Validation of GEANT4 Hadronic Generators versus Thin Target Data

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The GEANT4 toolkit is widely used for simulation of high energy physics (HEP) experiments, in particular, those at the Large Hadron Collider (LHC). The requirements of robustness, stability and quality of simulation for the LHC are demanding. This requires an accurate description of hadronic interactions for a wide range of targets over a large energy range, from stopped particle reactions to low energy nuclear interactions to interactions at the TeV energy scale. This is achieved within the GEANT4 toolkit by combining a number of models, each of which are valid within a certain energy domain. Comparison of these models to thin target data over a large energy range indicates the strengths and weaknesses of the model descriptions and the energy range over which each model is valid.

We will discuss improvements in the pre-compound, de-excitation, Bertini Cascade and Fritiof string models brought about by these validation tests. The pre-compound and de-excitation models get input from comparisons with low energy data on inclusive proton and neutron production. Several new features were added to the Bertini Cascade model in order to improve agreement with low and intermediate energy data. The Fritiof string model was compared to intermediate energy data to determine the low energy edge of its validity range.

Software has been developed to handle the large number of validation tests required to provide the feedback needed to improve the models. We will discuss the validation suites developed for the above work, including plans for an improved automated system which will encompass hadronic interactions at all energies below a few TeV.

KEYWORDS: Monte Carlo, event generator

I. Introduction

The GEANT4 toolkit¹⁾ has been used for the Monte Carlo simulation of LHC experiments over many years. It provides several models for hadronic processes each having its validity range in term of beam type or incident energy. For example, there are theory driven string models or parametrized models which are valid at high energies (for beam momenta above few ten's of GeV/c). At low energies there are cascade models or parametrized models to complement the high energy models. For any hadron the response depends on the simulation at both high and low energies. Detailed simulation also depends critically on the transport of low energy neutrons. The configuration of GEANT4 hadronic models is provided in term of Physics Lists²⁾. These lists are formed by combining several physics models which are applied to specific particles and to specific energy domains. For this it is essential to find out the range of applicability of these models by examining them against available data.

Validation of physics models is an integral part of commissioning the model within GEANT4 toolkit and has been performed from the very early days. This work is done either within the GEANT4 collaboration using published data or by users with a complete description of their detector setup. The earlier studies were done with thin and thick target data. Comparisons with thin target data is rather crucial because it directly compares the models against data without the effect of other processes like particle propagation or electromagnetic physics effects.

The earlier thin target results are done with (a) stopping particles (\bar{p} , π^-), (b) inclusive production of neutrons and protons in low energy (below 100 MeV/c) nuclear interactions with neutron, proton or photon beams, (c) medium energy data (100 MeV/c to 3 GeV/c) on mostly neutron (some proton and π^+) production in proton-nucleus collision, (d) high energy (> 100 GeV/c) data for inclusive π^{\pm} production in π^-/p interactions with nuclear target. These results are documented in reference^{3,4)}. LHC experiments routinely compared the results from the test beam studies with GEANT4 predictions to validate the Physics Lists within the framework of LCG simulation validation⁵⁾.

The hadronic test suite has been significantly extended and it now covers an energy range of the primary hadrons between 20 MeV and 400 GeV and allows validation of double differential cross sections for neutron, proton, charged pion and kaon production. Also GEANT4 has improved or incorporated several new models. The current work is devoted to test the new models and to validate all existing models with thin target data.

There has been an effort to standardize testing of hadronic models. This will have several advantages: (1) improve the consistency of the tests, (2) complete the tests within a definite time scale, (3) enable accessing the results in a central location, (4) share the tools and resources, (5) share the references for comparisons. The first version for display and publication is now available.

II. Data

This work includes several sources of data. The first set of data comes from a low energy experiment of spallation neutron production by protons on nuclear targets⁶). The double differential distributions are available in terms of neutron kinetic energy and emission angle for a number of elements from aluminum to thorium. The next set of data comes from a study of spallation products when a beam of iron is bombarded on liquid hydrogen target⁷).

An ITEP experiment⁸⁾ carried out an extensive set of measurements on inclusive neutron and proton production in hadron-nucleus collision at energies between 1 and 9 GeV/c. The experiment measured Lorentz invariant double differential cross section as a function of kinetic energy of the final state particle at fixed angles in the laboratory frame. There are three types of data. In the nuclear scan, measurements exist at 4 different emitted angles in 8-9 kinetic energy bins with 7.5 GeV/c proton beam on 12 nuclear targets ranging from beryllium to uranium. In the angular scan, two beam particles (7.5 GeV/c protons or 5.0 GeV/c π^-) are used with 4 nuclear targets (carbon, copper, lead and uranium) and inclusive production is measured at 29 different angles in 8-9 bins of kinetic energies. In the energy scan, the same set of targets are used while data exist at 4 different angles with proton, π + and π^{-} beams at 11/7/3 momenta. The typical statistical uncertainty in these data set is 1-10% while the systematic uncertainty is 5-6%.

There is a large set of data coming from the HARP experiment^{9,10)}. This experiment measured double differential distributions of inclusive pion production in protonnucleus collision. There are two sets of measurements one at large angle (0.35-2.15 radians) with five beam momenta between 3-12 GeV/c on seven nuclear targets (beryllium to lead) and the other in the very forward direction (0.03-0.21 radians) with six beam momenta between 3-12.9 GeV/c on nine different targets. The statistical uncertainty in these data sets is 1-10% while the systematic uncertainty is about 10%.

The BNL E802 experiment¹¹⁾ provides measurements made with proton beam at 14.6 GeV/c on nuclear targets. Published data exist on inclusive production of charged pions, kaons and proton for a variety of nuclear targets ranging from beryllium to gold. The measured quantities are Lorentz invariant cross sections as a function of transverse mass in bins of rapidity. Statistical uncertainties are between 5% and 30% while systematic uncertainties are 10-15%. In this study, comparisons are made for four targets: beryllium, aluminum, copper and gold.

III. Models

The LHC experiments routinely compared the results from the test beam studies with GEANT4 predictions to validate the physics lists within the framework of LCG (LHC Computing Grid) simulation validation⁵⁾. Based on these validation results, the LHC experiments have chosen QGSP_BERT as the default physics list. For the description of hadronic physics, this list uses three GEANT4 models. It uses Bertini Cascade model at low energies, low energy parameterization model at intermediate energies and quark gluon string model with the Pre-compound model at the back-end for high energies. The transition between Bertini Cascade and LEP models is made at 9.5-9.9 GeV and between LEP and QGS-Preco models at 12-25 GeV. This choice has made three hadronic models, LEP, QGS-Preco and Bertini Cascade as the primary candidates of detailed validation.

There has been some significant improvements in the Bertini Cascade model in the form of (1) correct normalization of the quasi-elastic cross sections, (2) improved partial cross sections, (3) addition of Coulomb barrier in the pre-compound and cascade phases. A review of the native GEANT4 pre-compound and de-excitation models has also been carried out. Comparisons are made with predictions of the following models inside GEANT4 using the release 9.3.p01 of April, 2010. Details of these models are documented in the physics reference manual¹². The primary set of models comprises of

LEP: low energy parametrized model derived from GHEISHA¹³⁾ and intended for incident energies below 25 GeV;

Bertini Cascade: Bertini intra-nuclear cascade model intended for momenta below 9 GeV;

QGS: quark-gluon string model intended for energies above 12 GeV.

In addition, the following three models are also considered:

Binary Cascade: data driven intra-nuclear cascade model intended for energies below 5 GeV;

CHIPS: quark level event generator based on chiral invariant phase space model;

FTF: Fritiof model implemented inside GEANT4 and intended for energies above 4 GeV.

The auxiliary models are chosen from the following considerations. The FTF model has been recently improved and used within an alternate physics list together with the Bertini Cascade model. This list, FTFP_BERT, is found to be a good substitute of the LHC default physics list QGSP_BERT. CHIPS provides an interesting alternative, being a model which can be applied at all energies thus needing no joining of models. Binary Cascade is a good substitute of the Bertini Cascade model with fewer parameters and better predictability,



Fig. 1 Differential cross section for inclusive neutron production at 30° , 60° , 120° and 150° in *p*-Iron interactions at 0.8 GeV/c as a function of neutron kinetic energy being compared with predictions of four GEANT4 hadronic models.

IV. Results

Figure 1 shows a comparison of model predictions of the two cascade models with inclusive neutron production cross section in proton-iron interactions at $0.8 \text{ GeV/c}^{6)}$. The cascade models give a good description of the data and the Binary Cascade model in particular fits the data very well at all angles.



Fig. 2 Inclusive production cross section for isotopes in *p*-Iron interactions at 750 MeV/c being compared with predictions of three GEANT4 hadronic models.

Figure 2 shows isotope production cross section from proton iron collision at 750 MeV/c. The cascade models are found to be in good agreement with the data.

ITEP data are compared with predictions of the six models: LEP, CHIPS, Binary and Bertini cascades and QGS, FTF models with the Pre-compound model in the back-end. As examples only four sets of comparisons are shown. Other comparisons also lead to similar conclusions.

Figure 3 compares model predictions to inclusive proton production at 59.1° and 119.0° in π^+ -Uranium interactions at 1.4 and 5.0 GeV/c as a function of proton kinetic energy. As can be seen from the figure, Bertini Cascade model is good in the forward hemisphere while it over-estimates in the backward hemisphere. Binary Cascade model is reasonable at low energies but underestimates at high energies. FTF-Preco does



Fig. 3 Ratio of data and six different GEANT4 hadronic model predictions for Lorentz invariant cross section of inclusive proton production at 59.1° (top row) and 119.0° (bottom row) in π^+ -Uranium interactions at 1.4 GeV/c (left column) and 5.0 GeV/c (right column) as a function of proton kinetic energy.

not work at low energies but gives reasonable description at the higher energy. QGS-Preco and CHIPS under estimates at all energies while LEP does not work at the lower energy.



Fig. 4 Lorentz invariant cross section for inclusive proton production at 59.1° (top row) and 119.0° (bottom row) in *p*-Carbon interactions at 1.4 GeV/c (left column) and 7.5 GeV/c (right column) as a function of proton kinetic energy being compared with predictions of five GEANT4 hadronic models.

Figure 4 compares model predictions to inclusive proton production at 59.1° and 119.0° in *p*-Carbon interactions at 1.4 and 7.5 GeV/c as a function of proton kinetic energy. As can be seen from the figure, Bertini Cascade model gives reasonable description of the data. Binary Cascade model is reasonable only at low energies in the forward hemisphere. FTF-Preco does not work at low energies and under estimates at the higher energy. QGS-Preco and CHIPS have poor agreement with the data.

Figure 5 (6) compares model predictions to inclusive neutron production at 119.0° (59.1° and 119.0°) in interactions of



Fig. 5 Lorentz invariant cross section for inclusive neutron production at 119.0° in π^- -nucleus collisions at 5.0 GeV/c as a function of neutron kinetic energy for carbon (top left), copper (top right), lead (bottom left), uranium (bottom right) targets being compared with predictions of five GEANT4 hadronic models.

 π^- (protons) with different nuclear targets at 5.0 (7.5) GeV/c as a function of neutron kinetic energy. As can be seen from the figures, Bertini Cascade model prediction agrees well with the data. Binary Cascade model predicts smaller cross section while FTF-Preco under predicts for heavier targets. QGS-Preco does not work while CHIPS predict larger cross sections for all the nuclei.



Fig. 6 Lorentz invariant cross section for inclusive neutron production at 59.1° (top row) and 119.0° (bottom row) in *p*-nucleus collisions at 1.4 GeV/c (left column) and 7.5 GeV/c (right column) as a function of neutron kinetic energy being compared with predictions of five GEANT4 hadronic models.

Figure 7 shows a comparison of the HARP data on inclusive π^- production in carbon target as a function of the pion momentum. The three models, QGS-Binary, FTF-Preco and QGS-Preco, provide similar predictions and are in reasonable agreement with the data above 1 GeV/c. The predictions of QGS-Preco is closest to the data. Bertini Cascade model predicts smaller cross sections at higher momenta.

Figure 8 shows a comparison of the HARP data on inclu-



Fig. 7 Differential cross section for inclusive π^- production in the forward hemisphere (in the angular region 50-250 mrad) in π^- -Carbon interactions at 12 GeV/c as a function of $\pi^$ momentum being compared with predictions of five GEANT4 hadronic models.



Fig. 8 Differential cross section for inclusive π^+ production in the forward hemisphere (in the angular region 30-210 mrad) in π^+ -Aluminum interactions at 13 GeV/c as a function of π^+ momentum being compared with predictions of six GEANT4 hadronic models.

sive π^+ production with aluminum target as a function of the pion momentum. The two models, QGS-Binary and FTF-Binary, provide good description of the data. QGS-Preco and FTF-Preco over estimate the cross section at lower momenta (below 2 GeV/c). Binary Cascade model cannot describe the data while Bertini predicts smaller cross sections at momenta above 3 GeV/c.

The BNL data are also compared with five different models. The Binary Cascade model is supposed to work only at much lower energy and is not used in this comparison. Again only a small subset of some representative comparisons are shown here.



Fig. 9 Lorentz invariant cross section for inclusive π^+ production in *p*-nucleus collisions at 14.6 GeV/c for beryllium (top row) and gold (bottom row) targets as a function of reduced transverse mass at rapidity values of 1.1 (left column) and 2.3 (right column) being compared with predictions of five GEANT4 hadronic models.

Figure 9 compares model predictions to inclusive π^+ production at rapidity values of 1.1 and 2.3 in interactions of protons with beryllium and gold targets at 14.6 GeV/c as a function of reduced transverse mass. Bertini clearly predicts a wrong shape in all these plots. It is to be noted that this energy is way above the validity range of the model. FTF-Preco is good for all rapidity (y) and transverse mass (m_T) values. LEP predicts larger cross sections at large y and m_T , while QGS-Preco predicts smaller cross sections at large m_T .

Figure 10 compares model predictions to inclusive proton production at four rapidity values from 1.1 to 2.3 in *p*-copper interactions at 14.6 GeV/c as a function of reduced transverse mass. Bertini gives a fair prediction of the data. FTF-Preco is good at small *y* values while it over predicts at large *y*. LEP predicts smaller cross section for low *y* and larger cross sections at large *y* and m_T . QGS-Preco and CHIPS predict smaller cross sections for all m_T values.

V. Validation Framework

A large collection of the GEANT4-based software and analysis tools has been developed for the validation of various aspects of the hadronic models. In order to carry out validation of a large number of models over the entire energy spectra, an automated validation framework is required. The framework



Fig. 10 Lorentz invariant cross section for inclusive proton production in p-Copper interactions at 14.6 GeV/c as a function of reduced transverse mass at rapidity values of 1.1 (top left), 1.5 (top right), 1.9 (bottom left) and 2.3 (bottom right) being compared with predictions of five GEANT4 hadronic models.

includes (1) execution of the tests, (2) merging the statistics (if required) and comparison of the results with references, (3) storing the results for future reference ir for publishing to the user community, (4) publishing the results. The requirement and the design documents for the framework is written and are available^{14, 15)}.

As a first step to complete the framework, the storage and publication part of the results are completed. The comparison results are stored in a database and the database schema is finalized. The database and the web application for display and publication are made to run on a central server. The display browser is implemented as a Java Server Page (JSP) web-application running on a Tomcat web application server.

Securing the web application and the database from malicious attacks is an important issue and they have been addressed in the design phase. A proper authentication system is integrated to the web application. Communication with the web application uses SSL. The web application is available at http://g4jsp.ifh.de:8080/G4HadronicValidation/.

VI. Summary

Systematic studies are being made by comparing results from several thin target experiments with predictions from different models of hadronic interactions inside the GEANT4 toolkit. The models showed their strengths and weaknesses when confronted with the data. These comparisons guide us to design a good physics list for high energy physics application.

Two promising models are realized - Bertini Cascade and FTF models for the lower and the higher ends of the energy explored. However, both these models have certain limitations. Bertini Cascade model under estimates proton and neutron production in the backward hemisphere for light nuclei. It also produces too many very low energy protons. FTF model, on the other hand, has some deficiency of predicting nucleon production. The results of the comparison are used in improving the model predictions.

A framework to automate the validation process is designed and a first implementation of storage and display of the results is now available.

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