Validation of Physics Models of Geant4 using Data from CMS Experiment

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Abstract. CMS has tuned its simulation program and has chosen a specific physics model of GEANT4 by comparing the simulation results with dedicated test beam experiments. CMS continues to validate the physics models inside GEANT4 using the test beam data as well as collision data. Several physics lists (collection of physics models) inside the most recent version of GEANT4 provide good agreement of the energy response, resolution of pions and protons. The validation results from these studies are used to make the choice of physics list and GEANT4 version for the CMS experiment.

1. Introduction
The CMS experiment [1] working at the Large Hadron Collider uses the GEANT4 toolkit [2, 3, 4] for its detector simulation software [5]. The simulation software as well as the GEANT4 code is evolving since CMS simulation code has been put into operation. There has been an active effort within CMS to evaluate the quality of simulation as one changes either the application software or the version of GEANT4.

Two sources of data are used for validating the software. Data exist from a test beam campaign during 2006 where a prototype of the CMS hadron calorimeter and one super-module of electromagnetic calorimeter was exposed to hadron beams of different types and of different energies. Results from this test beam are published [6, 7] and are used in earlier tuning of the CMS simulation program (described in [8, 9]). As a second source, collision data from the CMS experiment are used. Here low luminosity runs with zero bias or minimum bias triggers are analyzed from the 2016B run period. Similar analysis using isolated charged hadrons was done earlier in CMS [10].

These validation results consolidate the recent adaptation of the new GEANT4 version (10.2.p02) and the new Physics List (FTFP_BERT_EMM) for 2017 Monte Carlo production.

2. Evolution of CMS Simulation Software
CMS switched to a new framework and adopted GEANT4 ten years ago. CMS started with the physics list QGSP_FTFP_BERT_EML 1 for the first comparison with collision data using GEANT4 version 9.4.p02 and then moved to the version 9.6.p02. During the high (13 TeV) energy operation in 2015, CMS software changed the framework to multi-threading mode and

1 description of GEANT4 physics lists are given in [11]
started using GEANT4 version 10.0.p02 with the physics list QGSP_FTFP_BERT_EML. For its production plan of 2017, CMS plans to move to a new physics list FTFP_BERT_EMM and GEANT4 version 10.2.p02. The FTFP physics model has been substantially modified over the past few years to improve the quality of physics predictions and FTFP_BERT has become the recommended physics list from GEANT4 collaboration.

The physics list QGSP_FTFP_BERT combines QGSP (quark gluon string model with the Pre-compound model at the back-end), FTFP (Fritiof model implemented inside GEANT4) and Bertini Cascade (BERT) models for $\pi/K/p/n$ induced interactions with a fixed validity region for each of these models: Bertini Cascade being valid at $\leq 8$ GeV; FTFP valid between 6 and 25 GeV; and QGSP valid at $\geq 12$ GeV. The list FTFP_BERT uses FTFP and Bertini Cascade models with Bertini Cascade being valid at $\leq 5$ GeV and FTFP valid above 4 GeV. EML, EMM specify the physics models for electromagnetic processes. EML utilizes a simplified multiple scattering model for all detectors, while EMM uses the detailed multiple scattering model for sampling calorimeters and the simplified one for other detectors. Handling of multiple scattering is critical for sampling calorimeter.

GEANT4.10.2.p02 is chosen for producing Monte Carlo samples of 2017 run period because of the following considerations:

- it has full implementation of multi-threading mode;
- it is C++11 compliant and can be used with newest compilers;
- it includes many technical improvements and fixes;
- it is faster than 10.0 and requires less memory in general G4 benchmarks;
- it has improved physics predictions.

3. Comparison with Test Beam Data

Dedicated measurements were carried out with prototypes of the CMS calorimeter in the test beam facility at CERN [6, 7]. Two production wedges of the barrel hadron calorimeter (HB), one prototype module of the hadron endcap (HE), and eighteen trays of the outer hadron calorimeter (HO) were exposed to hadron beams in the H2 beam line of the Super Proton Synchrotron (SPS). The hadron calorimeter was preceded by a super-module of the barrel electromagnetic calorimeter (EB). The platform holding the modules could be moved along the $\phi$ and $\eta$ directions allowing the beam to be directed onto any tower of the calorimeter in order to mimic a particle trajectory from the interaction point of the CMS experiment. Monochromatic secondary and tertiary beams were used having a momentum between 2 and 350 GeV/c. Auxiliary beam counters were used to select pure beam interactions.

Both electromagnetic and hadron calorimeters were calibrated using 50 GeV electron beams. The energy response, resolution, and shower profiles were measured for different beam momenta. The analysis utilized particle identification using data from Time of Flight counters and Cherenkov detectors up to an energy of 9 GeV. The results consist of mean energy response (measured as the ratio of the total energy in the calorimeter to the beam momentum) as a function of beam momentum for different beam types and also the energy distribution for particles of a given type with a given momentum (all particles or particles which do not undergo inelastic interactions in the Electromagnetic Calorimeter). The test beam setup is described within CMS software and is used routinely to validate GEANT4 models.

3.1. Comparison of Mean Response

Figure 1 shows the mean energy response measured as the ratio of energy measured in the calorimeter to the beam energy as a function of the beam momentum for $\pi^-$ and $\pi^+$. $\phi$ is the azimuthal angle while $\eta$ is the pseudorapidity measured from the polar angle $\theta$ as $-\ln(\tan(\frac{\theta}{2}))$.
The measurements from the test beam experiment are compared with predictions from two physics lists, QGSP_FTFP_BERT_EML from GEANT4.10.0.p02 and FTFP_BERT_EMM from GEANT4.10.2.p02. The same figure also shows the ratio of Monte Carlo to data as a function of beam momentum. It is clear from the figure that the predictions from the physics list FTFP_BERT_EMM are closer to the data. This is particularly true at higher beam energies.

**Figure 1.** The top plots correspond to the mean energy response for $\pi^-$ (left) and $\pi^+$ (right) as a function of the beam momentum. The bottom plots are ratios of Monte Carlo predictions to the data for pions as a function of beam momentum. The black points refer to the data, while the red and blue points are Monte Carlo predictions from physics lists QGSP_FTFP_BERT_EML of GEANT4.10.0.p02 and FTFP_BERT_EMM of GEANT4.10.2.p02 respectively.

Figure 2 shows the mean energy response measured as the ratio of energy measured in the calorimeter to the beam energy as a function of the beam momentum for protons and anti-protons. The measurements are compared to the predictions from two physics lists, QGSP_FTFP_BERT_EML from GEANT4.10.0.p02 and FTFP_BERT_EMM from GEANT4.10.2.p02. The ratio of Monte Carlo to data is also shown in the same figure as a function of beam momentum. Again the predictions from the physics list FTFP_BERT_EMM give a better description of the data particularly at higher beam energies.

The level of disagreement between Monte Carlo and data is expressed as the difference of the weighted mean of the ratio (Monte Carlo to data) from 1. Table 1 summarizes this measure of disagreement for the two physics lists studied.

The level of agreement between data and Monte Carlo improves in the new model for pions and protons. Proton-proton collisions at high energies produce mostly pions. So a better
Figure 2. The top plots correspond to the mean energy response for protons (left) and antiprotons (right) as a function of the beam momentum. The bottom plots are ratios of Monte Carlo predictions to the data for p and \( \bar{p} \) as a function of beam momentum. The black points refer to the data, while the red and blue points are Monte Carlo predictions from physics lists QGSP\_FTFP\_BERT\_EML of Geant4.10.0.p02 and FTFP\_BERT\_EMM of Geant4.10.2.p02 respectively.

Table 1. The difference of the weighted mean of the ratio Monte Carlo to the data for mean energy response from 1 for different beam types.

| Physics List                         | Measure of disagreement for |
|-------------------------------------|-----------------------------|
|                                     | \( \pi^- \) | \( \pi^+ \) | p | \( \bar{p} \) |
| QGSP\_FTFP\_BERT\_EML (G4.10.0.p02)| (3.6±0.6)% | (1.9±0.5)% | (4.3±1.0)% | (3.5±0.8)% |
| FTFP\_BERT\_EMM (G4.10.2.p02)     | (1.8±0.7)% | (1.0±0.5)% | (2.2±1.1)% | (3.1±0.8)% |

agreement between data and MC is expected with the new physics list in the Geant4 version 10.2.p02.

3.2. Comparison of Energy Distributions

Figure 3 shows measured energy distributions in the calorimeter prototype for \( \pi^- \) at two beam momenta of 4 GeV and 8 GeV. The measured distributions are compared with Monte Carlo predictions from physics lists QGSP\_FTFP\_BERT\_EML of Geant4.10.0.p02 and FTFP\_BERT\_EMM of Geant4.10.2.p02. Both the physics lists studied here provide agreement better than 8% on average with the data. While the agreement is better for the mean energy...
response, the data seem to have a slightly longer tail than the Monte Carlo predictions.

![Figure 3](image1.png)

**Figure 3.** The plots correspond to measured energy distributions for $\pi^-$ at 4 GeV (left) and 8 GeV (right). The black points refer to the data, while the red and blue lines are Monte Carlo predictions from physics lists QGSP\_FTFP\_BERT\_EML of Geant4.10.0.p02 and FTFP\_BERT\_EMM of Geant4.10.2.p02 respectively.

Figure 4 shows measured energy distributions in the calorimeter prototype for protons at two beam momenta of 3 GeV and 6 GeV. The measured distributions are compared with Monte Carlo predictions from physics lists QGSP\_FTFP\_BERT\_EML of Geant4.10.0.p02 and FTFP\_BERT\_EMM of Geant4.10.2.p02. Both the physics lists studied provide agreement better than 10% on average with the data. Again the main source of disagreement is due to the tails of the distributions.

![Figure 4](image2.png)

**Figure 4.** The plots correspond to measured energy distributions for protons at 3 GeV (left) and 6 GeV (right). The black points refer to the data, while the red and blue lines are Monte Carlo predictions from physics lists QGSP\_FTFP\_BERT\_EML of Geant4.10.0.p02 and FTFP\_BERT\_EMM of Geant4.10.2.p02 respectively.

### 4. Comparison with Collision Data

Energy distributions of showers generated by isolated charged hadrons in proton-proton collision in the CMS experiment are compared with Monte Carlo predictions with different physics lists of Geant4. Data collected by the minimum bias and zero bias triggers in the low luminosity run of 2016 are considered.
Events are selected to have only one well reconstructed primary vertex which is close to the nominal interaction point. Good track candidates are then selected and tested if these are well isolated from other charged and neutral particles. Tracks are first selected on the basis of closeness of the track to the primary vertex in the transverse \((xy)\) plane as well as along the beam axis, the \(\chi^2\) of the track fit and number of tracker layers used in the measurements. It is important that the tracks do not interact before reaching the calorimeter surface. This is checked by looking at the number of missing hits in the inner and outer hit patterns of the reconstructed hits. All tracks with missing hits in the inner and outer hit patterns are rejected.

The tracks are extrapolated to the calorimeter surface and the calorimeter cell corresponding to the impact point is identified. A matrix of \(n \times n\) cells, corresponding to the granularity of the calorimeter cells, around the impact point is defined as signal zone and consequently a matrix of \(N \times N\) (with \(N > n\)) is defined as isolation zone. From a study of lateral shower profile of hadrons in the test beam and in simulation, signal zone is chosen to be a matrix of \(7 \times 7\) or \(11 \times 11\) crystals for the electromagnetic calorimeter (ECAL) and \(3 \times 3\) or \(5 \times 5\) towers for the hadron calorimeter (HCAL). The smaller size matrix provides better purity while the larger size provides larger containment.

The extrapolated cell needs to be well isolated from all other charged and neutral particles.

**Figure 5.** Mean energy response of the isolated track as a function of the track momentum when the track hit 4 different regions of the calorimeter: (top left) \(|\eta| < 0.52\), (top right) \(0.52 < |\eta| < 1.131\), (bottom left) \(1.131 < |\eta| < 1.653\) and (bottom right) \(1.653 < |\eta| < 2.172\). The black points are the data and the red and blue points refer to Monte Carlo predictions from physics lists QGSP\_FTFP\_BERT\_EML of Geant4.10.0.p02 and FTFP\_BERT\_EMM of Geant4.10.2.p02 respectively.
Isolation with respect to charged particles is obtained by extrapolating other charged particles (selected with slightly looser criteria) and examining if the extrapolated point is within a matrix of $31 \times 31$ crystals for the ECAL and $7 \times 7$ towers for the HCAL. Isolation against neutral particles is assured from a study of energy deposited in an annular region around the signal region. The energy in the annular region in the ECAL (between $15 \times 15$ and $11 \times 11$ crystals) is required to be smaller than 0.5 GeV and in the HCAL (between $7 \times 7$ and $5 \times 5$ towers) is required to be less than 2 GeV. The purity of the signal is found to be better than 90% from a study of Monte Carlo sample of minimum bias events.

Energy response is measured as the ratio of energy of the isolated track in the signal zone to the momentum of the track. Comparisons are done using the full spectrum of the energy responses or using the arithmetic mean of the distributions. Measurements are done for the mean energy response as a function of the track momentum in two parts of the barrel ($|\eta| < 0.52$, $0.52 < |\eta| < 1.13$), the endcap ($1.65 < |\eta| < 2.17$) and the transition ($1.13 < |\eta| < 1.65$) region. The granularity of the detectors and background conditions are different in these four regions.

Figure 5 shows the measurements of mean calorimeter response of isolated tracks corresponding to the larger signal zone as a function of the track momentum. The same measurements from data and Monte Carlo samples from two different physics lists are shown on the same plot. A good agreement is observed between data and the two Monte Carlo models for energies above 3 GeV in all the regions.

Figure 6 shows the ratios of mean calorimeter response in the Monte Carlo predictions to the data as a function of the track momentum. The ratio is consistent with 1 for the barrel detector at all energies. For endcap and the transition region, the agreement is consistent with 1 at energies above 4 GeV.

Deviation of the ratio from 1 is a measure of disagreement between data and Monte Carlo. Mean level of disagreement between data and Monte Carlo is shown in Table 2 for the two physics lists and for two different signal regions.

| Region    | ($E_{7\times7}+H_{3\times3})/p$ | ($E_{11\times11}+H_{5\times5})/p$ |
|-----------|--------------------------------|----------------------------------|
|           | G4.10.0.p02 | G4.10.2.p02 | G4.10.0.p02 | G4.10.2.p02 |
| Barrel 1  | $1.1 \pm 0.4\%$ | $2.4 \pm 0.4\%$ | $2.5 \pm 0.4\%$ | $2.6 \pm 0.4\%$ |
| Barrel 2  | $3.4 \pm 0.4\%$ | $3.6 \pm 0.4\%$ | $1.9 \pm 0.4\%$ | $2.2 \pm 0.4\%$ |
| Transition| $3.7 \pm 0.5\%$ | $4.9 \pm 0.5\%$ | $1.6 \pm 0.5\%$ | $2.2 \pm 0.5\%$ |
| Endcap    | $1.1 \pm 0.3\%$ | $4.1 \pm 0.5\%$ | $4.7 \pm 0.4\%$ | $1.6 \pm 0.5\%$ |

Both the physics lists are providing reasonable predictions for the mean energy response of the calorimeters. The level of disagreement between data and MC is between 2 to 5% depending on the region of the detector as well as the physics list used.

5. Summary
CMS experiment is planning to change the Geant4 version to 10.2.p02 as well as the physics list to FTFP_BERT_EMM for the future Monte Carlo production campaign. Predictions from this physics list as well from the current one (QGSP_FTFP_BERT_EML from Geant4.10.0.p02) are compared with the data.

Test beam data with identified particle types are used as one source of validation while isolated charged particles from collision data are used as the second source.
Figure 6. Ratio of Monte Carlo and data for the mean energy response of the isolated track as a function of the track momentum when the track hits one of the four different regions of the calorimeter: (top left) $|\eta| < 0.52$, (top right) $0.52 < |\eta| < 1.13$, (bottom left) $1.13 < |\eta| < 1.65$ and (bottom right) $1.65 < |\eta| < 2.17$. The red and blue points refer to Monte Carlo predictions from physics lists QGSP\_FTFP\_BERT\_EML of Geant4.10.0.p02 and FTFP\_BERT\_EMM of Geant4.10.2.p02 respectively.

There is a better agreement between the data and Monte Carlo predictions for the new version of physics list to be used by CMS for its future event production. Validation of physics within Geant4 will be continued using CMS data from the collisions as well as from past and future test beam experiments.

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