Recent improvements on the description of hadronic interactions in Geant4

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Abstract.
We present an overview of recent improvements of hadronic models in Geant4 for the physics configurations (Physics Lists) relevant to applications in high energy experiments. During last year the improvements have concentrated on the study of unphysical discontinuities in calorimeter observables in the transition regions between the models used in Physics Lists. The microscopic origin of these have been investigated, and possible improvements of Geant4 code are currently under validation. In this paper we discuss the status of the latest version of Geant4 with emphasis on the most promising new developments, namely the Fritiof based and CHIPS Physics Lists.

1. Introduction
In modern high energy physics (HEP) experiments Monte Carlo programs are employed not only in the initial phase of the life time of an experiment to assist its design, but also for studying the performance of the reconstruction algorithms that will be used for the data analysis. In some cases simulations are used also to derive corrections to unfold detector and reconstruction effects.

Geant4 [1, 2] is a toolkit for the simulation of passage of particles through matter. Its areas of application include high energy, nuclear and accelerator physics, as well as studies in medical and space science. It includes the algorithms to track particles in complex geometries with or without the effect of magnetic fields, interfaces to analysis (hits and digits) or persistency frameworks and advanced visualization capabilities. Most important, a complete set of physics models to describe both electro-magnetic and hadronic interactions up to energies to hundreds of GeV is available.

QCD is the well-established theory of strong interactions, but most of the hadronic interactions that occur when particles cross matter (e.g. detectors) are happening in the non-perturbative region of the theory, where the theoretical predictions are not computable. Various phenomenological models exist to describe hadronic interactions in some limited kinematic
regions, and to cover a wide energy range, from MeV to hundreds of GeV, various models have to be combined in a transportation code.

Geant4 provides a powerful framework to develop user specific algorithms describing hadronic interactions, and it comes with a variety of models with different performances in terms of physics precision and CPU needs, as well as different ranges of validity in terms of the energy and the type of the interacting particle. It is a user’s responsibility to assemble the models to cover all particles and energies interested in an application. However, a set of Physics Lists are available with pre-assembled models to cover all energies and particles of typical modern HEP experiments. These Physics Lists are routinely validated by models developers and compared with test-beam data from past and present experiments.

Geant4 has been developed and tuned with the current generation LHC experiments as primary users. Strong requirements have been set [3, 4]. In the past years mainly the ATLAS and CMS experiments have extensively compared the simulation predictions with the collected test-beam data. A summary of the results can be found in [5].

In the past years, LHC experiments (in particular ATLAS and CMS) studied the physics performances of the different Physics Lists and converged towards the use of the so-called QGSP_BERT Physics List as the default one. It gives the best results in terms of describing the data collected with the calorimeters during the test-beam campaigns.

Before describing the models, used by this Physics List, it is important to remember that the models parameters are tuned with thin target data (single interaction data) rather than test-beam data. The simulation of calorimeters is used to verify, at a global level, the quality of a Physics List (for an overview of some results on the validation of models see: [6, 7, 8, 9])

1.1. Main hadronic models

The Physics List QGSP_BERT which is used in production for ATLAS and CMS detector simulations, comprises the following physics models:

- Quark-Gluon String (QGS) model [10, 11, 12, 13, 14] for proton, neutron, pion and kaon interactions with nuclei at kinetic energies above 12 GeV, interfaced to Precompound (P) model [15] for the evaporation phase of the interaction.
- Low Energy Parameterized (LEP) model [16] for proton, neutron, pion and kaon interactions with nuclei at kinetic energies between 9.5 GeV and 25 GeV.
- Bertini cascade (BERT) model [17, 18], which includes intra-nuclear cascade, followed by precompound and evaporation phases of the residual nucleus, for proton, neutron, pion and kaon interactions with nuclei at kinetic energies below 9.9 GeV. Note that the Bertini model is not used for the simulation of secondary hadrons rescattering produced by the QGS model inside the nucleus.
- Parameterized (LEP + HEP) models for all remaining hadrons (i.e. hyperons and antibaryons) interactions.
- Parameterized capture and fission for low-energy neutrons.
- CHIPS model [20, 21, 22, 23] for the nuclear capture of negatively charged particles at rest.
- CHIPS model for elastic scattering of neutrons and protons; for elastic scattering of all other hadrons a parametrized model below 1 GeV and a revised elastic scattering model above 1 GeV are used.
- Glauber model [19] for quasi-elastic scattering for proton, neutron, pion and kaon interactions with nuclei at kinetic energies above 12 GeV; in all other cases parametrized models.
- Standard electromagnetic processes [24].
- CHIPS model for gamma-nuclear and electron-nuclear interactions.
Figure 1. Simulated response in a simplified scintillator/iron sampling calorimeter for negatively charged pions as a function of primary kinetic energy. Different Geant4 Physics Lists are shown for comparison. Statistical and systematic errors are also shown, in many cases they are smaller than the symbol size.

Figure 2. Simulated normalized response width in a simplified scintillator/iron sampling calorimeter for negatively charged pions as a function of primary kinetic energy (the interesting region at $E_{beam} = 10$ GeV is shown). Different Geant4 Physics Lists are shown for comparison.

- Parameterized model for muon-nuclear interaction.

There is a small transition region between BERT and LEP and a larger one between LEP and QGS. In these transition regions one of the models is chosen at random to compute the interaction with matter. The most promising alternatives to QGSP_BERT are the FTFP_BERT and CHIPS Physics Lists.

The FTFP_BERT Physics List is very similar to the QGSP_BERT one with the exception that it uses the well-known Fritiof model (FTF) instead of the QGS one to describe the interaction of highly energetic protons, neutrons, pions and kaons [25, 26]. While the QGS model is well-suited to describe interactions of projectile with kinetic energy $E_{kin} > 10$ GeV the FTF model can describe interactions starting from 4-5 GeV. Thus the string model can be coupled directly to the cascade model, that have a typical range of validity up to few GeV.

At high energy the CHIPS Physics List uses a one-dimensional parton multi-string model. The soft particles of a string fragment are absorbed by a target nucleus and handled by the low-energy model. A quasmon (parton plasma) is created and subsequently decayed. Finally, an evaporation model is used to de-excite the remnant nucleus. The advantage of the CHIPS Physics List is that it melds the high- and low-energy approaches in a coherent and unique theoretical framework. In addition, it can handle all types of projectiles, including kaons, antibaryons and hyperons. While QGSP_BERT and FTFP_BERT share the same data sets for cross sections, CHIPS has its own data set for the interaction of kaons, hyperons and anti-particles; and for the capture of neutrons.

Finally all three Physics Lists share the same implementation of electromagnetic processes.

2. Status of the simulations of hadronic interactions for High Energy Physics experiments

Starting from 2006 both ATLAS and CMS experiments have decided to use QGSP_BERT (or its variants) as the default Physics List for the simulation of hadronic interactions. This list gives the best results when comparing with test-beam data:
• The response to hadrons, defined as the ratio between the measured energy and the beam energy, is described at the level of 3%.

• The energy resolution \((\sigma/\langle E \rangle)\) is described by this list at the level of 10%, though if it is systematically smaller than measured data.

• With the addition of the Bertini intra-nuclear cascade, the shower shape description has substantially improved, however simulation still predicts shorter and narrower showers. Showers are shorter of about 10% (at a depth of \(10\lambda_I\) in the calorimeter) for pion projectile, while for protons the agreement is at the level of 30% [27, 28].

2.1. Transition between models

The CMS experiment has found that the calorimeter energy response in its HCAL test-beam setup, as a function of the pion beam energy, presents an unphysical discontinuity around 9-10 GeV. The ATLAS experiment confirmed the same problem for its calorimeter test-beam setups.

The origins of this discontinuity, shown in figure 1, have been studied in detail in the past two years. It is now clear that the effect is caused by the use of the parametrized models for particle interactions in the energy range \(9.5 < E_{kin} < 25\) GeV [29].

As a strategy to reduce the dependence on the parametrized models and to address the issue we have studied the performance of the FTFP\_BERT Physics List, which has a reduced dependence on the parametrized models and it has different transition regions; and the CHIPS one, that does not depend at all on these parametrization and does not have, by construction, any strong transition. Predictions of these Physics Lists in a comparison with QGSP\_BERT for simplified setups are discussed in the following section.

3. Results on simplified calorimeters

We have performed simulations of a \(10\lambda_I\) depth and wide sampling calorimeter (100 periods made of a 16.8 mm thick iron slab followed by 4 mm thick slab of scintillator). Impinging pions of different kinetic energies (from 1 to 500 GeV) have been simulated. Given its importance for the response in scintillator-based calorimeters the Birks’ attenuation effect has been implemented in the simulation with the parameters of [30]. Transportation of neutrons is stopped after 50 ns: this is the characteristic read-out time window in this kind of calorimeters\(^1\). A correction for front (albedo) and longitudinal leakage has been implemented. This correction varies with the primary particle’s momentum, but it is typically of the order of 1% of the deposited energy. The systematic error associated with this correction is much smaller than the statistical error.

3.1. Energy response

Figure 1 shows the response as a function of primary energy for the considered Physics Lists. Red circles illustrate the response for the LHC experiments default Physics List (QGSP\_BERT). The transition between models is clearly visible at around 10 and 25 GeV. Since these unphysical discontinuities are due to the use of the parametrized models, the results obtained with LHEP (a Physics List that uses parametrized models for all energies and all primary types) are also shown as reference. It becomes clear that the use of these models in QGSP\_BERT for the intermediate energy region has the effect of reducing the simulation response and of producing the unphysical discontinuities.

The FTFP\_BERT and CHIPS Physics Lists do not show these discontinuities and are much smoother. As discussed in section 2, the detailed simulations of the ATLAS and CMS calorimeters show that the response predicted by QGSP\_BERT Physics List is in agreement with

\(^1\) The response varies by about 3% increasing the neutron time-cut from 20 to 200 ns, this is the main systematic error in this analysis.
experimental data (typical test-beam have \( E_{\text{beam}} > 20 \text{ GeV} \), only few data points are available for lower energies). Thus, the FTFP\_BERT Physics List agrees with QGSP\_BERT which, in turn, agrees with the data. CHIPS response is too high (this Physics List is still considered as experimental one and its tuning with thin-target data is still ongoing).

3.2. Resolution
To study the smoothness of the energy resolution as a function of the beam energy, it is more convenient to show \( \sigma/E_{\text{beam}} \) instead of \( \sigma/\langle E \rangle \) since the response of QGSP\_BERT is not smooth. The results for the considered Physics Lists are shown in figure 2. Only in the region around the 10 GeV a small discontinuity is left. The transition effect is not particularly visible in this observable, and, once again, the FTFP\_BERT combination gives similar results to the other string-based Physics List. CHIPS model predicts smaller widths. Data prefer simulations with larger resolution, thus more studies are needed for the CHIPS model to reach an agreement with data.

3.3. Shower shapes
We have examined the hadronic shower dimension as a function of the primary energy. In order to efficiently summarize the longitudinal (\( \langle \lambda^2 \rangle \)) and lateral (\( \langle r^2 \rangle \)) dimensions for each event, we have calculated the second moment\(^2\) of the position of read-out cells with \( E_c > 0 \). The mean values of these quantities are shown in figures 3 and 4. For shower shape observables QGSP\_BERT has irregularities around 10 and 25 GeV. CHIPS predicts longer showers, which is in the direction of a better agreement with test-beam data. However, for this Physics List, showers are more compact in the lateral dimensions at low energies, while they tend to be wider at higher energies in comparison with the other two Physics Lists. CHIPS also predicts stronger fluctuations as a function of beam energy, further development is needed for the CHIPS models.

In general FTFP\_BERT Physics List gives similar results as the QGSP\_BERT one, but a transition between the Bertini cascade model and the Fritiof string model between 4 and 5 GeV

\[ \lambda^2 = \frac{\sum_{c \in \{\text{cells}\}} E_c \lambda_c^2}{\sum_{c \in \{\text{cells}\}} E_c} ; \quad r^2 = \frac{\sum_{c \in \{\text{cells}\}} E_c r_c^2}{\sum_{c \in \{\text{cells}\}} E_c} \]

with \( \lambda_c \) and \( r_c \) being the center of cell \( c \) in polar coordinates with respect to the shower center and shower axis.

\(^2\) First we read-out the energy deposited in the detector in small voxels of 5x5x5 cm\(^3\) of volume. For each event the characteristic shower dimensions have been calculated as:
4. Conclusions

In the past years the LHC experiments have compared in detail the prediction of the Geant4 simulations with test-beam data. The initial requirements set by LHC have been finally met. In particular the test beam experience has shown that at high energy the string based models describe reasonably well the experimental results. At low energies it has been shown that an intra-nuclear cascade code is a fundamental ingredient to improve the description of shower shapes.

New options have been created in Geant4 that are very promising. The FTFP\_BERT Physics List, with a much reduced dependence on the parametrized models (responsible for the discontinuities), shows a smooth response as a function of the primary energy. The Physics List is in a good agreement with the QGSP\_BERT predictions. The transition effect which is visible in FTFP\_BERT at 4 GeV for the shower shape observables will be addressed in the future, however, its impact on global physics performance is expected to be small.

The CHIPS Physics List is a good alternative to string and cascade based Physics Lists. It uses a coherent treatment of hadronic inelastic interactions which results in a very smooth behavior in all observed observables. Though at the moment its response is higher, and the resolution is lower with respect to QGSP\_BERT and FTFP\_BERT, improvements are expected in the future since it is still undergoing tuning with thin-target data.

In conclusion, Geant4 is used with success by many HEP experiments. The quality of its simulation of hadronic interactions is constantly improved and the most widely used Physics List QGSP\_BERT, has been stable since some years. Competitive models or new mixtures of models are emerging as promising alternatives. In most cases they give results similar of even better than QGSP\_BERT Physics List.

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