Validation of Geant4 Hadronic Generators versus Thin Target Data

S. Banerjee\textsuperscript{1}, G. Folger\textsuperscript{2}, A. Ivanchenko\textsuperscript{2,3}, V. N. Ivanchenko\textsuperscript{2,4,5}, M. Kossov\textsuperscript{2}, J. M. Quesada\textsuperscript{6}, A. Schälicke\textsuperscript{7}, V. Uzhinsky\textsuperscript{2}, H. Wenzel\textsuperscript{1}, D. H. Wright\textsuperscript{8} and J. Yarba\textsuperscript{1}

\textsuperscript{1}Fermilab, P.O.Box 500, Batavia, Illinois 60510, USA
\textsuperscript{2}CERN, CH1211 Geneva 23, Switzerland
\textsuperscript{3}Universite Bordeaux 1, CNRS/IN2P3, CENBG, 33175 Gradignan, France
\textsuperscript{4}Ecoanalytica, 119899 Moscow, Russia
\textsuperscript{5}Universite Metz, LPMC, 57078 Metz, France
\textsuperscript{6}Dep. Fisica Atomica, Molecular y Nuclear, University of Sevilla. Spain
\textsuperscript{7}DESY, Platanenallee 6, 15738 Zeuthen, Germany
\textsuperscript{8}SLAC, 2575 Sand Hill Road, Menlo Park, CA 94025, USA

E-mail: sunanda@fnal.gov

Abstract. 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.

Software has been developed to handle the large number of validation tests required to provide the feedback needed to improve the models. An automated process for carrying out the validation and storing/displaying the results is being developed and will be discussed.

1. Introduction

The GEANT4 toolkit\cite{1} 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 terms 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 tens 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 Lists\cite{2}. 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 the 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 ($\bar{p}$, $\pi^-$), (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 $\pi^+$) production in proton-nucleus collisions, (d) high energy (> 100 GeV/c) data for inclusive $\pi^\pm$ production in $\pi^-/p$ interactions with nuclear target. These results are documented in reference [3, 4]. LHC experiments routinely compared the results from their test beam studies with GEANT4 predictions to validate the Physics Lists within the framework of LCG simulation validation [3, 5].

The testing suite for hadronic models 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.

2. 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 targets [6] at the Saturne accelerator. The double differential cross sections 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 from the heavy ion synchrotron at GSI is bombarded on liquid hydrogen target [7].

An ITEP experiment [8] carried out an extensive set of measurements on inclusive neutron and proton production in hadron-nucleus collisions at energies between 1 and 9 GeV/c. The experiment measured the 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 a 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 $\pi^-$) 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, $\pi^+$ and $\pi^-$ beams at 11, 7 and 3 momentum values. The typical statistical uncertainty in these data sets 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 cross sections of inclusive pion production in proton-nucleus collisions. There are two sets of measurements: one at large angles (0.35–2.15 radians) with five beam momenta between 3 and 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 and 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 experiment [11] provides measurements made with a proton beam at 14.6 GeV/c on nuclear targets. Published data exist on inclusive production of charged pions, kaons and protons 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.

3. Models
The LHC experiments have validated the Geant4 predictions with their test beam studies and based on these validation results, have chosen QGSP\_BERT as the default physics list. For the description of hadronic physics, this list uses three Geant4 models. It uses the Bertini cascade model (BERT) at low energies (below 9 GeV), the low energy parametrization model (LEP) at intermediate energies (below 30 GeV) and the quark gluon string model (QGS) with the Pre-compound model (Preco) at the back-end for high energies (above 12 GeV).

There are two alternate physics lists which are considered by LHC experiment, FTFP\_BERT and CHIPS. FTFP\_BERT utilizes an improved version of Fritiof (FTF) model (intended for energies above 4 GeV) implemented inside Geant4 along with the Bertini cascade model and is found to be a good substitute for the LHC default physics list. CHIPS provides an interesting alternative, being a model which can be applied at all energies thus needing no joining of models. There is in addition Binary cascade model (BIC) which is a good substitute of the Bertini cascade model with fewer parameters and better predictability (working below 5 GeV).

Table 1 summarizes the models used in the three physics lists with specification for particle types and energy range of their applicability. There have 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 the 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 manual [12]. The following models validated in this paper: LEP, Bertini cascade, QGS, Binary cascade, CHIPS and FTF.

### Table 1. Models used in the physics lists with specification for particle types and energy range of applicability

| Physics List   | Particles     | Model Used     | Energy range          |
|----------------|---------------|----------------|-----------------------|
| QGSP\_BERT    | $\pi^\pm$, $K$, $p$, $n$ | Bertini, LEP, QGSP | 0.0 – 9.9 GeV, 9.5 – 25 GeV, > 12 GeV |
|               | Other particles | LHEP           | All energy            |
| FTFP\_BERT    | $\pi^\pm$, $K$, $p$, $n$ | Bertini, FTFP  | 0.0 – 5.0 GeV, > 4 GeV |
|               | Other particles | LHEP           | All energy            |
| CHIPS          | All particles  | CHIPS          | All energy            |

4. Results
Figure 1 shows a comparison of model predictions of the two cascade models (Bertini and Binary) with inclusive neutron production cross sections in proton-Iron interactions at 0.8 GeV/c[6].
Figure 1. Differential cross sections for inclusive neutron production at 30° and 60° in p-Iron interactions at 0.8 GeV/c as a function of neutron kinetic energy being compared with predictions of three Geant4 hadronic models.

Both the models give a good description of the data and the Binary cascade model (BIC) in particular fits the data very well at all angles.

Figure 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 the isotope production cross section from proton-Iron collisions 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 five models: LEP, CHIPS, Binary and Bertini cascades and FTF model with the Pre-compound model in the back-end. As examples only two 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, the Bertini cascade model is good in the forward hemisphere while it overestimates in the backward hemisphere. The Binary cascade model is reasonable at low energies but underestimates at high energies. FTF-Preco gives reasonable description at the higher energy. CHIPS underestimates cross sections at all energies while LEP does not work at
Figure 3. Ratio of data and different GEANT4 hadronic model predictions for Lorentz invariant cross section of inclusive proton production in $\pi^+$-Uranium interactions (a) at 1.4 GeV/c for protons at 59.1°, (b) at 5.0 GeV/c for protons at 119.0° as a function of proton kinetic energy.

the lower energy. The Bertini cascade model also provides reasonable description of inclusive proton production in proton-nucleus collisions for light as well as heavy targets. The Binary cascade model is reasonable only at low energies (with proton beams at or below 1.4 GeV/c) in the forward hemisphere. FTF-Preco gives somewhat poorer description than the Bertini cascade model at beam momenta around 7.5 GeV/c.

Figure 4. Lorentz invariant cross section for inclusive neutron production at 119.0° in $\pi^-$-nucleus collisions at 5.0 GeV/c as a function of neutron kinetic energy for (a) Carbon and (b) Uranium targets being compared with predictions of GEANT4 hadronic models.

Figure 4 compares model predictions to inclusive neutron production at 119.0° in interactions of $\pi^-$ with different nuclear targets at 5.0 GeV/c as a function of neutron kinetic energy. As can be seen from this figure, the Bertini cascade model prediction agrees well with the data. The Binary cascade model predicts smaller cross sections while FTF-Preco underestimates for heavier targets and CHIPS predicts larger cross sections for all the nuclei. Comparison with proton induced neutron production data also lead to similar conclusions.

Figure 5 shows a comparison of the HARP data on inclusive $\pi^+$ 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 the QGS-Preco model is closest to the data. The Bertini cascade model predicts smaller cross sections at higher momenta.

In describing inclusive $\pi^+$ production in aluminum target, the two models, QGS-Binary and FTF-Binary, provide good description of the data. QGS-Preco and FTF-Preco overestimate the
Figure 5. Differential cross section for inclusive $\pi^-$ production in the forward hemisphere (in the angular region 50–250 mrad) in $\pi^-$-Carbon interactions at 12 GeV/c as a function of $\pi^-$ momentum being compared with predictions of five GEANT4 hadronic models.

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.

Figure 6. Lorentz invariant cross section for inclusive $\pi^+$ production in $p$-nucleus collisions at 14.6 GeV/c for (a) beryllium target at rapidity value of 1.1, (b) gold target at rapidity value of 2.3 as a function of reduced transverse mass being compared with predictions of GEANT4 hadronic models.

Figure 6 compares model predictions to inclusive $\pi^+$ 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 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 reduced 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 \(m_T\).

The Bertini cascade model, however, gives a fair prediction of inclusive proton production at 14.6 GeV/c. Predictions from FTF-Preco gives a good match for inclusive proton production 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.

5. 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 includes (1) executing the tests, (2) merging the statistics (if required) and comparison of the results with references, (3) storing the results for future reference or for publishing to the user community, (4) publishing the results. The requirement and the design documents for the framework are written and are available[13, 14].

![Figure 7](image-url) Snapshot of the website demonstrating the display browser of the automatic validation framework.

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. Figure 7 provides a snapshot of the display browser.

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

6. 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 in designing optimal physics lists for high energy physics applications.

Two promising models are realized – the Bertini cascade and the FTF models for the lower and the higher ends of the energy explored. However, both these models have certain limitations. The Bertini cascade model underestimates 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 these comparisons 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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