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Simulation physics requirements from the LHC experiments

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(with input from the LHC experiments)

Abstract

In the framework of the LCG Simulation Physics Validation Project, we collect and revisit in this note the main physics requirements for the simulation packages (e.g. G4 and FLUKA), using inputs from the four LHC experiments. We try to quantify these requirements as much as possible.

This note should be considered as an evolving and regularly-updated document. It will be posted on the WEB and will be open to suggestions, additions, corrections.

1 Introduction

In the framework of the LCG Simulation Physics Validation Project, we collect and revisit in this note the main physics requirements for the simulation packages (G4, FLUKA, ...) using inputs from the four LHC experiments.

We try to quantify these requirements as much as possible. In some cases, quantitative statements cannot be made without additional (and often time-consuming) work. Therefore, we also mention some examples of issues which need to be addressed in the future.

It should be noted that the LHC experiments consider of utmost importance the availability of more than one simulation package (i.e. FLUKA, G4 with its various physics lists), especially for the description of hadron interactions. In this respect the physics requirements, and the capability of the various packages to cope with them, should provide useful information to understand the strengths and weaknesses of the various simulation engines.

The response of the various LHC sub-detectors to electrons, muons, pions can be studied with test beam data over the energy range from few GeV up to 300 GeV at the SPS (lower energies are available at the PS). In addition, well-known physics samples (e.g. $Z \to \ell^+\ell^-$ decays) can be used to understand and calibrate the detectors *in situ* at the LHC over a broader energy range than at the test beam (e.g. up to few hundreds GeV for the ATLAS and CMS calorimeters). However, the detector response to e.g. very-high energy particles (up to several TeV in ATLAS and CMS) cannot be directly checked with test-beam or collider data, and must therefore be predicted by the simulation.

The method to achieve an accurate detector modeling consists of comparing the simulation packages to data over the accessible (with adequate statistics) energy regions. This allows the physics content, the realism and the reliability of the simulation to be validated and improved. One has then to rely on the simulation to predict the detector behaviour outside the range covered by test-beam and/or control data samples.

Quantitative requirements on the needed simulation accuracy can be deduced by looking, for each performance issue (e.g. calorimeter linearity, particle identification), at the most sensitive LHC physics channel(s), and by asking that the simulation inadequacy does not become the dominant limitation in the study of that channel at the LHC.

The requirements listed below are grouped by experiment (ATLAS and CMS are discussed together) and, for each experiment, by sub-detector.

In general, calorimetric measurements set requirements on global shower features. Validations of these features are being performed, in the experiments and in the LCG Simulation Physics Validation Project, mainly by comparing test-beam data with G4 and FLUKA simulations of the test-beam set-up. Tracking devices are concerned mainly by the interactions of (often low-energy) particles with thin layers, and therefore by individual microscopic collisions. The simulation validation in this case relies on both, test-beam measurements and so-called "simple benchmark" studies (see Ref. [1] as an example). It should be noted that a complete and sensible validation demands that the considered packages describe well not only a large number of relevant observables, but also their correlations (e.g. the correlation between the energy fraction released by a shower in a longitudinal compartment of the calorimeter and the shower shape in that compartment).

Obviously, an accurate validation of the simulation codes requires good-quality test-beam data. Effects like beam contaminations, electronic noise, etc., need to be well understood in order to achieve the desired precision in the comparisons. Therefore simulation requirements translate also into requirements on the test-beam data quality.

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2 ATLAS and CMS

The two general-purpose experiments have similar physics goals, and therefore are discussed together, although the different technologies of the various sub-detectors imply slightly different requirements in a (very) few cases.

Many of the requirements below are extracted from Ref. [2].

2.1 Inner Detectors

In the LHC trackers, the sensitive layers are usually quite thin (e.g. 300 μ in some cases) and granular, which requires accurate modeling of individual microscopic collisions down to very low energies. In addition, the environment is very crowded, due to the high density of particles which produce many hits in the active layers. Therefore, if particle interactions are not accurately described, occupancies and Pattern Recognition performance could be wrongly estimated by large factors.

Given these challenging and unprecedented conditions, both experiments feel that detailed studies and comparisons with the two main simulation packages (G4 and FLUKA) are needed, especially for low-energy particles, in order to reach confidence that the above issues are under control.

The main requirements can be summarised as follows:

- All relevant physics processes need to be included in the simulation: ionisation, δ-ray production and propagation, multiple scattering, photon conversion, electron Bremsstrahlung, transition radiation and subsequent propagation of the X-rays in the detector material (relevant for ATLAS), synchrotron radiation (relevant mainly for CMS), hadronic interactions, neutron interactions, etc.

- Particle tracking should be stopped (and the energy released locally) only when the residual range is smaller than the detector space resolution, otherwise the occupancy would be underestimated. The typical resolution of the ATLAS and CMS Pixel/Si detectors is 10-20μm. For comparison, an electron of 100 keV has a residual range of 50 μm in Silicon. This requirement is even more stringent in the ATLAS TRT detector, due to the longer particle range in gas. It is estimated that hadrons should be tracked down to 1 MeV or below.

- Electronic thresholds can be very low, e.g. 10 keV in the ATLAS pixel readout, 20 keV in both the ATLAS and CMS Si strips, and 200 eV in the ATLAS TRT. Single physics processes in the active elements involve even lower energy deposits (e.g. the threshold is $\sim$10 eV in the TRT gas). Energy releases down to these values should be correctly simulated (e.g. using PAI-like models).

- In the ATLAS TRT an accurate description of δ-ray production is needed, both in the active straws and outside, since this is the main background to Transition Radiation. The required accuracy in the energy range of a few keV is about 1%, as obtained from many years of test-beam studies.

- Synchrotron radiation by electrons in the high-field CMS tracker is a process that the simulation must reproduce correctly. This process is included in G4, but has not yet been validated by the experiment.

  Synchrotron radiation may also produce X-rays in the ATLAS TRT; this was estimated analytically to contribute <10% to the transition radiation signal itself many years ago, but should be checked with the present versions of the simulation packages.

- Hadronic interactions, in particular of low-energy particles, must be modeled in detail. Some of the low-energy hadrons are absorbed by the tracker material, thereby reducing the reconstruction efficiency. Nuclear break-up gives rise to large local energy depositions which can produce saturation of the readout electronics. These and other effects need to be well simulated for a reliable estimate of the tracker response, of the occupancy and of the Pattern Recognition performance.

  More quantitatively, 10% of 1-5 GeV pions are not reconstructed properly at $|\eta| \sim 1.7$ in the ATLAS Inner Detector [3], given the large amount of material. These numbers, obtained with GFLUKA, should be reassessed with G4 and FLUKA. The accuracy required is again of order a few percent and includes distortions to the track caused by quasi-elastic interactions.

- A reliable estimate of the impact of the neutron fluence in the inner cavity on the occupancy, and therefore on the Pattern Recognition efficiency, can only be made by merging the neutron background hits with hits from the primary *pp* collisions (see Section 2.5), in a similar way to what is done to simulate the impact of the high-luminosity pile-up on hard-scattering processes.

- Backsplashes from early showers in the EM calorimeter have an impact on the occupancy of the outermost tracker layers. In the past G3 was compared to measurements performed with an ATLAS TRT prototype and was found to underestimate the hit multiplicities by a factor of up to $\sim$2 [4]. Such comparisons should be repeated with G4 and FLUKA.

The simple-benchmark studies mentioned in Section 1 are particularly helpful to validate the simulation for many of the above issues.

Because of the complex environment, and of the numerous and ambitious requirements listed above, the simulation of complete LHC *pp* events in the ATLAS and CMS trackers may become a highly CPU-consuming task (although still less consuming than the calorimeter simulations). Both experiments require that the physics needs listed above be implemented with an acceptable time performance.

2.2 EM calorimeters

The simulation should reproduce the energy deposited by electrons and photons in the calorimeters and in the passive material (upstream, cracks, etc.) from $\sim$100 MeV (pile-up level) up to the TeV scale. It should also model the energy and position resolutions, and the shower lateral and longitudinal profiles. The latter are important e.g. for particle identification, and to predict the energy released in the upstream material and the longitudinal leakage beyond the calorimeter active volume. Knowledge of such energy losses is in turn essential to correct the calorimeter response.

Given the rôle of EM calorimeters for precision physics at the LHC (e.g. $H \rightarrow \gamma\gamma$ studies, W-mass measurement, etc.), the required precision is between few permil [5] and 1% in most cases and for most observables. Such a precision would match e.g. the expected few permil detector response linearity and uniformity.

Particle identification, e.g. e/jet separation, and accurate estimates of the pile-up levels require that the simulation package describes well hadron showers not only in the hadron calorimeters (see below) but also in the EM part. Therefore the requirements listed in the next Section apply also to the EM calorimeter case.

Pion, muon and electron test-beam data can be used to validate the simulation from $\sim$1 GeV up to $\sim$300 GeV.

2.3 Hadron calorimeters

Pion test-beam data and *in situ* control samples, like $Z + 1jet$ events, can be used to understand the detector performance up to a few hundreds GeV. From this range up to a few TeV, the calorimeter response to pions and jets, in particular non-linearities due to non-compensation, has to be modeled by the simulation.

- A deviation of the calorimeter response to jets of 1.5% at 4 TeV (compared to the Monte Carlo predictions) can fake a Compositeness scale Λ of $\sim$30 TeV in the study of the di-jet cross-section vs p_T [6]. This would impair the LHC ultimate reach of Λ $\sim$40 TeV. Assuming that control samples (e.g. Z+jet events) have enough statistics to normalise the simulation to the data up to 500 GeV, the above-mentioned Compositeness physics argument implies that the simulation should reproduce the e/h ratio of the calorimeters at the few percent level [2]. This should ensure that the simulation inadequacy is not the main limitation in these physics studies, compared e.g. to the knowledge of the jet fragmentation function.

- Shower longitudinal and lateral profiles should be reproduced with accuracy, since this affects for instance the estimations of the energy lost in the upstream material and in cracks, and of the leakage beyond the calorimeter volume. A poor description could fail in e.g. reproducing tails in the missing E_T spectrum observed in the data (e.g. for QCD multijet events), thereby opening the door to (wrong) claims for New Physics. On the low-energy side, the quality of the simulation of the shower profile has an impact on the determination of the cell occupancy coming from pile-up events (and correlations between cells), and therefore on the effects of cell threshold cuts on a physics event. More quantitative statements in these cases are only possible with (time-consuming) additional work, e.g. by studying channels like $A/H \to \tau\tau$, which require good missing E_T resolution, and the high-energy tails in multi-jet events.

Other issues, such as the precision required in the simulation of the pion energy resolution, need more studies to be properly addressed. They are however in large part covered by the two requirements listed above.

2.4 Muon Spectrometers

In this case requirements are more stringent for ATLAS than for CMS because of the open air-core layout of the ATLAS Spectrometer. The large amount of iron embedding the CMS Muon chambers renders the background problems less serious.

- Muon catastrophic energy losses in the calorimeters and punch-trough of hadronic debris of the calorimeter showers produce background hits in the external Muon Spectrometer. These affect the occupancy of the chambers and can create confusion for the Pattern Recognition. In the past, the G3 simulation was compared to data from the dedicated RD5 experiment [7], and the agreement was judged to be satisfactory [8]. According to these studies, the rate of shower muons and punch-throughs in the ATLAS Spectrometer is well below the rate of real muons (prompt or from decays). However, these studies should be repeated with G4 and FLUKA, because of the possible implications on e.g. the Pattern Recognition performance. Comparisons of G4 with ATLAS muon test-beam data taken with various absorbers in front of the chambers have started [9] and should also allow validation of the simulation of muon catastrophic energy losses. More quantitative requirements could be derived e.g. from detailed studies of the Pattern Recognition performance in the presence of the above-mentioned backgrounds.

- A good description of muon multiple scattering is important especially for CMS, because of the large amount of iron in the CMS Spectrometer. For muons of momentum ∼100 GeV, the precision should be better than 10%, otherwise the measurement will be dominated by multiple scattering uncertainties.

- The so-called radiation background is a gas filling the experiment cavern, consisting (mainly) of low-energy (≤1 MeV) photons and neutrons. Neutrons are produced in the interactions of the collision debris with the forward detectors and machine elements. The photons (typical energy 300-500 keV) come mainly from radiative capture of these neutrons, and produce hits in the external Muon chambers through Compton scattering on the chamber walls and gas. This background is not correlated in time with the *pp* interactions. It has an impact on the detector ageing and occupancy and on the performance of the Pattern Recognition. Therefore it should be accurately modeled, including e.g. a correct simulation of the propagation and emission times of neutrons and photons in the cavern and inside the detector elements. In the past, the uncertainty on the FLUKA simulation of the ATLAS radiation background has been estimated (very conservatively) to be a factor of ∼5 [2]. By comparing FLUKA, MARS and GCALOR, CMS has deduced an uncertainty of ∼3. A common effort has started between LHCb and LCG physicists (see below) to compare GCALOR, FLUKA and G4 for the radiation background modeling in LHCb, and should tell us if the above uncertainties can be reduced (the hope is to achieve a factor of ∼2 or smaller). Inputs are also expected from the previously-mentioned simple benchmark studies.

2.5 Radiation background simulation

A simulation environment is needed where hits from the radiation background and hits from the main *pp* collision can be merged. This is necessary in particular for the Muon Spectrometers and Inner Detectors, in order to obtain a reliable estimate of e.g. of the impact of the occupancy on the performance of the Pattern Recognition. This calls either for an integration of the package used for radiation studies into the overall simulation environment, or for a unique simulation able to describe the LHC event down to thermal neutron energies.

3 LHCb

The LHCb physics goals [10, 11], i.e. the study of CP violation and other rare phenomena in B-meson decays with very high precision, impose several detector requirements: a high track reconstruction efficiency; a $\pi - K$ separation capability from a few GeV up to around 100 GeV; a proper-time resolution of about 40 fs; high trigger efficiencies not only for final states including leptons, but also for fully-hadronic events.

This entails a number of physics requirements on the simulation packages used for the detector response studies.

3.1 Tracker-like devices

The tracking of charged particles in the magnetic field (of values up to 1.5 T) should be of high precision. In particular, the tracking of particles inside the Vertex Locator (extending approximately up to 1 m from the interaction point and consisting of a number of Silicon sensors) should have at least the precision of order a few microns. This seems to be achievable with the present implementation of G4.

The energy loss process in the Silicon should well reproduce both the most probable value and the width of the distribution. This should be true for a large range of momenta (from a few MeV up to several hundred GeV) and of thicknesses of the Silicon sensors (from 200 μm to 600 μm). A specific requirement is that, because of technical reasons (use of a simplified geometry), it should be possible to switch off δ-ray production in G4 (as it is possible in G3) and replace it with a parametrized description. First attempts to do this by adjusting the range cut values have not been fully successful, and (unacceptable) discrepancies between the experimental measurements and the G4 simulation at the 10% level have been observed.

3.2 Ring Imaging Cherenkov detectors

The relevant quantities that must be well simulated for such detectors are the Cherenkov angle resolution (of order of 1 mrad) per hit and the number of hits (N) per charged track. The resolution per Cherenkov ring is related to the number of hits as $1/\sqrt{N}$. For all three radiators (aerogel, C4F10, CF4), we are able to obtain the expected resolutions with the current implementation of electromagnetic, optical and hadronic processes in G4.

Furthermore, due to a large number of Cherenkov photons potentially generated, the CPU-time performance plays a key role for some of the optical processes. This has been improved with respect to the original G4 implementation by customizing some of the processes.

3.3 Calorimeters

The important aspects of the calorimeter simulation in LHCb [12] are discussed one by one below.

3.3.1 Electron identification

Studies of physics channels with electrons (e.g. $B \rightarrow J/\Psi X$, with $J/\Psi \rightarrow e^+e^-$) show that the background is dominated by real electrons from secondary interactions (photon conversion, showering, etc.). One can therefore conclude that the final result is not very sensitive to the e/h separation capabilities. Moreover, combined e/h separation in LHCb includes the information from the RICH, the Preshower detector (Prs), and the Electromagnetic (ECal) and hadronic (HCal) calorimeters, which makes the dependence of the final result on errors coming from a single device less pronounced. A possible consequence is that LHCb is not so sensitive to the e/h ratio in the calorimeters. From all calorimetric devices (Prs, ECal and HCal), the largest relative contribution to the e/h separation comes from the Prs. Therefore, the largest uncertainty on the e/h separation in LHCb is expected to come from the modeling of hadron interactions in the 2.5 X_0 of the lead converter in front of the Prs scintillator.

3.3.2 HCal resolution and HCal trigger

The relative contribution of the HCal in the offline physics analysis is very small. The HCal-based trigger, however, is one of the most important triggers for a large number of physics channels in LHCb. Moreover, this trigger is expected to dominate the overall level-zero bandwidth, and therefore its performance (background rejection versus efficiency) is sensitive to the HCal energy resolution near the energy threshold. The description of the resolution in the high energy regime is less important, whereas it is crucial for $E_T \sim$3 GeV. For instance, a 10-15% discrepancy in the energy resolution between simulation and data would lead to a wrong estimate of the trigger efficiency for the $B_d^0 \rightarrow \pi^+\pi^-$ channel by $\sim$5%.

Since the LHCb HCal is a thin device (the energy measurement is not the main goal), the modeling of the longitudinal shower development in the simulation is particularly important.

3.4 Machine background

Events where all relevant sources of background are included are important to evaluate the overall performance of the detector. The muon detector can be particularly affected, for example, by the muon halo from the machine. This background is generated separately by dedicated simulations of beam losses and transport along the machine elements. The resulting beam halo distribution needs to be folded with the simulation of *pp* collisions. Currently it is treated as an additional generator in the LHCb simulation. The time difference between this background and the *pp* collisions has to be taken into account in the simulation of the detector response.

3.5 Radiation studies

The performance of the detectors and electronics will be affected by the radiation environment in which they will operate. In order to evaluate the reliability of the various systems and their performance, it is important to know the dose accumulated over time as well as the fluences and spectra of the various particles. The simulation has to provide description of both electromagnetic and hadronic processes in a wide range of energies. In the case of neutrons, the range has to extend from thermal to the TeV energies. The physics simulation has also to allow the evaluation of the production of radioactive nuclei in the various detector elements during the experiment operation. This is necessary to estimate the activity in the experiment for interventions on the detector during controlled accesses or shutdowns.

Obviously, the above requirements apply also to the other LHC experiments.

4 ALICE

ALICE has used G3 and FLUKA during the design and optimization phases, in particular to perform simulations related to the Technical Design Reports of the sub-detector systems. Production has by now started for most of the detectors. In parallel, the ALICE Offline Team is developing the reconstruction and analysis code. The process is mainly driven by the production and analysis of simulated data serving as input to the Volume II of the ALICE Physics Performance Report (PPR), to be published at the end 2004. A major production using G3 will start at the beginning of February 2004. Through its Virtual Monte Carlo Interface, ALICE can in the near future also produce simulated data using FLUKA or G4 without changing the user data. Using the TGeo geometry modeler from ROOT, direct comparison between the different transport codes based on exactly the same geometry description will be possible.

4.1 Validation

The ALICE Offline Team thinks that the validation of the simulation packages and their continuous improvement can only be achieved through a judicious combination of simple benchmarks and test-beam verifications, as it is indeed happening in the LCG Simulation Physics Validation Project. We require that one focuses on the underlying physics in order to avoid the programs developing into a set of experiment-specific tools with plug-in parameterisations.

4.2 Requirements

Specific requirements of ALICE on the simulation packages can be deduced from the influence of the simulation accuracy on the overall systematic error on physics measurements. For most of our physics signals, studies of these errors have not yet been performed. The main reason is that in most cases the errors are either dominated by the effect of the high particle multiplicities and related detector occupancies or by statistics due to the limited luminosity in Pb-Pb runs.

Multiplicity effects can be studied by embedding tracks from a low-multiplicity environment (pp) into A-A data. A clearer picture will evolve from the analysis performed for the PPR.

Shortcomings of the simulation packages and their possible effect on the data analysis can already be anticipated qualitatively in some cases, but cannot be quantified at this stage. This is discussed below.

4.2.1 Muon Spectrometer

The main challenge in the reconstruction of muon tracks measured with the ALICE Muon Spectrometer comes from the relatively high occupancy of the Cathode Pad Chambers. This occupancy results from secondary particles produced at the end of hadronic showers induced by primary particles with energies ranging from 1 GeV to several TeV. The upper bound is given by the energy of beam-halo particles producing background in addition to that coming from the primary collisions. The Front and Small Angle Absorbers have been optimized with FLUKA to reduce the respective longitudinal and lateral punch-throughs to a minimum.

Effects of the occupancy on the tracking efficiency can be quantified by embedding tracks from low-multiplicity events (pp) into Pb-Pb events. ALICE is interested in state-of-the-art simulations of the predicted background levels before start-up, in order to be able to anticipate possible problems. Accurate predictions (at the 10% level) of both the background rate and the angular and momentum distributions of background particles are needed, e.g. in order to optimize the shielding layout.

The background sources described above are to a large extent uncorrelated with the muon signal. Additional background results from δ-rays and electrons from bremsstrahlung and direct pair-production produced by the high-energetic (up to 300 GeV) muons themselves. The electrons can produce signals overlapping with the muon signal and decrease the resolution. Since this effect can only be quantified using simulations, an accurate modeling of these electrons (rate, momenta, angular distributions) is necessary.

4.2.2 Central Tracking (ITS and TPC)

The ALICE inner tracking system consists of six layers of Silicon detectors. The simulation requirements are a subset of those formulated by ATLAS and CMS (see above). The simulation of ionization losses, in particular in the relativistic rise, will influence particle identification with the Time Projection Chamber and the Transition Radiation Detector. Hence, accurate dE/dx simulations, at the level of $\sim$1%, are needed.

4.2.3 Transition Radiation Detector (TRD)

The simulation of correlated background (δ-rays, bremsstrahlung and direct pair-production produced by high-energetic electrons) is important for a detailed understanding of the electron measurement and identification capabilities (resolution, efficiency, pion rejection). The ALICE TRD uses polypropylene fiber mats as radiator. The accurate simulation of transition radiation from such an irregular medium represents a real challenge. The signal response can be obtained and parameterized from test-beam data. However, to obtain the actual response in a high-multiplicity background environment a microscopic simulation is essential.

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