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Recent Developments and Validation of Geant4 Hadronic Physics

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Abstract. In the past year several improvements in Geant4 hadronic physics code have been made, both for HEP and nuclear physics applications. We discuss the implications of these changes for physics simulation performance and user code. In this context several of the most-used codes will be covered briefly. These include the Fritiof (FTF) parton string model which has been extended to include antinucleon and antinucleus interactions with nuclei, the Bertini-style cascade with its improved CPU performance and extension to include photon interactions, and the precompound and deexcitation models. We have recently released new models and databases for low energy neutrons, and the radioactive decay process has been improved with the addition of forbidden beta decays and better gamma spectra following internal conversion.

As new and improved models become available, the number of tests and comparisons to data has increased. One of these is a validation of the parton string models against data from the MIPP experiment, which covers the largely untested range of 50 to 100 GeV. At the other extreme, a new stopped hadron validation will cover pions, kaons and antiprotons. These, and the ongoing simplified calorimeter studies, will be discussed briefly. We also discuss the increasing number of regularly performed validations, the demands they place on both software and users, and the automated validation system being developed to address them.

1. Introduction

Geant4 [1] is a toolkit for the Monte Carlo simulation of the passage of particles through matter. Its areas of application include high energy physics (HEP), nuclear and accelerator physics, as well as studies in medical and space science. One of the most challenging tasks that Geant4 is modeling hadronic interactions in a wide range of energies. For this reason the Geant4 suite of hadronic physics models is one of its key components.

Since Geant4 can not offer a single hadronic model to cover the entire energy domain from zero to the TeV scale for all known processes and all know of particles, models have to be combined to cover large energy range. This concept is know as a physics list, where every two adjacent models may have an overlap in their validity range.

While the fabrication of a physics list is, in principle, a choice of a user, the toolkit is distributed with a number of pre-fabricated physics lists, for the convenience of many user applications. These physics lists are supported by the Geant4 development team and can be recommended for specific physics tasks.

In the recent past many improvements in the Geant4 hadronic physics models have been triggered and motivated by important feedback from various experiments that include such as

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LHC experiments as ATLAS and CMS, HARP-CDP experiment at CERN and MIPP experiment at Fermilab, and CALICE collaboration.

Developments have concentrated on several models for inelastic hadronic interactions. These include the Fritiof parton string model at the higher energy range to the Bertini intranuclear cascade for the intermediate energy range to the Precompound model at lower energies. Special attention has been given to ensure smooth transtion from one model to another. At the same time, functionalities of these models have also been extended to allow modeling of capture and annihilation processes. Substantial progress has also been made in the area of modeling low energy neutron transport.

These efforts have led to the possibility to replace older software components in the physics lists and to migrate to the most up-to-date and better performing models, while still offering in the distribution more traditional physics lists for reference and for backward compatibility.

Work is also ongoing in other areas, for example development and improvement of models for simulation of spallation reactions such as the Intranuclear Cascade model (INCL).

At the same time, several older hadronic models will be preserved and maintened within Geant4, as they remain useful for some specific applications.

Model development and improvement work is tightly coupled with extensive efforts to validate Geant4 physics with experimental data. A large collection of tests ranges from vary basic validation at the single process level and comparison with thin target experimental data to the validation of full blown physics lists and comparison with results from LHC experiments.

As the number of regularly performed validation tests increases and the collection of results grows, storing them and making them available to the users community becomes another challenge on its own. To address it, the collaboration has designed and deployed an automated validation system, which will also be covered in this paper.

2. Key Developments in the Geant4 Hadronic Physics Domain

2.1. Fritiof String Model

Fritiof Model (FTF) is a High Energy string model that simulates hadron-hadron, hadron-nucleus and nucleus-nucleus interactions. It is primarily meant for higher energy end, up to 1TeV, however with the recent improvements it can be extended into the intermediate energy range as low as 3GeV.

Interest in this model has been renewed about 3 years ago, when it was discovered that the alternative string model in Geant4 could not be extended below ∼15GeV while the validity of lower energy cascade models could not go higher than 10GeV. This required incorporation in the physics lists of a crude parametric model to fill up the gap, which resulted in discontinutities in some of the physics observables, as it will be shown later in this paper.

The FTF model includes elastic hadron-nucleon scatterings, binary reactions in hadron-nucleon interactions, and a separate simulation of single diffractive and non-diffractive events. It can also model nuclear reactions, based on the Reggeon theory of neuclear destruction; after the initial high energy interaction occurs, the cascading process is simulated as a repeated exchange of quarks between nucleons.

With parameters tuning, this allows to describe cross sections for for different final states in reactions such as πp-interactions, Kp-interactions, and pp-interaction. For example, FTF can well describe cross sections as a function of energy for reactions such as $pp \rightarrow pp\pi^0, pp \rightarrow np\pi^+, pp \rightarrow pp\pi^+\pi^-, pp \rightarrow np2\pi^+\pi^-$. The model also gives results in good agreement with the nuclear reaction data, in paricular with the HARP-CDP [2] experimental data on pion and proton productions in the interactions of projectile protons and pions of momenta 3, 5, 8, 12 and 15 GeV/c with Be, Cu, Ta and Pb targets.

With the recent improvements the FTF model can directly overlap with so called cascade models, such as Bertini intranuclear cascade, which eliminates the use of earlier crude parametric

models.

Recent features of the FTF model also include extentions into the area of modeling annihilation processes for anti-baryons, which will be revisited later in this paper.

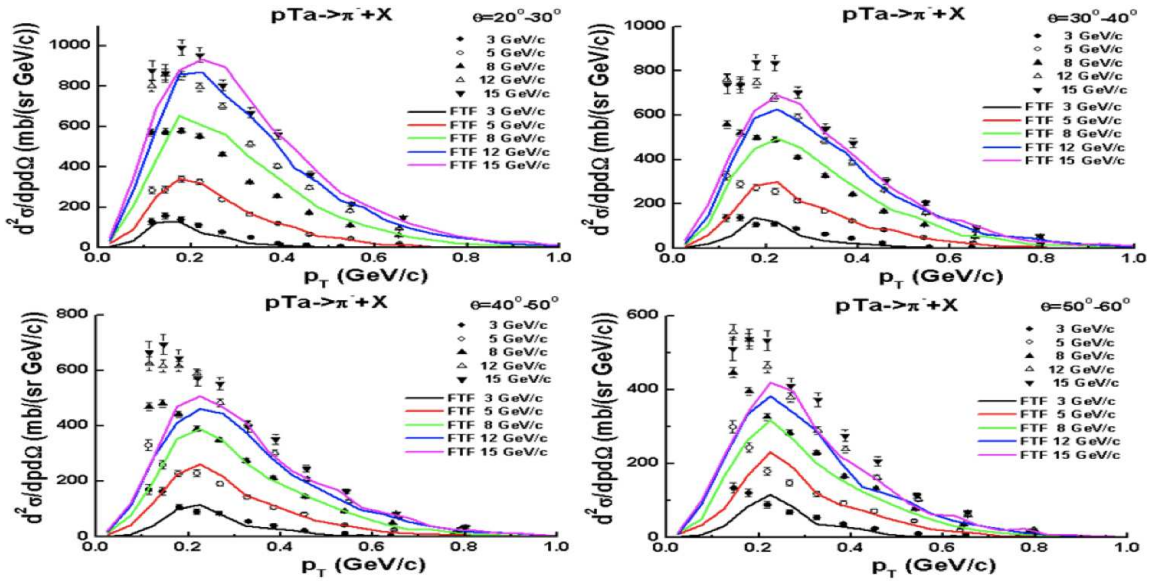

Figure 1. Invariant cross section for inclusive π^- production at four different angles in proton interactions with Beryllium as a function of p_T for five different energies. The data are compared with simulated results by FTF model.

Figure 1 shows how FTF model predictions compared with the HARP-CDP experimental data on the invariant cross section for the inclusive π^- production in proton Beryllium

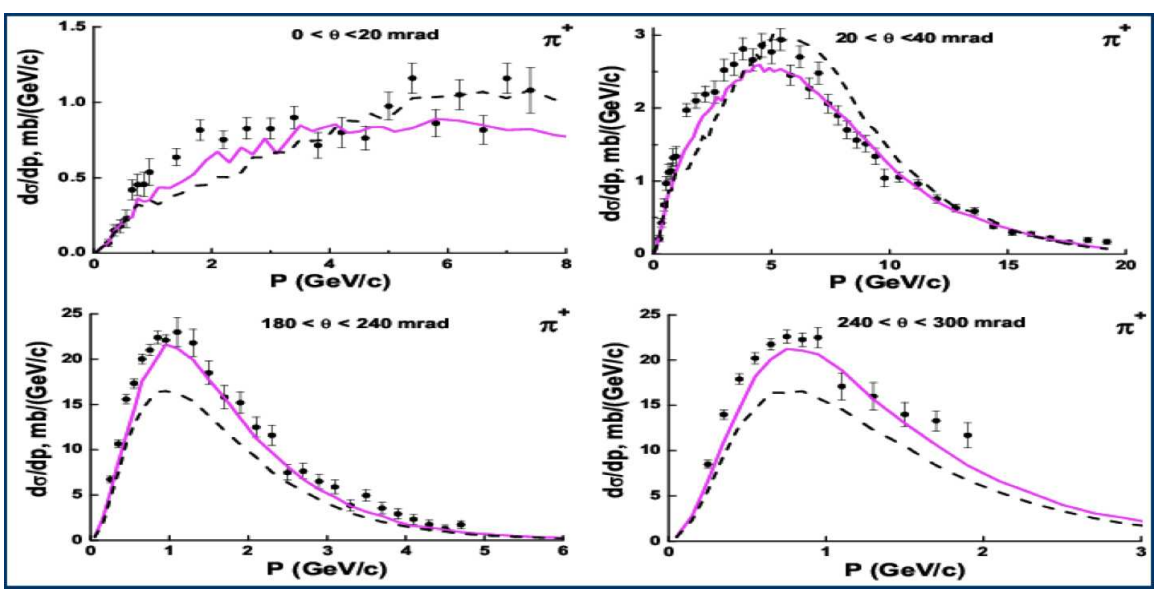

Figure 2. Invariant cross section for inclusive π^+ production in proton interactions with Carbon at 31GeV/c as a function of momentum. Results are shown at four different angles. Simulation results is shown for the new (magenta) and old (dashed black) versions of FTF.

interactions as a function pf p_T for five different beam energies; the data and the simulation results are shown for four different angles of the secondary π^-. The comparison indicates that FTF model gives good predictions at smaller angles but somewhat deviates from the experimental data in the backward hemisphere, especially at higher beam energies.

Figure 2 shows improvements between two versions of Geant4 of the simulation results by the FTF model for the invariant cross section for the inclusive π^+ production in proton Carbon interactions at 31GeV/c as a function of momentum, and compared to the NA61 [3] experimaental data.

Figure 3 shows simulation results for FTF and for other Geant4 hadronic models that are valid for the same energy range. Simulation results are compared with the recent experimental data [4] on the exclusive neutron production in proton interaction with Carbon, Uranium, and Berylluim targets, at 56 GeV/c, 57 GeV/c, and 120 GeV/c respectively.

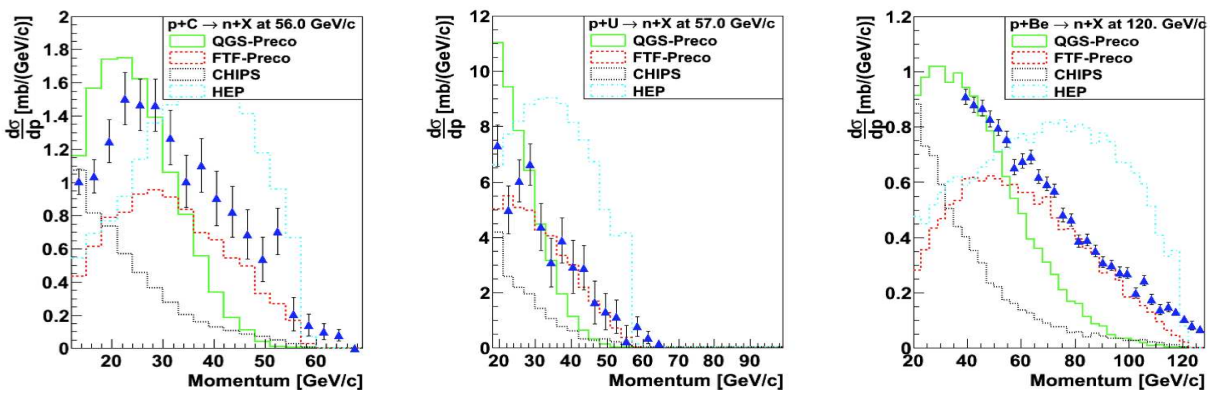

Figure 3. Invariant cross section for inclusive neutron production in proton interactions with Carbon, Uranium, and Beryllium as a function of momentum.

Although none of the models can give perfect overall fit with the data, however, FTF provides the closest match.

Development of the FTF model in the near future will focus on further improvements of its physics performance, as indicated by the feedback from the validation efforts.

Together with the Bertini Cascade model, described in the next section, FTF is the core component of the new physics list FTF_BERT that, from now on, is going to be recommended as the principal production physics list for the HEP experiments.

2.2. Bertini Intranuclear Cascade Model

Bertini intranuclear cascade model is valid for proton, neutrons, pions, kaons, and hyperons in the kinetic energy range up to 10GeV.

The early version of the code, initially developed as a standalone package, has been adapted in the Geant4 more than a decade ago, and has been extensively redesigned and much improved over these years.

The software now supports rescattering of high-energy string-fragmentation cascades using the Bertini-style model. The nuclear structure parametrization (a zone-based integrated Woods-Saxon potential) has been adjusted to use physically meaningful units, and incorporates a simple model of the cascade trailing effect. Angular distributions for intracascade two-body scattering have been improved. Direct gamma-nucleon interactions have also been incorporated into the model software. In addition to its own internal version to model precompound and deexcitation process, it also offers an interface to Geant4 standard Precompound package. The model is now

implemented in a fully energy- and momentum-conserving way, to within 1 per mil for a typical 1 GeV projectile momentum.

The agreement of both thick-target (sampling calorimeter) simulations and thin-target production cross-sections to experimental data are significantly better than in earlier GEANT4 releases.

The model has also been extended to model capture processes for pions, kaons, and Sigma-hyporons, which will be described in more details later in the paper.

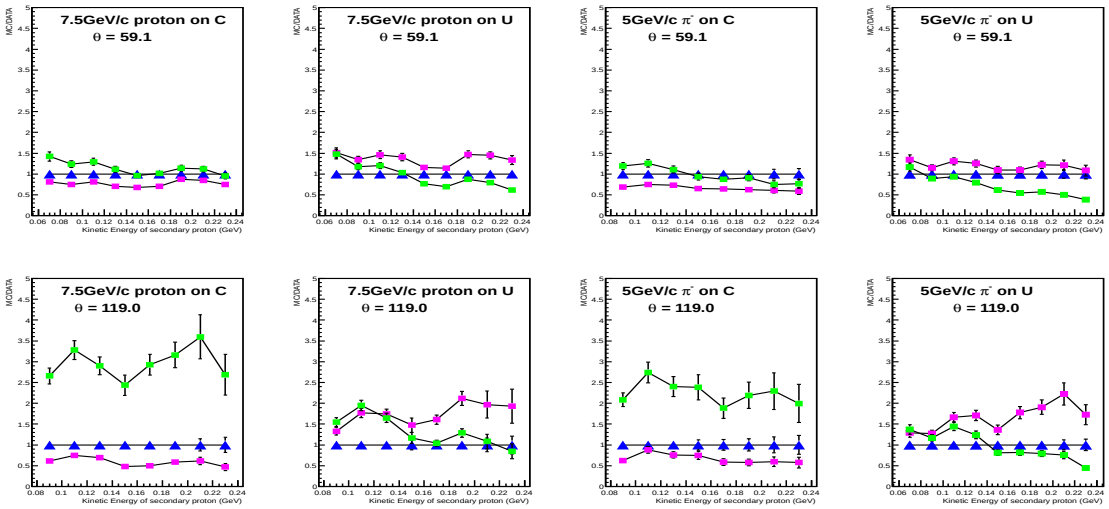

Figure 4. Invariant cross section for inclusive protons production at two different angles in proton and π^- interactions with Carbon or Uranium as a function of kinetic energy. All spectra are normalized to the experimental data (blue). Simulation results include Bertini Cascade (magenta) and FTF (green).

Figure 4 shows Bertini simulation results compared with the thin target experimental data [5] and with the FTF simulation in the energy range between 5GeV and 7GeV, where the two models overlap in validity. This figure shows differential cross-section of the inclusive proton production in proton or π^- beam interactions with Carbon or Uranium thin target as a function of kinetic energy of the secondary proton. All results are normilized to the experimental data, and are shown at two different angles of the outcoming particle. While both models are valid in this energy range, the Bertini model shows better agreement with the data than FTF, especially in the backward hemisphere.

Further tuning of the Bertini model will remain one of the Geant4 priorities in the near future.

This model has been employed in the Geant4 current production physics lists for the HEP and in several other physics lists. Together with the FTF model, it will remain one of the core components of the principal production physics lists.

2.3. Precompound Model

The Precompound model is used to model the nucleus de-excitation after the initial higher energy interaction. It is valid in the range below 200MeV, for any excited nucleus. When simulating showers induced by high energy hadron in matter, this model is greatly responsible for the lower energy component of a shower; thus, it is highly important for proper representation of observables such as calorimetric energy resolution and energy response.

In the recent past improvements have been made on several aspects of this model. For example, since the precompound state is a competition between particle emission and internal transition between exciton states, modern data are used to improve estimate of the emission probabilities and exit conditions. Other upgrades include improved calculation of the density of state and revision of modeling of de-excitation processes, such as fission, Fermi breakup of light nuclei, Weisskopf-Ewing evaporation and photon evaporation. Also, new Generarilized Emission Model is now used to model emission of heavy fragments, which improves nuclear fragment spectra from decays.

2.4. High Precision Low Energy Neutron Transport

Significant improvement has been made in the area of modeling low energy neutron transport with Geant4. The toolkit offers its own fairly accurate package, which has been upgraded to higher precision, by interfacing Geant4 to the low energy nuclear data from Evaluated Nuclear Data File (ENDF) libraries, developed at the Lawrence Livermore National Laboratory (LLNL). The interface provides Geant4 with cross sections for neutrons hitting various isotopes and with the final state products from the reactions. During simulation, Geant4 initially requests cross sections based on the materials in the geometry. Neutrons are then tracked according to their mean free path. At the end of a track, Geant4 queries the library for the final state products of the reaction and registers them into a stack for further tracking.

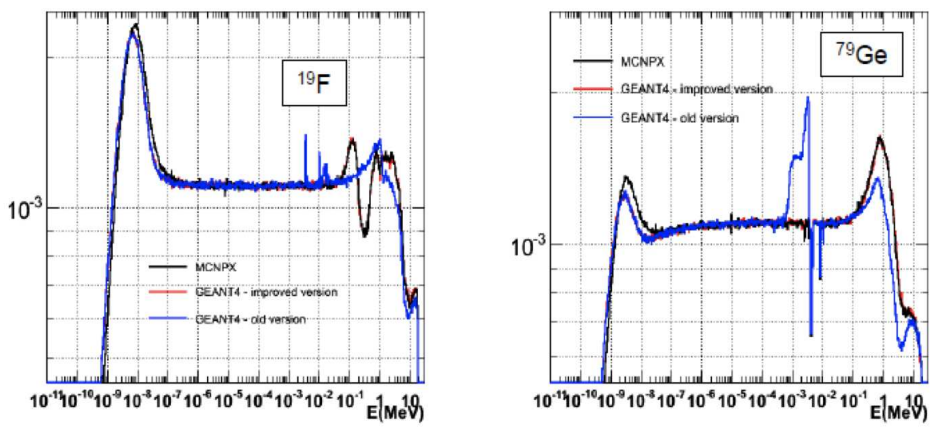

Figure 5. Kinetic energy spectra of a secondary neutron after projectile neutron interactions with ^{19}F or ^{79}Ge isotopes. Simulation is shown for old(blue) and recent (red) versions of HP neutron transport, and are compared with results from MCNPX Monte Carlo package.

Figure 5 shows simulated results for the secondary neutron kinetic energy after initial neutron interacts with Fluoride or Germanium isotopes.

The simulation includes the most recent version of Geant4 and an earlier version, as well as results from MCNPX [6] Monte Carlo package. One can see that the most recent version of Geant4 gives results that agree well with the output of MCNPX, while an earlier version of Geant4 indicates non-negligible deviations.

Later in this paper it will also be shown that the upgrade in the area of low energy neutron transport also improves the simulation of the transverse profile of hadronic showers.

2.5. Capture and Annihilation Processes

Until several months ago Geant4 could offer only two options for modeling capture and annihilation processes. One was a very simplistic, crudely parametrized code, where only model for muons was realistic and was giving reasonable agreement with the experimental data. This model is used for muons in all pre-fabricated physics lists. The other one was an option incorporated in the implementation of the so called CHIPS [**?**] model, which is also available in Geant4 and is currently used in most physics lists for all particles where applicable, except muons. It must be noted that, while CHIPS model gives results that are closer to the data than the simplistic code, it still has serious limitations and deficits. Due to this, in the recent months work has been done to extend both FTF and Bertini Cascade models to simulate annihilation processes for anti-baryons (FTF) and capture processes for mesons (pions and kaons) and for Σ^- hyperon (Bertini).

Figure 6 and Figure 7 show sample results to illustrate the case.

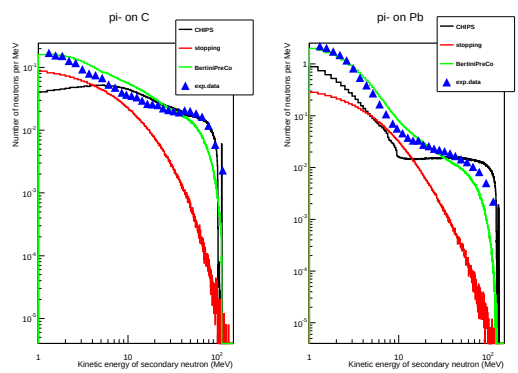

Figure 6. Average number of secondary neutrons produced in π^- capture on Carbon or Lead nuclei as a function of neutron kinetic energy. Simulation results by Bertini (green), CHIPS (black) and simplistic (red) models are compared to the experimental data (blue).

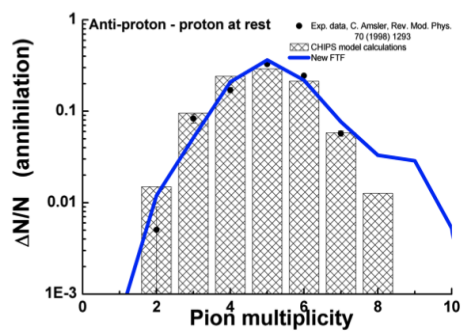

Figure 7. Average multiplicity of pions produced in anti-proton annihilation in Hydrogen. Simulation results from FTF (blue) are compared to the data (black dots) and CHIPS results (shaded area).

Figure 6 shows secondary neutron spectra produced in pi- interaction with Carbon or Lead target as a function of the secondary neutron kinetic energy. Simulation results are shown for Bertini Cascade model (combined with Precompound model) and compared with experimental data [8] and with results by simplistic and CHIPS models. It is clear that results from the Bertini model agree with the data much better than those of the alternative models. Figure 7 shows average multiplicity of secondary pions produced in anti-proton interactions with Hydrogen. Results include simulation by FTF and CHIPS models, and compared with experimental data [9]. FTF simulation fits with the experimental data at least as good as or better than the CHIPS one, and is much better than the simplistic model.

It must be noted that both Bertini and FTF models are also substantially more efficient than CHIPS in terms of CPU. This two models will be used for modeling annihilation and capture physics, instead of CHIPS, in the principal production physics lists, starting the next major release of Geant4.

2.6. Other Models

2.6.1. Intranuclear Cascade Model The Liège Intranuclear Cascade model (INCL) is a basically parameter-free, time-like Monte Carlo cascade model, which can be applied to nucleon-, pion- and light-ion-induced reactions in the kinetic-energy range up to 3 GeV per nucleon.

The model has been initiually incorporated in Geant4 since several years, and has much improved over the recent past [10].

Most recent version of it, the INCL++, can be used for modeling nucleon- and pion-induced reactions. It includes modeling of de-excitation of the INCL++ cascade remnants. improvements to the underlying physics, good description of the pre-equilibrium-like emission of light charged particles (up to $A = 8$) using a dynamical phase-space coalescence algorithm, and smooth connection to a fusion model for covering lower-energy range of ~ 100 MeV. In the near future the model will be extended to light-ion-induced reactions.

Detailed description of the new development in this area will soon be available in a dedicated publication [11].

2.6.2. Low and High Energy Parametrized Models Low and High Energy Parametrized models (LEP/HEP) are the veteran models of Geant4. They represent a C++ translation and port of an earlier Gheisha code [12]. The model has been used in many applications at the beginning of the Geant4 career. It is also quite efficient in terms of CPU. But it is a relatively crude parametrization, largely based on calorimetric measurements from 1980's, and it lacks of many certain up-to-date knowledge in hadronic physics.

2.6.3. Quark Gluon String Model Quark Gluon String model (QGS) [13] is an earlier alternative to the FTF string model. As already mentioned before, it can give reasonably good agreement with a variety of experimental data, but its low validity range is $\sim$15GeV, which prevents from smoothly interfacing it with cascade nodels that work well in the range up to 10GeV. However, in the past years this model has been employed as a core of the QGSP family of production physics lists.

2.6.4. Binary Cascade Model Binary cascade model [14] is a theory-driven alternative to Bertini cascade model. It gives fairly accurate results in the energy range up to 2GeV, but yeilds to Bertini model at higher energies.

2.6.5. Chiral Invariant Phase Space Model Chiral Invarinat Phase Space model (CHIPS) is described in details in the dedicated publication [7]. In Geant4 it is currently used for modeling gamma-nuclear interactions, nuclear capture of negatively charges hadrons, quasi-elastic scattering processes, p-A and n-A elastic scattering processes, and for kaon and hyperon nuclear cross sections. However, it is being gradually replaced in main production physics lists by recent developments, including those presented in this paper.

3. SimplifiedCalo Suite for the Validation of the Physics Lists

Each new Geant4 version features refinements of physics models and improvements in computing performance. These improvements and upgrades need to be tested not only for a particular model, but also on the level of full scale physics lists that include multiple processes for different particles, in applications that are similar to the realistic detector simulations of running experiments and ongoing R&D. An example of a particularly demanding use-case are High Energy Physics calorimeters. A testing suite has been developed to test physics lists with different physics parameters and includes several calorimetric applications, such as LHC calorimeters materials and technologies, ZEUS compensating calorimeter concept, CALICE

calorimetry ideas, and several other sampling calorimeter concepts. The high statistics tests are performed for public release of Geant4 and for internal development releases. They provide results on most important observables for calorimetric measurements, such as energy response, energy resolution, and shower longitudinal and lateral profile. Simulation results are compared against experimental data wherever possible. Figure 8 shows simulated results and test beam data for a sampling calorimeter made of Copper absorber and Liquid Argon as an active medium. It presents calorimeter response as a function of beam energy.

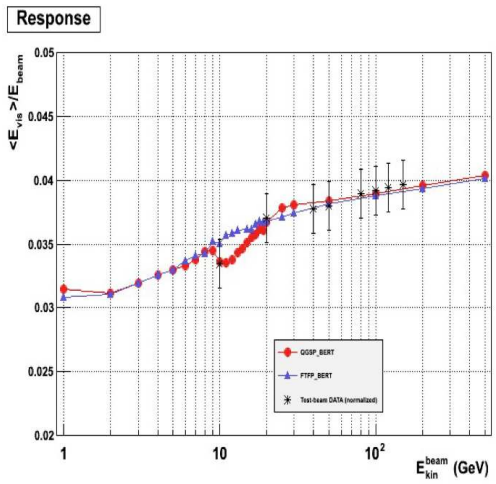

Figure 8. Response of a Copper and Liquid Argon Calorimeter to a pion beam as a function of energy.

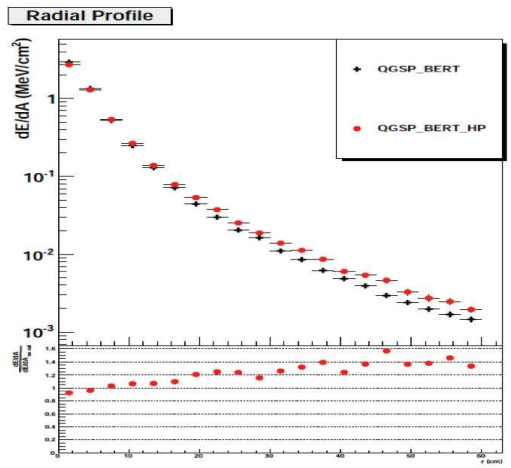

Figure 9. Energy desposit by a pion induced shower in a Lead and Liquid Argon calorimeter as a function of distance from the shower axis.

Simulation results are shown for the new and most recommended physics list FTFP_BERT and are compared with the results from another physics list, based on the alternative string model (QGS). The unphysical deep in the response function simulated with QGS model disappears in the FTF-based results, because of the recently improved smooth interface between FTF and the Bertini Cascade models, as it has already been mentioned in previous sections. Figure 9 shows simulated results for a sampling calorimeter made of Lead absorber and Liquid Argon as an active medium. The figure shows the lateral profile of a hadronic shower, i.e. energy deposit in the calorimeter as a function of distance from the shower axis. Geant4 has long been criticized for modeling shower transverse profile to be too narrow in comparison to the experimental results. The new simulated results are presented for the physics list QGSP_BERT_HP that employs recent upgrade in modeling low energy neutron transport via interface to the ENDL database and are compared with the physics list QGSP_BERT that does not employ those improvements. The new result indicate that the simulated lateral profile of a hadronic shower is wider with the use of the new low energy neutron simulation package.

4. Consolidation of the Geant4 Validation Results

As the physics simulation in Geant4 improves or older models are replaced by newer and better ones, the amount of validation results grows and presents a serious challenge of collecting and organizing the materials in one central repository and to make this data generally and easily available, not only for the internal use in the collaboration but also for community of users.

To achieve this goal a JavaEE/JSP based framework that uses a postgreSQL data base as back-end has been designed and implemented. The framework consists of four components:

- PostgresSQL database stores collections of the tests, such as images, tags, descriptions, references, etc.
- Java/JSP class library provides an interface to the database that allows to access and manages the objects, without exposing details of the database to end users.
- Web Application is based on the Java/JSP library and can run on a Tomcat or Glassfish web application server. It is used to display the tests and also provides Geant 4 experts with tools to upload, edit or delete a test.
- A separate utility allows the development team to upload into the database a large volume of test results in a one-step process. The input for this utility is a text file containing XML representations of the objects to be uploaded to the data base.

The collection of Geant4 validation materials is available at the following URL:
http://g4validation.fnal.gov:8080/G4HadronicValidation

5. Summary

Geant4 offers a rich collection of models to simulate hadronic physics, that are being continuously improved and validated against experimental data. Significant progress has been recently made in this domain, driven not only by feedback from the current LHC experiments but also from past experiments and from the R&D for the proposed projects.

While Geant4 can not offer a single hadronic model to cover the entire energy range, as each model has certain limitation in its validity, the models, however, can be sucsessfully combined to cover practically any use-case. This is particularly due to the work invested into smooth interface of every two models that have an overlap in validity.

Current key developments in the Geant4 hadronic physics domain are the following:

- Fritiof string model for the high energy end
- Bertini Cascade model for the intermediate energy range
- Precompound model to handle excited nuclei and the lower energy range
- Extention of these models that allow to simulate annihilation and capture processes
- High precision low energy neutron transport

Geant4 will also support older physics models, for various physics studies, as well as for reference and backward compatibility.

A large collection of prefabricated physics lists makes full use of the available hadronic physics models. These physics lists are distributed with each public release of Geant4, and provide users with choice suitable for their tasks and applications. The physics lists are stable but not frozen, as the Geant4 collaboration aims to improve them with the feedback from experiments.

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