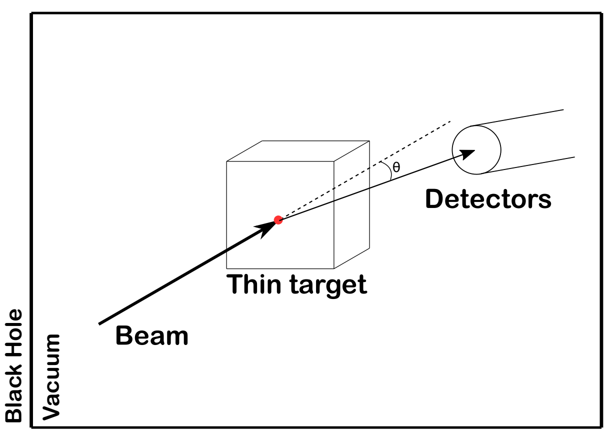

Figure 1: A sketch of the geometry considered. A beam hits a rectangular target perpendicularly, and yields are measured in the plane of the beam at varying angles.

The geometry consists of a rectangular target such that the incoming beam is normal to one of the surfaces of the target. The target thickness is then adjusted according to the situation in each experiment, and its transversal (to the beam) dimensions are kept fixed.

FLUKA is a fully integrated Monte Carlo simulation package for the interaction and transport of particles and nuclei in matter. It can be used to calculate physical observables and their distributions across a set of variables. The Monte Carlo method takes its name from the famous Casino in Monaco; the connection is that they function in virtue of the same principle: Average values are attained in the limit of infinite samples of the underlying probability distribution. The procedure undertaken in FLUKA simulations can be summed up with the following algorithm, simulating the events of a single particle at a time,

1. Set up the given initial conditions.
2. If the particle is in vacuum: Evolve it in time until it meets a material boundary.
3. Determine the cross section at the current energy and sample a step length after which an interaction occurs (with physical arguments, it can be shown that the step length is exponentially distributed).
4. Sample the energy loss (ionization) and change in direction (multiple scattering) along the step. These processes cause changes in the cross sections considered in the code. Furthermore, when the interaction occur, any additionally generated particles are added.
5. Repeat from step 2 until the particle energy is below a given threshold, or the particle exits geometry.

By repeating this procedure, the underlying distribution of outcomes is simulated.

Physics Models

In order to simulate the collisions in step 4 in the aforementioned Monte Carlo algorithm, models of nuclear reactions are required to give the distribution of outcomes from which to sample. Numerous such models exist. In nucleus-nucleus collisions, FLUKA relies on three distinct models, each operating in a different beam energy range E_B:

- $E_B \leqslant 125 \pm 25$ MeV/nucleon: The Boltzmann Master Equation (BME) model [3].
- $125 \pm 25 \leqslant E_B \leqslant 5000$ MeV/nucleon: An extensively modified version [13] of the relativistic Quantum Molecular Dynamics (rQMD) model [14].

- $E_B \geqslant 5000$ MeV/nucleon: The DPMJET-III model [15].

We will mainly investigate the interface between the BME and rQMD models, and leave the DPMJET-III out of scope.

In the BME model, the nucleons are distributed in binned momentum space according to their energies, and the energy level occupancies follow the Pauli principle. Time evolution is given by numerical integration of the so-called Boltzmann Master Equation, and a range of mechanisms, depending on the spatial offset of the beam direction to the target particle, may lead to the emission of secondary fragments.

In the rQMD model, each nucleon is represented as a Gaussian wave function with its Fermi kinetic energy inside the potential of all other nucleons. Phenomenologically, this potential V is made up of three terms,

$$V = V_{\text{int}} + V_{\text{sym}} + V_{\text{surf}},$$

where V_{int} represents an internucleonic interaction term, V_{sym} represents a term that incorporates the proton-neutron asymmetry, and V_{surf} represents effects present around the surface of the nucleus, of special importance to its stability. Hence, each nucleus is made up of a direct production of the wave-functions of its constituent nucleons, and its evolution is taken as the production of the evolution of each constituent nucleon.

Benchmarking

With FLUKA, we have exclusively calculated double differential cross sections of the creation of fragments with respect to laboratory angle and fragment energy. Subsequently, the results were compared with experimental data. The data used were published in the articles [5]-[9] in the 1970s and 1980s. Experiments with beam energies around the transition between the BME and rQMD models were prioritized. Furthermore, as the focus is on heavy ions, experiments with heavy beam particles and target particles were favoured. The experimental data were available in the EXFOR library [11] or were extrapolated from the articles using the tool `webplotdigitizer` [12]. The graphical interface `flair` [10] has been used to prepare the FLUKA input files. On table 1 is given an overview of the experimental data against which FLUKA has been benchmarked, along with the beam-target composition, beam energy E_B, the fragments whose differential cross sections are measured, and the angles at which they are detected.

Paper	**Reaction**	E_B [MeV/n]	**Fragments measured**	**Lab angles** [°]
Jacak 1987 [5]	Ar+Au	42, 92, 137	from p to ^{12}C	30, 50, 70, 90, 110, 130
-	Ar+Ca	42, 92, 137	from p to ^{12}C	30, 50, 70, 90, 110, 130
-	Ne+Au	156	p, d, t, ^{3}He, ^{4}He	50, 70, 90, 110, 130
-	Ne+Al	156	p, d, t, ^{3}He	50, 70, 90, 110, 130
Auble 1983 [6]	O+Sn	100	^{3}He, ^{4}He	6, 12, 18, 24, 45, 85
-	O+Ni	51.8, 100, 147	p, d, t, ^{3}He, ^{4}He	12, 45
Hasselquist 1985 [7]	Ar+Au	92	p, d, t, ^{3}He, ^{4}He	45, 67, 90
-	C+Au	30	p, d, t	47, 56, 71, 90
-	C+Au	30	d, t	15, 45, 75, 90, 105
-	C+Al	30	p, d, t	45, 56, 71, 90
Poskanzer 1975 [8]	O+U	1050	^{3}He, ^{4}He	20, 60
Fukuda 1984 [9]	N+Th	15	p, d, t	10, 20
-	N+Th	15	^{4}He	20, 33, 44, 55

Table 1: Overview of the data that FLUKA double differential cross sections have been benchmarked against. E_B denotes the beam energy per nucleon.

For each experiment, we have carried out the calculation using the FLUKA production version 2011.2x.6 and the newer development version 2018.2. In turn, the changes made since the last production version can be assessed.

BME/rQMD Comparison

As mentioned earlier, in nucleus-nucleus interactions, FLUKA uses the BME model at beam energies below 125±25 MeV/nucleon, an extensively modified and improved version of the relativistic molecular dynamics rQMD-2.4 model [13] (original code from [14]) at beam energies between 125±25 MeV/nucleon and 5 GeV/nucleon as well as the DPMJET model [15] at higher energies. Our focus is on the former two models. For testing purposes, one may adjust the energy at which FLUKA switches between the BME and rQMD models. With this, one can compare the results from a calculation based purely on the BME model with one that is based exclusively on the rQMD model.

For the simulations where only BME was used, the transition energy is set to 200 MeV/nucleon; sufficiently above the beam energies such that the rQMD model does not contribute. Similarly, for rQMD calculations, the transition is set to 75 MeV/nucleon. In this report we show only selected examples of the analyzed reactions and results. The first comparison, with protons from the 100 MeV/nucleon O+Sn data from [6] can be seen on figure 1 with calculations from FLUKA development version 2018.2. Simulations and experimental data are shown at the laboratory angles of 6°, 12°, 18°, 24°, 45° and 85°. Subfigure (a) shows the results of a BME only, subfigure (b) rQMD only, and subfigure (c) the results of the default hybrid with a 125 MeV/nucleon ± 25 MeV/nucleon transition. Firstly, we note that the BME only case agrees exactly with the hybrid calculation; this is because the beam energy of 100 MeV/nucleon is exactly at the lower bound of the transition energy, so by default, FLUKA exclusively uses the BME model in this case. It is seen that both the BME and rQMD models underestimate the energy of the maximum in the cross sections; however, the peaks are less accentuated in the BME model, which consequently yields predictions closer to the experimental data at the smaller angles, although refinements are still needed in order to better agree with the experimental data.

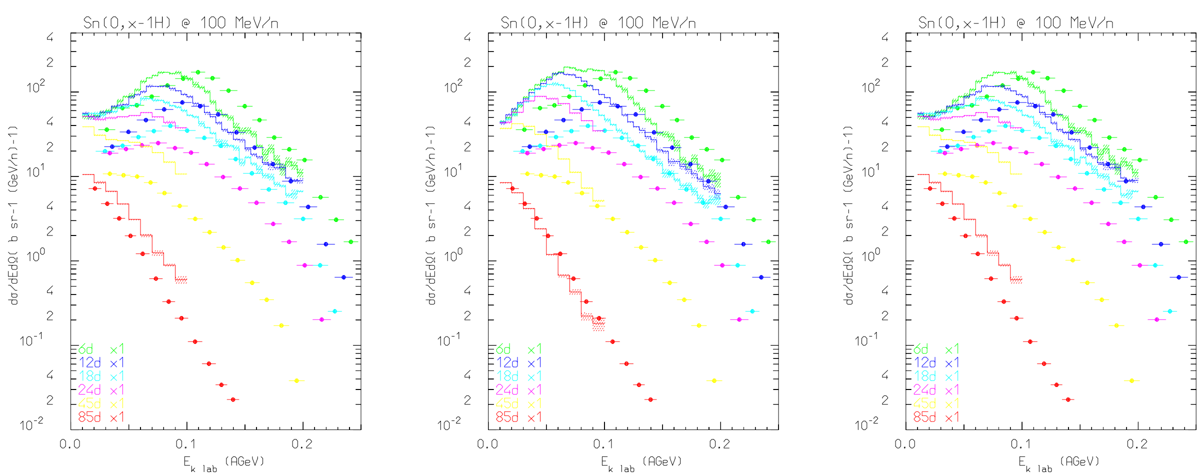

Figure 2: The dependence on emitted fragment energy of the double differential cross sections of protons emerging from a 100 MeV/nucleon beam of oxygen impinging on a tin target. The points are data from [6] and the lines represent FLUKA simulations (development version 2018.2) based on different models. Left: BME model. Middle: rQMD model. Right: Smearing of BME and rQMD.

A comparison of the models' predictions on helium fragments from the 137 MeV/nucleon Ar+Au reaction of [5] is shown on figure 2, calculated with the FLUKA development version 2018.2. This energy is within the range in which FLUKA gradually switches from BME to rQMD; consequently, it is seen that the default calculations with smearing (right) are different from the exclusively BME and rQMD calculations (left and middle). All three calculations deviate from experiment with about an order of magnitude at energies close to zero, but gradually approach the experimental values with increasing energy. Notably, there is a distinct peak in the BME calculations at energies of 0.12, 0.11 and 0.09 GeV/nucleon for the angles 30°, 50° and 70°, respectively. This is probably due to a lack of secondary fragments produced at intermediate energies (i.e. between 0 and 137 MeV/nucleon) in incomplete fusion processes. However, further studies will be carried out to find the potential sources of such findings in the BME configuration. Furthermore, the BME cross sections decrease significantly at energies slightly lower than the peak energies, which is also not seen in the experimental data. However, the 30° and 50° rQMD calculations approach the experimental data with increasing fragment energy without the distinct peak of the BME calculation, although a significant underestimation of the total yield was found. From this, it is evident that the default FLUKA result is a direct combination of the two models.

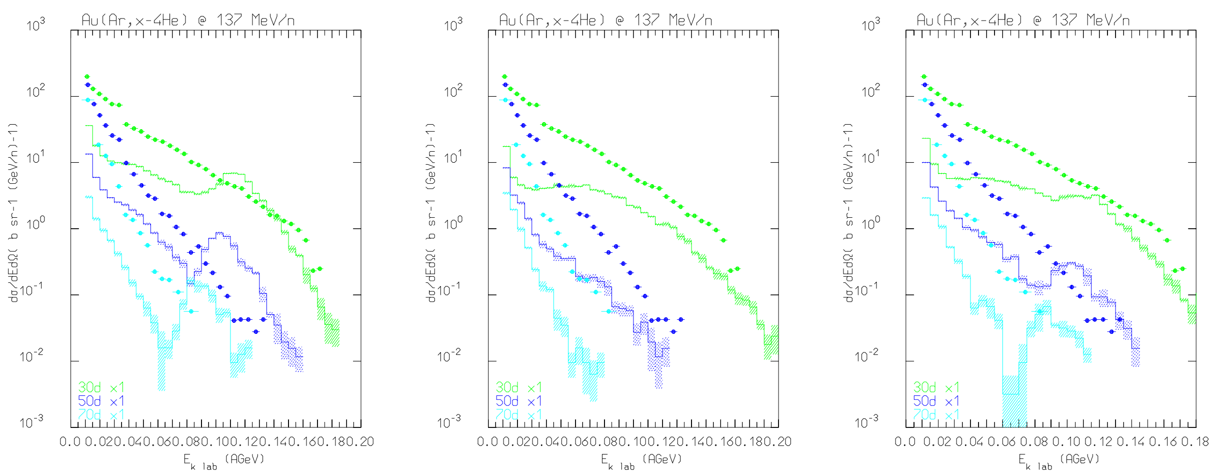

Figure 3: The dependence on emitted fragment energy of the double differential cross sections of ^{4}He particles emerging from a 137 MeV/nucleon beam of argon impinging on a gold target. The points are data from [5] and the lines represent FLUKA simulations (development version 2018.2) based on different models. Left: BME model. Middle: rQMD model. Right: Smearing of BME and rQMD.

Version Comparison

In this section, we compare the two most recent FLUKA versions, namely the development version 2018.2 and the production version 2011.2x.6. The comparison is carried out with the data from protons from the 92 MeV/nucleon Ar+Au experiment of [5] at the angles 30°, 50° and 70°. The results can be seen on figure 3, where the left subfigure shows the results of the production version 2011.2x.6 and the right subfigure shows the results of the development version 2018.2. It is seen that the production version predictions are reasonable at low fragment energies, but diverge increasingly from the experimental data at larger energies. The development version predictions agree well with experiment at energies below some 0.06 GeV/nucleon, after which they also deviate from experiment, although they also give appreciably better predictions than the production version at large fragment energies. Notably, a distinct improvement is the ability of the development version to predict the wide peaks around 0.06 GeV/nucleon much better than the production version.

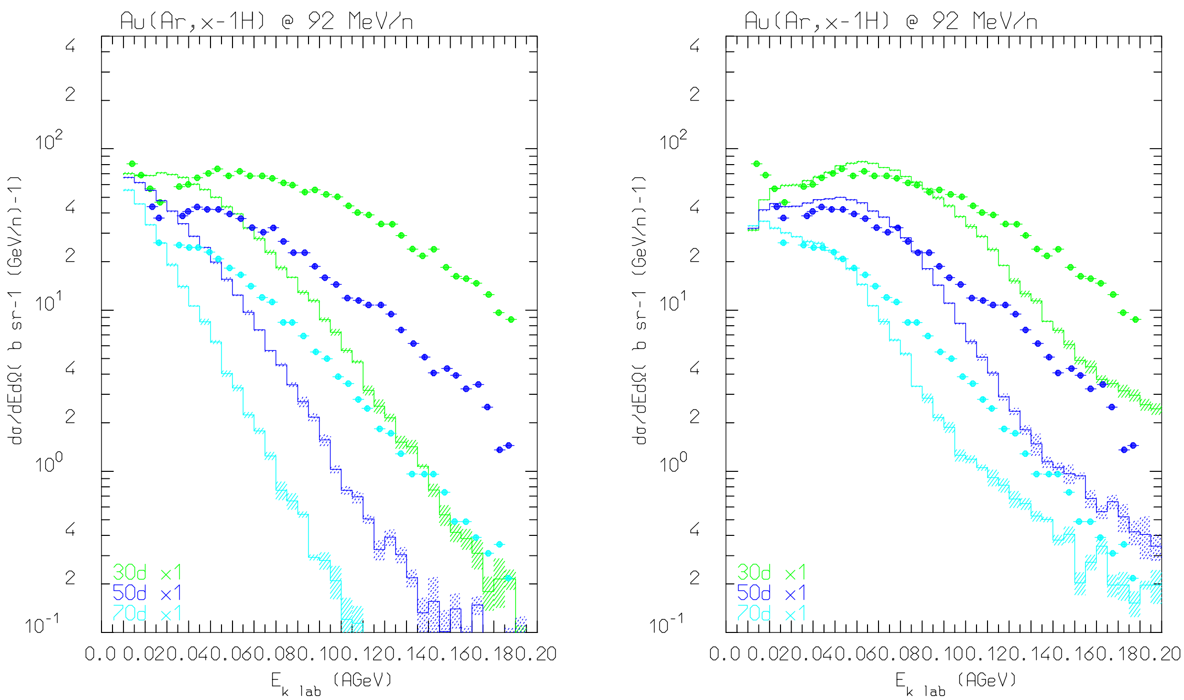

Figure 4: The dependence on emitted fragment energy of the double differential cross sections of protons emerging from a 92 MeV/nucleon beam of argon impinging on a gold target. The points are data from [5] and the lines represent FLUKA calculations with two different versions. Left: FLUKA production version 2011.2x.6. Right: FLUKA development version 2018.2.

Conclusion

We have benchmarked double differential cross sections of the creation of light and heavy fragments in fixed-target experiments from calculations of FLUKA against several sets of experimental data, the complete overview of which is found in table 1. With emphasis on testing the capabilities of the Boltzmann Master Equation (BME) [3] and Relativistic Quantum Molecular Dynamics (rQMD) [4] models, we have presented comparisons of calculations based explicitly on BME, rQMD and a combination with a gradual transition between the two (as implemented by default in FLUKA), respectively. Furthermore, we have compared the results of the FLUKA production version 2011.2x.6 and the FLUKA development version 2018.2, which illustrated that the development version is an appreciable improvement to the older production version. Still, the FLUKA development version predictions occasionally deviate substantially from experimental data. All cases listed in table 1 have been investigated. Thus, this work can be used to identify the cases in which FLUKA deviates from experiment, which may then provide clues on how to improve the underlying nuclear reaction models.

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