CERN-LCGAPP-2010-02
July 20, 2010
Version 1.0

Status of GEANT4 hadronic physics for the simulation of LHC experiments at the start of LHC physics program

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Abstract

In this short note we summarize the status of GEANT4 hadronic physics for the simulation of LHC experiments, based on an extended physics validation program carried out in the last ten years. The data used come from thin-target published results and LHC test-beam set-ups with electron, pion and proton beams. No LHC collider data are yet utilized; rather, the expectations for the physics quality of GEANT4 hadronic simulations for the first analyses at the start of the LHC physics program are discussed. Several physics lists are considered, for GEANT4 versions 9.2 (used currently in ATLAS, CMS and LHCb simulations) and 9.3 (latest version, released in December 2009).

1 Introduction

An extensive physics validation program for the detector simulation of LHC experiments based on GEANT4 [1] has been carried out in the past ten years.

In this note we aim to give a short summary of the results of this validation activity. We concentrate on hadronic physics, and in particular on hadronic showers on calorimeters, which is relevant for the simulation of jets and τ leptons.

A first report [2] on hadronic physics validation with LHC test-beam data, written in 2004, was based on GEANT4 version 5.2 and considered the two physics lists LHEP and QGSP. Our present note is an update of that report, based on the two latest GEANT4 versions, 9.2 and 9.3, and with a wider choice of physics lists.

As described in detail in our previous notes [3, 4], we use only thin-target published results to tune the GEANT4 hadronic models, whereas thick-target (e.g. calorimeter test-beam set-ups) data are used to assess the overall physics quality of physics lists. Our conclusions are based on the following four LHC calorimeter set-ups:

- ATLAS Tilecal calorimeter (iron-scintillator);
- ATLAS Hadronic End-Cap (HEC) calorimeter (copper-liquid argon);
- ATLAS Combined Test-Beam (CTB): accordion electromagnetic calorimeter (lead-liquid argon) in front of the Tilecal hadronic calorimeter;
- CMS hadronic calorimeter (brass-scintillator): both alone, and with the electromagnetic calorimeter (PbWO4 crystals) in front.

Some of these set-ups have been described in [2]; for the others, together with the comparisons between GEANT4 simulations and test-beam data, can be found in the presentations made at the LCG Physics Validation meetings, available in [5], and in published papers and public notes of ATLAS [6] and CMS [7] collaborations.

Although we do not cover in this note the GEANT4 electromagnetic physics, it is important to note that a detailed validation of electromagnetic physics is necessary in order to validate the simulation of hadronic showers. This is because of the presence of an electromagnetic component inside any hadronic shower, originating from $\pi^0 \rightarrow \gamma\,\gamma$ and ionization of charged hadrons. Moreover, electrons or muons are used for the calibration of calorimeters.

The structure of the note is the following. We start with a brief description of some of the physics lists of interest for high-energy applications. The results of the comparisons between the GEANT4 simulations with some of these physics lists and test-beam data are then summarized for each calorimeter observables: response, energy resolution, longitudinal shower profile and lateral shower profile. In Section 7, non-calorimeter observables, like multiplicities and spectra of produced particles, of interest for hadronic interactions happening in detector trackers, are discussed. Finally, we conclude with a summary and an outlook for the future of GEANT4 hadronic physics validation.

2 Physics Lists

Any GEANT4 application has to provide a physics list, where all the particles present in the simulation, their physics processes, and the production thresholds are specified. A number of pre-packaged Reference physics lists are available for user convenience. We described here the main hadronic models used in some of the Reference physics lists of interest in high-energy physics, as present in GEANT4 version 9.3. All values refer to the kinetic energy of the primary particle in the interaction.

LHEP : for pion-, kaon-, proton- and neutron-nucleus inelastic interactions the Low Energy Parameterized (LEP) model is used below 55 GeV, and the High Energy Parameterized (HEP) model is used above 25 GeV.
For all other hadrons (hyperons and antibaryons) and nuclei the LEP model is used below 25 GeV, and the HEP model is used above 20 GeV.

QGSP_BERT : for the inelastic cross-sections:

- Barashenkov evaluations are used for pion-nucleus interactions;
- Axen-Wellisch evaluations are used for proton- and neutron-nucleus interactions;
- the same as in LHEP physics list is used for kaon-, hyperon- and antibaryon-nucleus interactions.

For the final-state model of pion-, kaon-, proton- and neutron-nucleus inelastic interactions:

- Bertini intra-nuclear model followed by nucleus de-excitation (called "BERT" from now on) is used below 9.9 GeV;
- LEP is used between 9.5 GeV and 25 GeV;
- Quark-Gluon-String model followed by Precompound and evaporation models for the nucleus de-excitation (called "QGSP" from now on) is used above 12 GeV.

For the final-state model of hyperon- and antibaryon-nucleus inelastic interactions, the same as in LHEP physics list is used.

FTFP_BERT : the same inelastic cross-sections as QGSP_BERT are used.
For the final-state model of pion-, kaon-, proton- and neutron-nucleus inelastic interactions:

- BERT model is used below 5 GeV;
- Fritiof model followed by Reggeon cascade and Precompound and evaporation models for the nucleus de-excitation (called "FTFP" from now on) is used above 4 GeV;

- for the final-state model of hyperon- and antibaryon-nucleus inelastic interactions, the same as in LHEP physics list is used.

CHIPS : for the inelastic cross-sections of pion-, kaon-, proton-, neutron-, hyperon- and antibaryon-nucleus inelastic interactions, new CHIPS-specific interpolations are used.
For the final-state model of all inelastic interactions, a new approach is used: first a 1-dimensional parton multi-string is applied; then its soft secondaries are absorbed by the target nucleus; "quasmons" are formed; then, decay of the quasmons in nuclear matter with final CHIPS evaporation.
There is no transition between different models in CHIPS physics list.
This physics list is not available before GEANT4 version 9.3.

QGS_BIC : the same inelastic cross-sections as QGSP_BERT are used.
For the final-state model of proton- and neutron-nucleus inelastic interactions:

- Binary (BIC) intra-nuclear model, followed by Precompound and de-excitation, is used below 9.9 GeV;
- LEP is used between 9.5 GeV and 25 GeV;
- QGSP is used above 12 GeV.

For the final-state model of pion-nucleus inelastic interactions:

- BIC, followed by Precompound and de-excitation, is used below 1.3 GeV;
- LEP is used between 1.2 GeV and 25 GeV;
- QGSP is used above 12 GeV.

For the final-state model of kaon-nucleus inelastic interactions:

- LEP is used below 25 GeV;
- QGSP is used above 12 GeV.

BIC model, followed by Precompound and de-excitation, is used also for the rescattering (inside the nucleus) of secondaries particles produced by the Quark-Gluon-String model.
For the final-state model of hyperon- and antibaryon-nucleus inelastic interactions, the same as in LHEP physics list is used.

Other alternative physics lists, some of which could be deprecated or removed in future GEANT4 releases, are the following:

QGSC_BERT : the same inelastic cross-sections as QGSP_BERT are used.
For the final-state model of pion-, kaon-, proton- and neutron-nucleus inelastic interactions:

- BERT model is used below 9 GeV;
- Quark-Gluon-String model, with the CHIPS quasmon algorithm for the nucleus fragmentation, is used above 6 GeV.

For the final-state model of hyperon- and antibaryon-nucleus inelastic interactions, the same as in LHEP physics list is used.

QGSP_FTFP_BERT : the same as QGSP_BERT, with LEP replaced by FTFP (i.e. Fritiof + Reggeon cascade + Precompound and de-excitation) in the interval $6-25$ GeV, with transition with BERT between $6-8$ GeV (whereas the transition with QGS remains the same, between $12-25$ GeV).
This physics list is not available before GEANT4 version 9.3.

QBBC : The same inelastic cross-sections as QGSP_BERT are used for all hadrons, except for antibaryons which are treated as in CHIPS.
For the final-state model of proton- and neutron-nucleus inelastic interactions:

- BIC model, followed by Precompound and de-excitation, is used below 1.5 GeV;
- BERT is used between 1 GeV and 5 GeV;
- FTFP is used between 4 GeV and 25 GeV;
- QGSP is used above 12.5 GeV.

An alternative (to LEP and CHIPS) cross-section and final-state model for neutron capture (HP-like but much faster) is used exclusively in this physics list.
For the final-state model of pion-nucleus inelastic interactions:

- BERT is used below 5 GeV;
- FTFP is used between 4 GeV and 25 GeV;
- QGSP is used above 12.5 GeV.

For the final-state model of kaon- and hyperon-nucleus inelastic interactions:

- BERT is used below 5 GeV;
- FTFP is used above 4 GeV.

FTFP_BERT_TRV : the same as FTFP_BERT, but with the transition between FTFP and BERT in the region $6-8$ GeV (i.e. FTFP is used above 6 GeV, and BERT below 8 GeV).
This physics list is not available before GEANT4 version 9.3.

QGSP_BERT_TRV : the same as QGSP_BERT, but with the transition between LEP and QGSP between $10-15$ GeV (i.e. LEP starts at 9.5 GeV and ends at 15 GeV and QGSP starts at 10 GeV).
This physics list is not available before GEANT4 version 9.3.

QGSP_BERT_NOLEP : the same as QGSP_BERT, but with QGSP starting from 8.5 GeV and avoiding LEP.
This physics list is not available before GEANT4 version 9.3.

FTF_BIC : The same inelastic cross-sections as QGSP_BERT are used.
For the final-state model of pion-, proton- and neutron-nucleus inelastic interactions:

- BIC model, followed by Precompound and de-excitation, is used below 5 GeV;
- FTFP is used above 4 GeV.

For the final-state model of kaon-nucleus inelastic interactions:

- LEP is used below 5 GeV;
- FTFP is used above 4 GeV;

The BIC model, followed by Precompound and de-excitation, is also used for the rescattering (inside the nucleus) of secondaries particles produced by the Fritiof model.
For the final-state model of hyperon- and antibaryon-nucleus inelastic interactions, the same as in LHEP physics list is used.

QGSP_BIC : Similar to QGS_BIC, but without using BIC for pions and for the rescattering of secondaries particles produced by the Quark-Gluon-String model.

For some of the above physics lists, variants exist which include:

- High-Precision (HP) treatment of low-energy neutrons, $E_{kin} < 20\,MeV$.
Example: QGSP_BERT_HP.
- Alternative multiple scattering model: faster but less precise.
Example: QGSP_BERT_EMV.
- Alternative choice of default production range thresholds that could enhance CPU performance with a limited affect on precision.
Example: QGSP_BERT_EMX.
(Note that QBBC is the only physics list which uses this variant of electromagnetic physics without having the explicit suffix "_EMX" in its name.)
- Alternative choice of electromagnetic physics for the most precise description of low-energy effects. Example: QGSP_BIC_EMY.

Some general observations:

- Elastic hadron-nucleus scattering (i.e. coherent elastic with the whole nucleus): LHEP and CHIPS have their own cross-sections and final-state models; all other physics lists use a mixture of these two approaches (in particular CHIPS elastic is used for proton- and neutron-nucleus interactions) and a new Glauber-type model for all hadrons at high-energies.
- Quasi-elastic hadron-nucleus scattering (i.e. elastic scattering with individual nucleons): all QGS-based physics lists use the quasi-elastic implementation provided by CHIPS; all FTF-based physics lists have their own version of the quasi-elastic scattering.
- Nuclear capture of negatively charged hadrons: all physics lists, with the only exception of LHEP, uses the CHIPS implementation for this process.

- Neutron capture and fission: all non-HP physics lists use LEP for these processes, with the only exception of CHIPS and QBBC which have their own implementations.

- Gamma-nuclear interactions: all physics lists use CHIPS for this process.

In the following sections we summarize the validation results for only a few of the above physics lists which are the most interesting for LHC physics analyses.

3 Response

The measured mean total energy in a calorimeter normalized to the beam energy is referred here as the response of the calorimeter.

In Geant4 version 9.2, the physics list QGSP_BERT is the closest to the pion test-beam data for the response. The agreement is within $2-3$ %, with QGSP_BERT response higher than in the data [8, 9].

The beam energies available in the LHC test-beams were either below 9 GeV, or above 20 GeV. By studying the response in the simulation as a function of the beam energy, for small steps in the whole range (even when experimental measurements did not exist), CMS has found unphysical discontinuities in QGSP_BERT [10]. ATLAS confirmed the same behaviour [11]. Other physics lists, like FTFP_BERT and FTF_BIC, showed less pronounced discontinuities but were farther from data ($\sim$ $5-7$ % higher than data).

The beam energy values at which the discontinuities in the response happen correspond to the transition regions between hadronic models. In the case of the QGSP_BERT physics list, the transition between BERT and LEP models occurs between 9.5 and 9.9 GeV. The transition between FTF and cascade models, i.e. BERT in the case of FTFP_BERT, and BIC in the case of FTF_BIC, occurs between 4 and 5 GeV.

We have studied the problem of the transition between hadronic models, and in the Geant4 version 9.3 (released in December 2009) some significant improvements have been achieved:

- The Fritiof model has been retuned (using thin-target data), improved (with the inclusion of quark-exchange) and extended to lower energies (by coupling to a Reggeon cascade). FTFP_BERT physics list provides now a response very close to QGSP_BERT and a smooth behaviour as a function of the beam energy. The variant FTFP_BERT_TRV is also interesting, whereas FTF_BIC needs further work and is not recommended.

- Replacing LEP with the new FTFP in QGSP_BERT, and with transition with BERT in the interval $6-8$ GeV, has produced a new physics list, QGSP_FTFP_BERT, which has a response very close to QGSP_BERT and smooth.

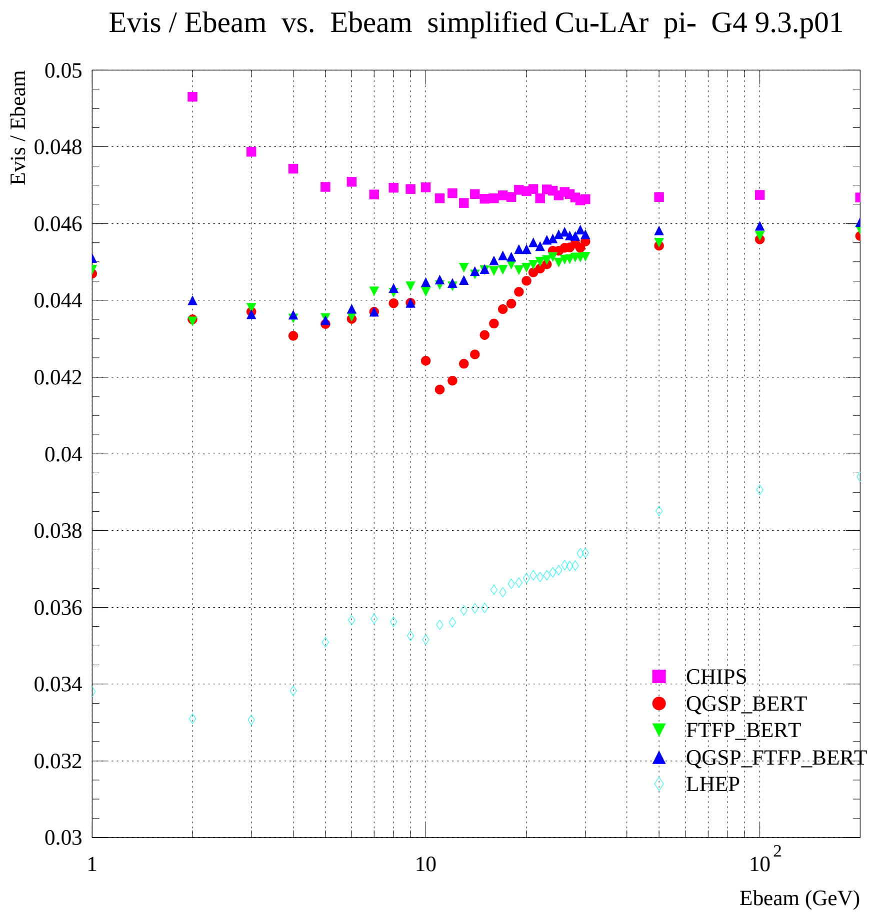

Figure 1: Energy response as a function of the beam energy for a π^- beam on a simplified copper-liquid argon calorimeter, for GEANT4 version 9.3.p01.

- The new physics list CHIPS shows a smooth response as a function of the beam energy, as expected due to the absence of a rigid transition threshold between its string and fragmentation components. In the first, experimental version of CHIPS, the response is too high, but tuning with thin-target data is still ongoing and improvements are expected in the next versions.

Figure 1 shows the energy response as a function of the beam energy for a π^- beam on a simplified copper-liquid argon calorimeter, for GEANT4 version 9.3.p01.

For the response of protons, the agreement between simulation and test-beam data is more or less at the same level as for pions, although protons have been tested less extensively.

4 Energy resolution

The physics list QGSP_BERT describes the calorimeter energy resolution for pions within ~ 10 % [8, 9]. The energy resolution is typically narrower in the simulation than in data.

Similar energy resolutions are produced in GEANT4 version 9.3 by the following physics lists: FTFP_BERT, QGSP_FTFP_BERT and FTFP_BERT_TRV. The experimental physics list CHIPS produces a too narrow energy resolution, but tuning with thin-target data is in progress.

For the energy resolution of protons, the agreement between simulation and test-beam data is more or less at the same level as for pions, although protons have been tested less extensively.

5 Longitudinal shower profile

The QGSP_BERT physics list produces pion longitudinal shower profiles that are shorter than data by ≤ 10 % up to about 10 λ (the typical thickness of hadron calorimeters) [8, 9].

Proton longitudinal shower profiles are significantly shorter than observed in test-beam data: $\sim$ 30 % up to about 10 λ. We interpret this as a deficiency of the modeling of diffraction processes in QGS: we have started validating them with thin-target data.

For the physics lists of interest in GEANT4 version 9.3 the longitudinal shower profiles are described as follows:

- QGSP_FTFP_BERT is very similar to QGSP_BERT for both pion and proton showers. This shows that replacing LEP with FTF does not affect the longitudinal shower profile.

- FTFP_BERT and FTFP_BERT_TRV physics lists have very similar longitudinal profiles, for both pion and proton showers, in good agreement with data, within about $\pm$ 10 % up to about 10 λ. This shows that changing the transition region between FTF and BERT has negligible effect on longitudinal shower profiles.

- CHIPS physics list produces longitudinal profiles longer than data by $\sim$ 20 % up to about 10 λ, for both pion and proton showers. This could be due to the overestimation of diffraction in the present CHIPS inelastic interactions.

6 Lateral shower profile

There is only one LHC calorimeter test-beam result for the lateral profiles of pion and proton showers: the ratio of the energy measured in the bottom and central modules of the ATLAS TileCal set-up with beam sent at 90° [12]. Based on it, we can draw the following conclusions.

The physics list QGSP_BERT produces pion and proton lateral shower profiles that are narrower than data by $\sim$ 15 %.

In GEANT4 version 9.3, CHIPS physics list describes very well the lateral profiles of both pion and proton showers. QGSP_FTFP_BERT is very close to QGSP_BERT; similarly for FTFP_BERT in the case of pion showers, whereas it is closer to data in the case of proton showers.

7 Other observables: multiplicity and spectra

Up to now we have considered observables relevant for hadronic showers in calorimeters. These are important for jets and τ leptons, which are of great interest for ATLAS and CMS physics analyses. Although most of the hadronic interactions happen in calorimeters, a few hadronic interactions do occur also in tracker detectors. In the case of the LHCb experiment, the hadronic interactions in the tracker need to be well understood, because secondary pions and kaons could be confused with the ones originating either in the B decays or in the hadronization of the $b-$quarks, which are part of the signal or the flavour tag in physics analyses.

In the case of pion inelastic interactions, the physics list QGSP_BERT is expected to provide a reasonable description of data below $9.5\,GeV$, where Bertini model is utilized, and above $\sim 25\,GeV$, where QGS is utilized. In the intermediate region, between 9.5 and $25\,GeV$, the LEP model is used and therefore a less accurate simulation of inelastic pion interactions is expected. It is worth considering one of the following alternative physics lists for a better simulation of inelastic pion collisions at all energies: FTFP_BERT, QGSP_FTFP_BERT, and CHIPS (the latter only for GEANT4 versions not older than 9.3.p01).

In the case of kaon inelastic interactions, all the GEANT4 physics lists, with the only exception of CHIPS, are using the same inelastic kaon cross-sections as LHEP, which are not accurate; the final state, instead, is treated similarly as for pions. Although so far we have carried out only few validations of models with kaons, we expect the CHIPS physics list to be the most accurate for these type of particles. We are planning to extend our validation tests with kaons.

For hyperons (Λ, Σ, Ξ and Ω), and antibaryons ($\bar{p}$, $\bar{n}$, $\bar{\Lambda}$, $\bar{\Sigma}$, $\bar{\Xi}$ and $\bar{\Omega}$) the cross-sections and modeling of final states are less reliable than for kaons, with less experimental data available for validation, and fewer modeling choices. There are only two different physics lists: LHEP and CHIPS. All other physics lists are equivalent to LHEP, on both cross-sections and final states, as far as hyperons and antibaryons are concerned. (The only exception is QBBC for the final state of hyperon-nucleus interactions, in which BERT and FTF are used.) For these particles (as for kaons) we expect the CHIPS physics list to be the most accurate. At least for antiprotons, we are planning to validate the simulation, whereas for the other particles it is difficult to find useful data.

8 Summary and outlook

For Geant4 version 9.2, used by ATLAS, CMS and LHCb simulations for the first LHC physics data, the physics list QGSP_BERT should provide a reasonable simulation of pion showers, likely the best available in 9.2 release.

The pion response is expected to be a few percent higher than data, with an unphysical discontinuity as a function of the beam energy between 9.5 and 9.9 GeV (due to the transition between LEP and BERT models). The pion energy resolution is slightly ($\sim$ 10 %) narrower than data. The pion showers are moderately more compact than in data: $\sim$ 10 % shorter in the longitudinal profile up to about 10 λ, and $\sim$ 15 % narrower in the lateral profile.

For protons, the agreement between QGSP_BERT physics list in Geant4 9.2 and data is of lower level than for pions. In particular, the proton longitudinal shower profile is $\sim$ 30 % shorter than data up to about 10 λ: we think that this is caused by an inaccurate modeling of the diffraction process in QGS.

Regarding multiplicities and spectra of secondary particles produced by inelastic pion-nucleus and proton-nucleus interactions, of interest for simulation of detector trackers, the agreement between data and simulation is expected within a factor of two, with unphysical discontinuities in the transition region around 10 GeV.

For other hadrons, such as kaons, hyperons and antibaryons, very few benchmarks are available for validation, therefore the quality of their simulation is quite uncertain.

For Geant4 version 9.3, QGSP_BERT physics list produces results very close to the ones of version 9.2. However, an emerging alternative is the physics list FTFP_BERT, which produces results quite similar to QGSP_BERT, but with smoother behaviour as a function of the beam energy, and longer proton longitudinal shower profiles in better agreement with data. To explore the systematics of model transitions it is worth to consider also the following two physics lists: QGSP_FTFP_BERT and FTFP_BERT_TRV.

A new physics list, CHIPS, is also potentially interesting: although it should be still considered as experimental, with a response too high and energy resolution too narrow, it shows a smooth behaviour as a function of the beam energy, reasonable longitudinal hadronic shower profiles and promising lateral hadronic shower shapes. Moreover, it could potentially offer the best description of kaon, hyperon and antibaryon hadronic interactions available in Geant4 .

We are also preparing a new physics list (QGSP_BERT_CHIPS) which is as QGSP_BERT, but with CHIPS used for kaon-nucleus cross-sections (but not for the final-states), and hyperon- and antibaryon-nucleus cross-sections and final-state modeling.

Looking at the future of hadronic physics validation for GEANT4 , we see two interesting directions:

- thin-target validation: HARP results and LHC collision data on hadronic interactions in tracker detectors can be very useful to improve and tune the inelastic hadronic cross-sections and final-state models. It is important to note that most of the energies involved in these measurements cover the transition region ($\sim\ 3\ \div\ 15\ GeV$) between high-energy and low-energy models, which is the most difficult, and hence interesting, region to model.

- calorimeter validation (thick-target): CALICE (calorimeters for the ILC detector) test-beam data, and isolated tracks in minimum-bias LHC events can be utilized to validate physics lists. In the latter case, from the point of view of GEANT4 it should be a confirmation of what has been measured in test-beam set-ups, whereas for the LHC experiments it would be an essential cross-check of their understanding of the whole detector. The highly-granular calorimeter prototypes investigated by the CALICE collaboration can measure unprecedented details of hadronic showers. For instance, it is possible to study the first interaction in great detail; it is also possible to correlate the lateral shower profile with the longitudinal profile. We think that these "tracking calorimeters" could provide a link between the microscopic thin-target information and the traditional macroscopic calorimeter observables: hopefully, this could lead to a significant improvement of the simulation of hadronic physics.

9 Acknowledgment

We would like to thank the following people: S. Banerjee, T. Carli, M. Cascella, G. Corti, J. Damgov, D. Elvira, E. Garutti, K.J. Grahn, V. Grichine, A. Howard, A. Kiryunin, S. Kunori, B. Lutz, S. Piperov, M. Simonyan, P. Speckmayer, P. Strizenec, I. Vivarelli, J. Yarba, T. Yetkin, and D. Ward.

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