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Full Simulation of CMS for Run-3 and Phase-2

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Abstract. In this contribution we report the status of the CMS GEANT4 simulation and the prospects for Run-3 and Phase-2. Firstly, we report about our experience during the start of Run-3 with GEANT4 10.7.2, the common software package DD4hep for geometry description, and VecGeom runtime geometry library. In addition, FTFP_BERT_EMM Physics List and CMS configuration for tracking in magnetic field have been utilized. For the first time, for the Grid mass production of Monte-Carlo, this combination of components is used. Further simulation improvements are under development targeting Run-3 such as the switch to the new GEANT4 11.1 in production, that provides several features important for the optimization of simulation, for example the new transportation process with built-in multiple scattering, neutron general process, custom tracking manager, G4HepEm sub-library, and others. We will present evaluation of various options, validation results, and the final choice of simulation configuration for 2023 production and beyond. The performance of the CMS full simulation for Run-2 and Run-3 will also be discussed. CMS development plan for the Phase-2 GEANT4 based simulation is very ambitious, and it includes a new geometry description, physics, and simulation configurations. The progress on new detector descriptions and full simulation will be presented as well as the R&D in progress to reduce compute capacity needs.

1 Introduction

The Compact Muon Solenoid (CMS) experiment is one of the experiments at the Large Hadron Collider (LHC) at CERN. CMS Software (CMSSW) is a software collection used by the CMS experiment to acquire, produce, process, and analyze data. For the full simulation, including modellings of (i) the interaction region, (ii) the penetration of particles through the hierarchy of volumes that compose the CMS detector and of the accompanying physics processes, (iii) the effect of multiple interactions per beam crossing and the effect of events

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overlay (a.k.a. pile-up simulation) and (iv) the detector's electronics response (a.k.a. digitization), cmssw utilizes CMS detector simulation software to handle the mentioned modellings Geant4-based [2],[3],[4],[5]. Like all complex software environments, the CMS simulation software and Geant4 have been subject to evolutionary changes to improve accuracy, efficiency, and compatibility [6]. CMS remains proactive in its approach, diligently assessing the quality of its simulations every time there is an update. The development applies not just to updates in the main application software but also to changes in Geant4's versions, its underlying components, and other details like geometry descriptions, which are crucial for accurate simulations.

This proceeding delves into the current status of the CMS simulation environment in the context of the LHC Run-3 [1]. We will present insights into the validation results and overall software performance, particularly in light of recent modifications to the CMS simulation application. These results comprehensively understand how evolutionary changes impact large-scale scientific experiments and the measures taken to ensure consistent and high-quality outcomes.

2 Evolution of CMS simulation software

The CMS experiment operates on two primary timescales: the current LHC Run-3 and the upcoming Phase-2 upgrades. These Phase-2 enhancements are significant detector improvements tailored for the high luminosity LHC (HL-LHC) conditions, anticipated to be operational by 2029. To support both the Run-3 and Phase-2 initiatives, CMS has implemented various modifications in its simulation application and infrastructure. Users across both applications depend on a comprehensive Geant4-based detector simulation for accurate outcomes. Throughout the development of cmssw, there have been updates to Geant4 and its associated components. In addition to routine upgrades of the operating systems—encompassing Scientific Linux 5, Red Hat Enterprise 6, Centos 7, and Alma 8 and 9, and updates to compiler versions, there are updates on:

- For LHC Run-2 [8]:
  - versions of Geant4 from 10.0.p02 used in 2015 to 10.4.p03 used for CMS Run-2 Ultra-Legacy processing
  - geometry for each year, to reflect the real detector configuration
  - multithread mode which is in production since 2017
  - configuration for physics including physics list and Hadron Forward (HF) calorimeter shower library,
  - methods to reduce number of simulation steps and/or number of tracks to be processed including cut optimization and Russian roulette method
- For LHC Run-3 [9] and Phase-2:
  - versions of Geant4 from 10.7.p02 for 2022 to the current 11.1.p01. CMS benefits from newer processes of Geant4, especially from faster computations – less instructions and still achieve the same result, for example, Geant4 Gamma General Process
  - migration to DD4hep geometry description (complete migration for Run-3)
  - usage of the Link Time Optimization (LTO) build

The Fig.1 shows an evolution of cmssw, Geant4 and its components.

A rigorous validation process is initiated each time Geant4 and its associated components undergo an update [7]. This validation encompasses three distinct methods: (i) the simulation

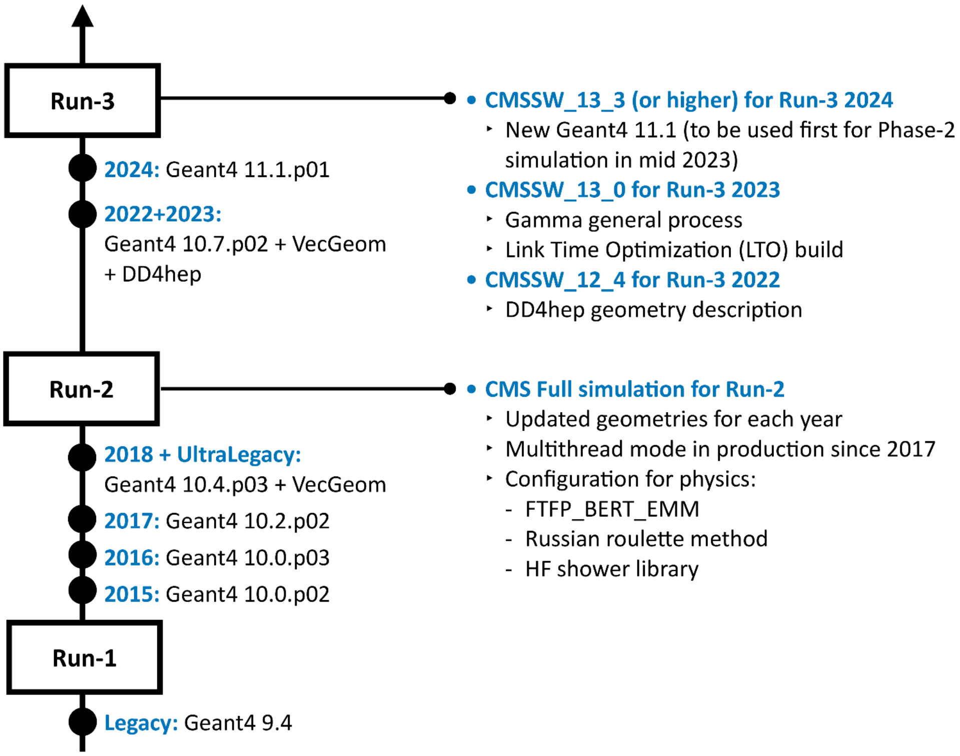

Figure 1. Evolution of CMS software, GEANT4, computing environment from LHC Run-1 to the current LHC Run-3.

group conducts validations using test beam data, (ii) validation using 2016's low pile-up data, and (iii) central validation performed by various groups, including the Detector Performance Groups (DPGs), Physics Object Groups (POGs), and the Physics Analysis Group (PAGs). Beyond these validations, software performance metrics are systematically measured across all major software releases.

3 Software validation

3.1 Comparison with test beam data

The initial validation utilized test beam data from the H2 beam line of CERN's Super Proton Synchrotron (SPS) [10]. As illustrated in Fig.2, a barrel electromagnetic calorimeter (EB) was positioned ahead of two production wedges from the hadron barrel calorimeter (HB). Subsequently, the outer hadron calorimeter (HO) was affixed to the adjustable platform. This configuration mirrors the geometric relationship seen in the CMS experiment. The platform's bidirectional mobility in the ϕ and η directions enabled the beam to target any calorimeter tower, replicating a particle's path from the CMS experiment's interaction point. Four scintillation counters, placed three meters before the calorimeters, collaborated in a subset coincidence to act as the trigger. The experiments employed monochromatic secondary and tertiary beams with momenta spanning from 2 to 350 GeV/c. Additional beam counters were incorporated to guarantee the capture of pure beam interactions.

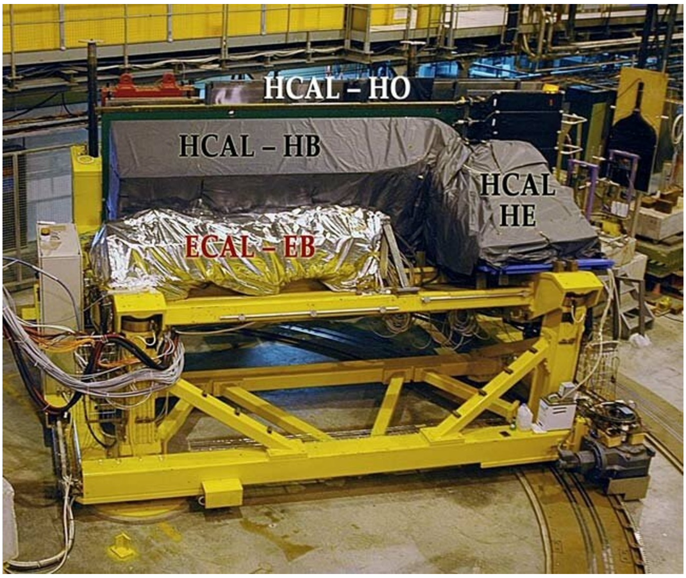

Figure 2. An overview of the H2 test beam area showcasing the HB, HE, HO, and ECAL EB components, all meticulously mounted on a versatile moving platform [10].

To compare between test beam data and Monte-Carlo simulation, the mean energy response is used. It is quantified as the ratio of the calorimeter's total energy to the beam momentum, and is evaluated as a function of beam momentum across different beam types to discern disparities between data and MC. Figs.3 and 4 present the outcomes for pion and kaon beams, respectively. A notable concurrence is observed between Data and Monte-Carlo for both positive and negative pions, though variances arise with the kaon. Nevertheless, given the prevalence of pions in high-energy proton collisions, a congruence between the actual data and MC simulations from the CMS experiment is anticipated.

3.2 Comparison of experimental and simulated collision data

This study delves into a comparison between energy distributions produced by isolated charged hadrons in proton-proton collisions, as evidenced in the CMS experiment, and the theoretical forecasts derived from various Geant4 physics modules. The analysis draws on data accumulated in the low-luminosity phase of 2016, initiated by both minimum and zero bias triggers [12]. In summary of the analysis,

1. **Run**: Only runs marked as 'good', which all CMS sub-detectors are fully operational, are used.
2. **Events and primary vertex**: Events contain only one high-quality primary vertex are selected. This vertex is required to be consistent with the nominal interaction point.
3. **Track candidate**: To ascertain track candidates, the tracks must remain discernibly isolated from other charged and neutral particles. Selection parameters for these tracks encompass their closeness to the primary vertex in both transverse and longitudinal directions relative to the beam, the chi-squared value of their trajectory, and the count of tracker layers utilized in the readings. To ensure the integrity of the tracks, they are

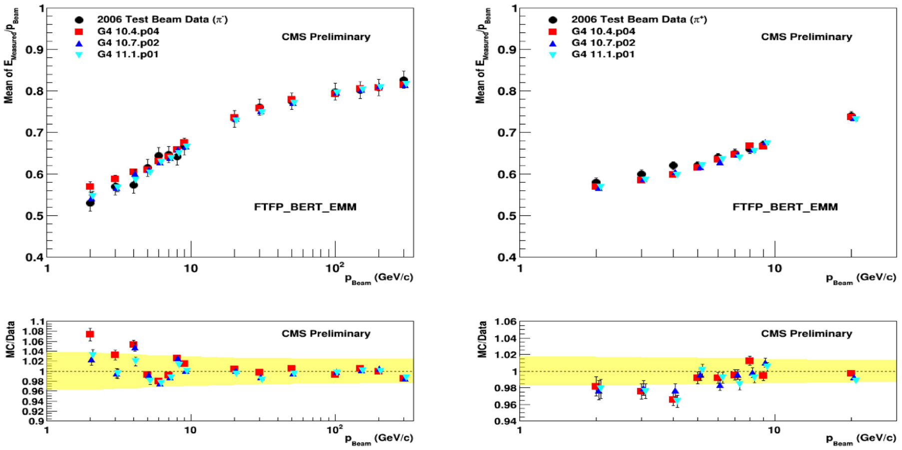

Figure 3. (Top) The mean response for negative (left) or positive (right) pions as a function of momentum compared to MC predictions; (bottom) Ratio of MC to data for negative (left) or positive (right) pions as a function of momentum. The yellow band shows one standard deviation of the data [11].

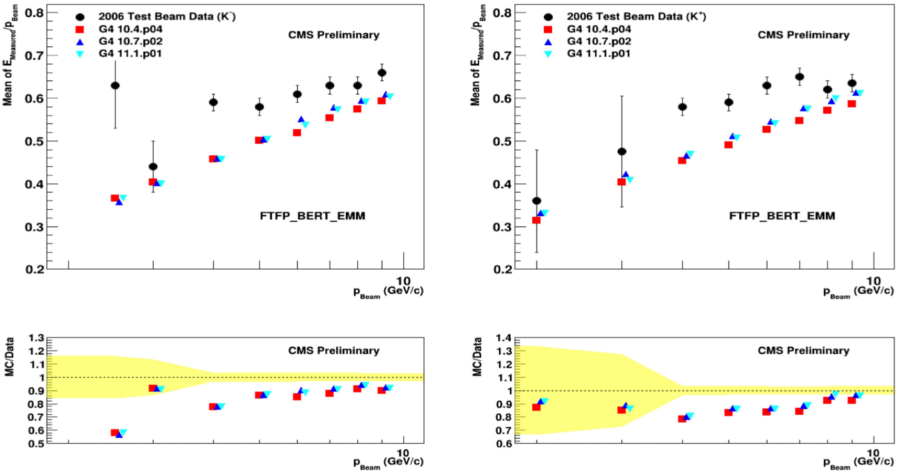

Figure 4. (Top) The mean response for negative (left) or positive (right) kaons as a function of momentum compared to MC predictions; (bottom) Ratio of MC to data for negative (left) or positive (right) kaons as a function of momentum. The yellow band shows one standard deviation of the data [11].

scrutinized for the absence of interactions pre-calorimeter encounters by checking for missing indications in their internal and external hit patterns. Any track evidencing such omissions is duly omitted from further analysis.

4. **Energy and signal region**: The chosen tracks are subsequently extrapolated to the surface of the calorimeter, at which point the corresponding cell of impact is discerned. We delineate a signal zone comprising n×n cells and an encompassing isolation zone of N×N cells, wherein N exceeds n. Drawing from in-depth analyses of hadron shower

profiles, the signal zones are designated as either 7×7 or 11×11 cells for the ECAL and 3×3 or 5×5 towers for the HCAL.

5. **Isolation**: We ascertain that the identified cell in the calorimeter remains uninfluenced by other particles. For charged entities, this confirmation is achieved by ensuring that no additional charged particles intersect within a 31×31 crystal matrix in the ECAL or a 7×7 tower matrix in the HCAL. In the case of neutral particles, it is imperative that the energy deposition within an annular vicinity surrounding the signal cell remains under 0.5 GeV for the ECAL and 2 GeV for the HCAL. Our computational analyses project a signal purity surpassing 90%.

In this analysis, the ratio of calorimeter energy measurement to track momentum for isolated charged hadrons is compared between data and Monte-Carlo simulation in 4 different regions of calorimeters including (i) $|\eta| < 0.52$, (ii) $0.52 < |\eta| < 1.04$, (iii) $1.04 < |\eta| < 1.39$, and (iv) $1.39 < |\eta| < 2.01$. Fig.5 shows the ratio of the mean energy response in 11x11 matrix of ECAL and 5x5 matrix of HCAL between MC and data. The complete result can be found in [11].

A good agreement between data and MC with Geant4 10.7.p02 and 11.1.p01 has been observed. The level of disagreement is between 1.3% and 3.4% in these two versions. The result shows an improvement from Geant4 10.4.p03.

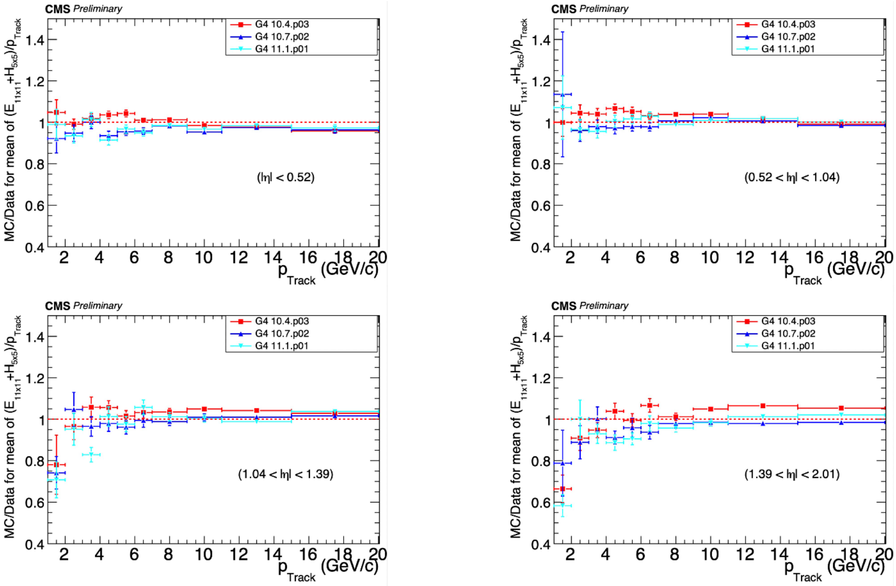

Figure 5. The ratio of the mean energy response in a wide matrix of ECAL and HCAL between MC and data for four regions of the calorimeter: central barrel (top left); side barrel (top right); transition region (bottom left); endcap (bottom right). [11]

3.3 Central validation

To validate Geant4 11.1, CMS called a wide validation to DPGs, POGs and PAGs. The Monte-Carlo vs Monte-Carlo was done with the same cmssw release, but different versions of Geant4 (10.7.p02 vs 11.1.p01). The validation shows a good agreement between them.

4 Software performance

The CPU time performance has been measured for Run-2 (13 TeV) with CMSSW 10_6_X to 11_3_X and Run-3 (14 TeV) with CMSSW 12_0_X to 13_2_X [13]. The historical trends plot is shown in Fig.6. Four physics processes including (i) minimum bias, (ii) $t\bar{t}$, (iii) $Z \rightarrow ee$, and (iv) beyond standard model T1tttt ($\tilde{g}\,\tilde{g} \rightarrow 2 \times t\bar{t}\,\tilde{\chi}_1^0$) processes have been used for this measurement. One would observe the reduction of CPU runtime across 4 years in the historical trend plot. Main improvements come from the Geant4 migration from versions 10.4 to 10.7 (CMSSW 11_3_X) and to 11.1.p01 (CMSSW 13_1_X), the change of the computing platform operating system from CentOS 7 (SLC7) to Alma Linux 8 (EL8) (CMSSW 12_4_X) and the usage of the Link Time Optimization (LTO) build method since CMSSW 13_0_X. The improvement has been seen by 27% in BSM T1tttt, 32% in $t\bar{t}$ and $Z \rightarrow ee$, and 36% in the minimum bias process.

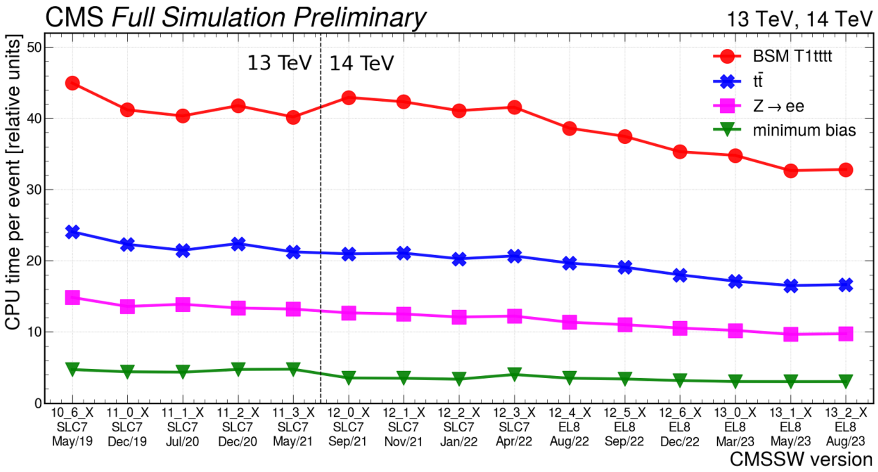

Figure 6. Historical trends of Full Simulation CPU time performance of Run-2 (13 TeV) with CMSSW 10_6_X to 11_3_X and Run-3 (14 TeV) with CMSSW 12_0_X to 13_2_X of minimum bias, $t\bar{t}$, $Z \rightarrow ee$, and beyond standard model T1tttt ($\tilde{g}\,\tilde{g} \rightarrow 2 \times t\bar{t}\,\tilde{\chi}_1^0$) processes. The average CPU run time per event in relative units of the event simulation is shown for 500 events on single threaded jobs.

5 On the way to CMS Phase-2 simulation

There are several ongoing development for CMS Phase-2 simulation including migration to CMS Phase-2 DD4hep geometry, studying new approaches for electromagnetic physics to speed up the simulation without compromise of physics result. For example,

1. new G4TransportationWithMsc introduced in Geant4 11.1.0. The new process specialises the transportation process combined with multiple-scattering
2. custom tracking manager, this is to simplify e-gamma transportation in Geant4
3. G4HepEm external library [14]

In addition, CMS also follows the R&D for GPU usage, such as Accelerated demonstrator of electromagnetic Particle Transport (AdePT) [15] or Celeritas [16] to implement HEP detector physics on GPU accelerator, targeting for HL-LHC.

6 Summary

CMS is actively developing and validating new simulation software. GEANT4 version 11.1.p01 has been integrated into CMSSW, with the aim of being used for the Mid-Year Phase-2 production, as well as for Run-3 in 2024. Updates to GEANT4 and its components have led to comprehensive software validations. CPU performance has also been assessed. The software validations involved comparisons between Monte-Carlo versions (specifically, GEANT4 10.4.p03, 10.7.p02, and 11.1.p01) and two sets of data. These data sets include the 2006 test beam data from the combined CMS barrel calorimeter with prototype hadron and electromagnetic calorimeters, and the low pile-up collision data at $\sqrt{s} = 13$ TeV collected in 2016. The data and Monte-Carlo simulation have been found to be in good agreement. In terms of CPU performance, Run-3 exhibited higher performance compared to Run-2.

Ongoing developments are underway for CMS Phase-2. These include a migration to DD4hep, which was carried out for Run-3, and research and development efforts are being made to incorporate GPU usage for simulations. The aim is to expedite the simulation process.

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