CMS Experience with Recent Versions of Geant4

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Geant4 Technical Forum

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Geant4 status in CMS

- For Run-2 Geant4 10.4.3 is used
  - VecGeom
- For Run-3 Geant4 10.7.2 is adopted
  - VecGeom + DD4hep
- CMS plan to migrate to Geant4 11.1.X in 2023
  - It is expected to have VecGeom + DD4hep + G4HepEm
- Validation of Geant4 11.0 is an important step for this goal
  - Today we report on first results and some observed problems

CMS validation of new Geant4 versions

CMS checks all releases of Geant4 including the reference releases using official CMS codes(CMSSW). However, since Geant4 version 10.7.ref08, there were backward incompatible changes for which a new DD4hep library was required. This became available recently and we restarted testing the versions with 10.7.ref09. All tests are made with 6 versions of Geant4 together with DD4hep version 1.19, CLHEP version 2.4.5.1, and VecGeom version 1.1.18. We tested with Native Geant4 geometry as well as with VecGeom geometry.

We carried out tests with GEANT4.10.7.ref09 (will not be discussed today), GEANT4.11.0, GEANT4.11.0.p01, GEANT4.11.ref01 and GEANT4.11.ref02

The validation is carried out using 2 sources of data:
- 2006 test beam with CMS calorimeter prototypes (hadron beams of different types and different energies)
- Collision data from the CMS experiment utilizing zero bias or minimum bias triggers from low luminosity runs

For testing 2 workflows are used: Run3 geometry (2021) and one recent Phase2 geometry (2026D88), each for 5 physics lists: FTFP_BERT, FTFP_BERT_EMM, FTFP_BERT_EMN, FTFP_BERT_EMY, and FTFP_BERT_EMZ

Warnings

CMS tries to define the geometry with right material composition. For performance issues, several passive components are combined and is defined by an approximately correct shape but with a composite material

In some material definitions, the same component used to appear more than once, and it never complained in earlier Geant4 releases.

```
<CompositeMaterial name="TIB_SSMCModConn" density="1.23046*g/cm3" method="mixture by weight" symbol=" ">
  <MaterialFraction fraction="0.03675">
    <rMaterial name="tibtidcommonmaterial:TIBTID_HybridTails" />
  </MaterialFraction>
  <MaterialFraction fraction="0.01862">
    <rMaterial name="materials:T_Kapton" />
  </MaterialFraction>
  <MaterialFraction fraction="0.00418">
    <rMaterial name="trackermaterial:T_Copper" />
  </MaterialFraction>
  <MaterialFraction fraction="0.12499">
    <rMaterial name="trackermaterial:T_FR4" />
  </MaterialFraction>
  <MaterialFraction fraction="0.01191">
    <rMaterial name="trackermaterial:T_FR4" />
  </MaterialFraction>
  <MaterialFraction fraction="0.16248">
    <rMaterial name="materials:Polyethylene" />
  </MaterialFraction>
  <MaterialFraction fraction="0.37555">
    <rMaterial name="materials:T_Bronze" />
  </MaterialFraction>
  <MaterialFraction fraction="0.24997">
    <rMaterial name="materials:Polyethylene" />
  </MaterialFraction>
  <MaterialFraction fraction="0.01556">
    <rMaterial name="materials:T_Bronze" />
  </MaterialFraction>
</CompositeMaterial>
```

Warnings for overlaps in VecGeom case

```
-------- WWWW ------- G4Exception-START -------- WWWW -------
*** G4Exception : GeomNav1002
      issued by : G4Navigator::ComputeStep()
Stuck Track: potential geometry or navigation problem.
   Track stuck, not moving for 10 steps.
   Current  phys volume: 'TECModule3'
    - at position : (-384.3906135793612,360.5600415896217,2426.9609999995)
      in direction: (-0.1579913514657975,0.1398702501211166,0.9774840387408211)
     (local position: (526.8757991295599,-12.71140002577118,-0.0640000050007293))
     (local direction: (0.2110070758652714,0.0009838402921873903,0.9774840387408211)).
   Previous phys volume: 'TECModule3RphiWafer'

   Likely geometry overlap - else navigation problem !
    *** Trying to get *unstuck* using a push - expanding step to 1e-07 (mm) ...
         Potential overlap in geometry !

TrackID=1 ParentID=0  mu-; Ekin(MeV)=49829.4; time(ns)=8.24921; status=0
    position(mm): (-384.391,360.56,2426.96);
direction: (-0.157991,0.13987,0.977484)
    PhysicalVolume: TECModule3; material: Air
    stepNumber=395; stepLength(mm)=0; weight=1
*** This is just a warning message. ***
-------- WWWW -------- G4Exception-END --------- WWWW -------
```

Warnings for stack tracks – native geometry and FTFP_BERT_EMY physics

```
-------- WWWW ------- G4Exception-START -------- WWWW -------
*** G4Exception : Transport-001-ExcessSteps
      issued by : G4Transportation::AlongStepDoIt
 Transportation is killing track that is looping or stuck.
   Track is e- and has 108.774 MeV energy  ( pre-Step = 108.774 )
   momentum = (-28.0329,4.63155,105.526) mag= 109.284
   position = (-23.5591,34.7703,217836) is in volume 'RP_220_Left_Station',
 its material is 'Air' with density = 0.001214 g/cm^3
 Total number of Steps by this track: 110
 Length of this step = 1239.97 mm
 Number of propagation trials = 1 ( vs maximum = 10 for 'important' particles )
   ( Number of *calls* of Transport/AlongStepDoIt = 559202987 )

TrackID=296581 ParentID=295881  e-; Ekin(MeV)=108.774; time(ns)=727.331; status=0
   position(mm): (-23.5591,34.7703,217836);
   direction: (-0.256514,0.0423809,0.965611)
   PhysicalVolume: RP_220_Left_Station; material: Air
   stepNumber=110; stepLength(mm)=1239.97; weight=1; creatorProcess: conv; modelID=10030
*** This is just a warning message. ***
-------- WWWW -------- G4Exception-END --------- WWWW -------
```

Warnings for surface normal


```
-------- WWWW ------- G4Exception-START -------- WWWW -------
*** G4Exception : GeomNav0003
        issued by : G4Navigator::GetGlobalExitNormal()
 WARNING> Expected normal-global-frame to be valid,  i.e. a unit vector!
   - but |normal|    = 0  - and |normal|^2 = 0
  which differs from 1.0 by -1
    n = (0,0,0)
 Global point: (675.7494075,264.4095634,3298.185688)
 Volume: HGCalEEConnector1Fine
============================================================
    State of Navigator:
The current state of G4Navigator is:
  ValidExitNormal= 1
  ExitNormal      = (0,0,0)
  Exiting         = 1
  Entering        = 0
  BlockedPhysicalVolume= None
  BlockedReplicaNo      = -1
  LastStepWasZero       = 1

 Current Localpoint = (5.9862075,-25.60641,1.865688)
 PreviousSftOrigin  = (675.74941,264.40956,3298.1857)
 PreviousSafety     = 0
Current History:
History depth=11
Level=[0]: Phys Name=[DDDWorld] Type=[N]
Level=[1]: Phys Name=[CMSE] Type=[N]
Level=[2]: Phys Name=[CALO] Type=[N]
Level=[3]: Phys Name=[CALOEC] Type=[N]
Level=[4]: Phys Name=[CALOECTSRear] Type=[N]
Level=[5]: Phys Name=[CALOECRear] Type=[N]
Level=[6]: Phys Name=[HGCalService] Type=[N]
Level=[7]: Phys Name=[HGCal] Type=[N]
Level=[8]: Phys Name=[HGCalEE] Type=[N]
Level=[9]: Phys Name=[HGCalEELayer86] Type=[N]
Level=[10]: Phys Name=[HGCalEEWafer1Fine] Type=[N]
Level=[11]: Phys Name=[HGCalEEConnector1Fine] Type=[N]

============================================================
Value obtained from stored global-normal is not a unit vector.

TrackID=1070958 ParentID=1070955   e-; Ekin(MeV)=0.0269937; time(ns)=11.596; status=0
    position(mm): (675.554,264.404,3294.46);
    direction: (-0.546887,-0.177274,0.818222)
    PhysicalVolume: HGCalEEConnector1Fine; material: HGC_EEConnector
    stepNumber=12; stepLength(mm)=0.00419028; weight=1; creatorProcess: eIoni; modelID=1001d
*** This is just a warning message. ***
-------- WWWW ------- G4Exception-END -------- WWWW -------
```

Abnormal End of Run with VecGeom

Most of the workflows for the version with VecGeom geometry could not finish normally. Some jobs exit after failure (GEANT4.11.0, GEANT4.11.0.p01) and some jobs (GEANT4.11.0.ref01, GEANT4.11.0.ref02) enter endless loops and need to be terminated by hand.

```
-------- EEEE ------- G4Exception-START -------- EEEE -------
*** G4Exception : GeomNav0003
      issued by : G4Navigator::ComputeStep()
Stuck Track: potential geometry or navigation problem.
  Track stuck, not moving for 25 steps.
  Current  phys volume: 'PixelForwardOuterDiskCFInnerRing'
   - at position : (-84.10362716324558,-22.45623867972706,-304.9649729190022)
     in direction: (-0.9111671286658983,-0.4120265431180305,-0.002931109849161457)
    (local position: (-84.10362716324558,-22.45623867972706,-3.164972919002139))
    (local direction: (-0.9111671286658983,-0.4120265431180305,-0.002931109849161457)).
  Previous phys volume: 'PixelForwardDiskZminus'

  Likely geometry overlap - else navigation problem !
 Track *abandoned* due to excessive number of Zero steps. Event aborted.

TrackID=17958 ParentID=17863  gamma; Ekin(MeV)=41.3985; time(ns)=0.990675; status=0
   position(mm): (-84.1036,-22.4562,-304.965); direction: (-0.911167,-0.412027,-0.00293111)
   PhysicalVolume: PixelForwardOuterDiskCFInnerRing; material: FPix_CFSkin_OuterInnerRing
   stepNumber=30; stepLength(mm)=1e-07; weight=1; creatorProcess: Decay; modelID=-1

-------- EEEE -------- G4Exception-END --------- EEEE -------
```

Abnormal End of Run with Native Geometry

```
------ WWWW ------- G4Exception-START -------- WWWW -------
*** G4Exception : GeomNav0003
      issued by : G4Navigator::ComputeStep()
Stuck Track: potential geometry or navigation problem.
  Track stuck, not moving for 951 steps.
  Current  phys volume: 'PixelForwardInnerDiskInnerRing'
   - at position : (35.13106957477028,-11.12342362405783,-315.9830578963742)
     in direction: (0.9961932776019362,0.07205235822723381,0.04906537816634005)
    (local position: (-35.13106957477028,11.12342362405783,-3.983057896374191))
    (local direction: (-0.9961932776019362,-0.07205235822723387,0.04906537816634018)).
  Previous phys volume: 'PixelForwardDiskZminus'

  Likely geometry overlap - else navigation problem !
 Track *abandoned* due to excessive number of Zero steps. Event aborted.


TrackID=34237 ParentID=28  neutron; Ekin(MeV)=4.1458; time(ns)=2.78465; status=0
    position(mm): (35.1311,-11.1234,-315.983); direction: (0.996193,0.0720524,0.0490654)
    PhysicalVolume: PixelForwardInnerDiskInnerRing; material: C_C_InnerInnerRing
    stepNumber=972; stepLength(mm)=0; weight=1; creatorProcess: pi-Inelastic; modelID=23000
*** This is just a warning message. ***
-------- WWWW -------- G4Exception-END ---------- WWWW -------
```

Comparison for Tracking Efficiencies
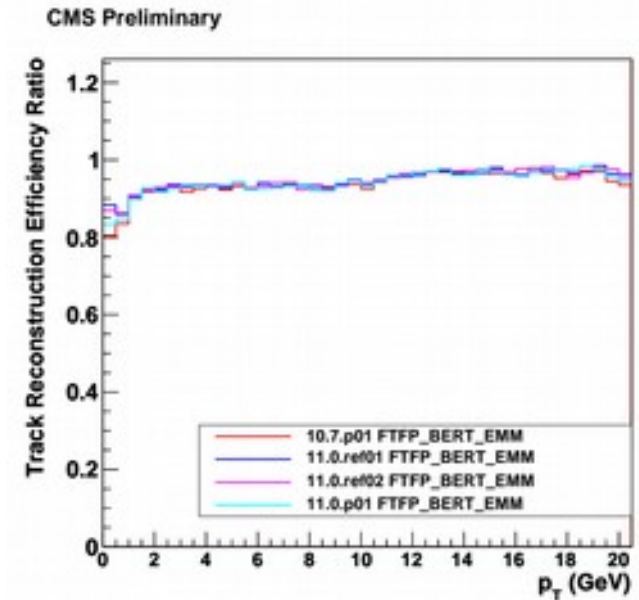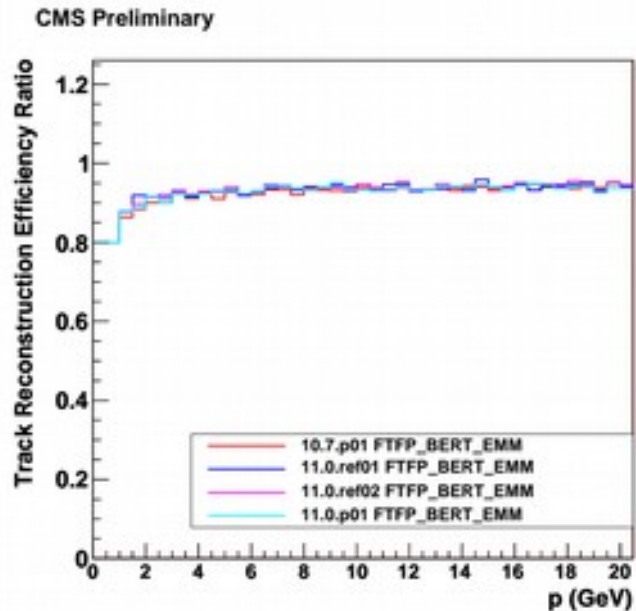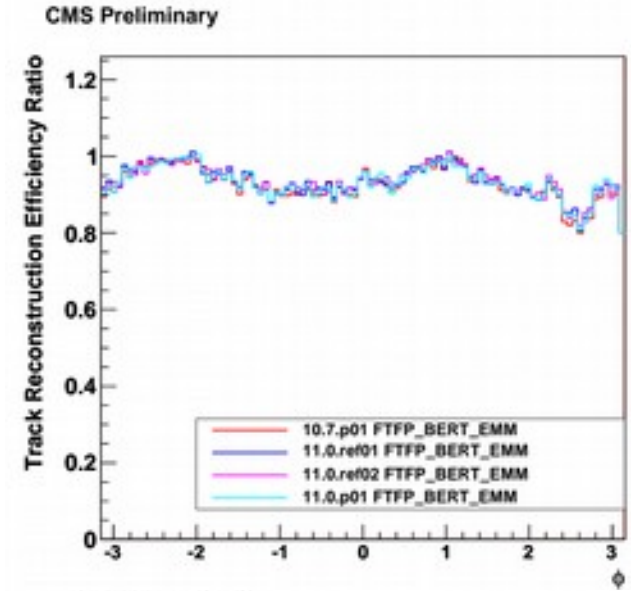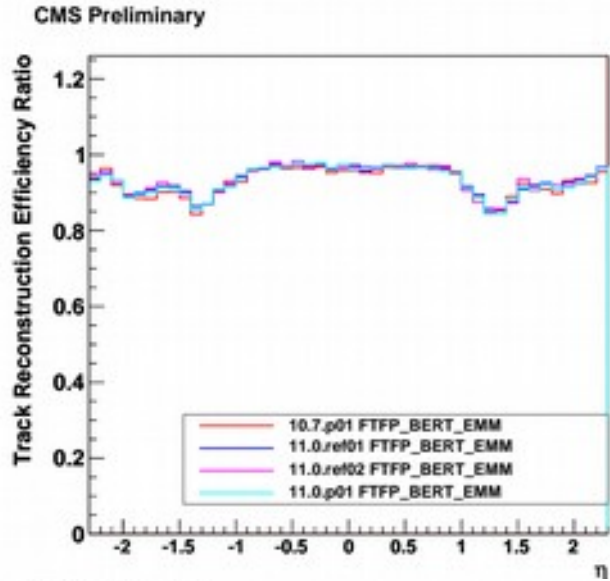
- Efficiencies with Geant4 versions 10.7.p01 and all from 11.0.. agree well

Test Beam 2006 Simulation

- 2006 Test Beam data were calibrated using 50 GeV electron Beam with the full detector (for EB calibration) or just with the HCAL prototype (for HB calibration)

- A similar procedure is normally carried out for MC samples. However, for this Geant4 version we see a significant shift of energy scale:

- which causes energy scales for EB to be 1.017 (10.7.p02), 1.019 (all versions of 11.0)
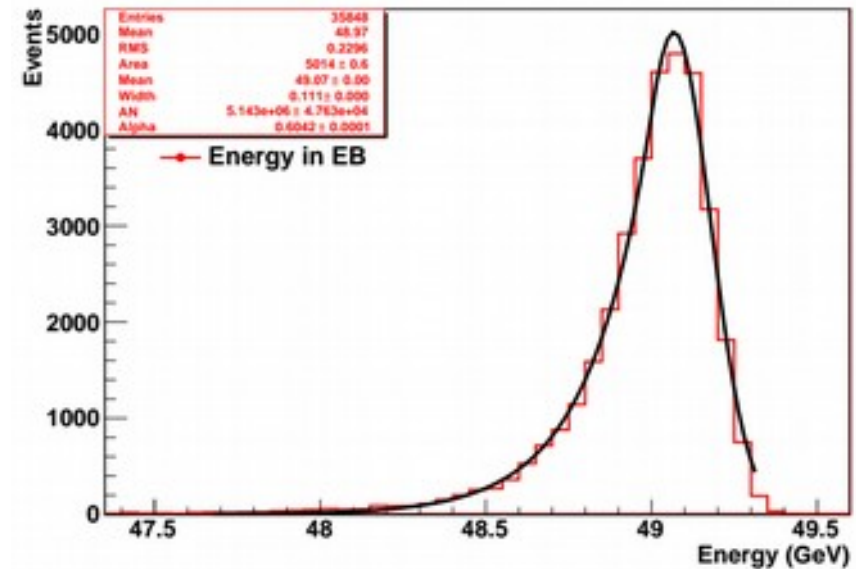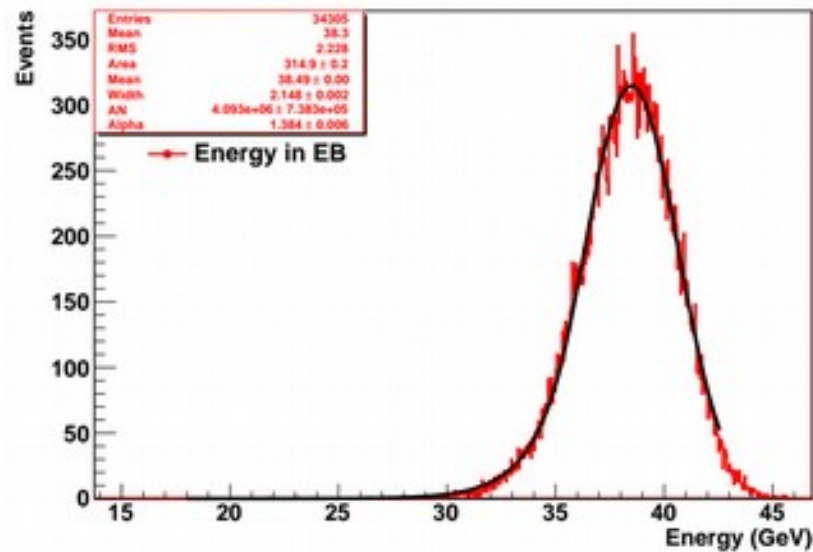
Test Beam 2006 Simulation

- The same story holds for energy scale of the hadron calorimeter, which causes energy scales for EB | HB to be 105.9 (10.7.2), 110.1 (all versions 11.0)
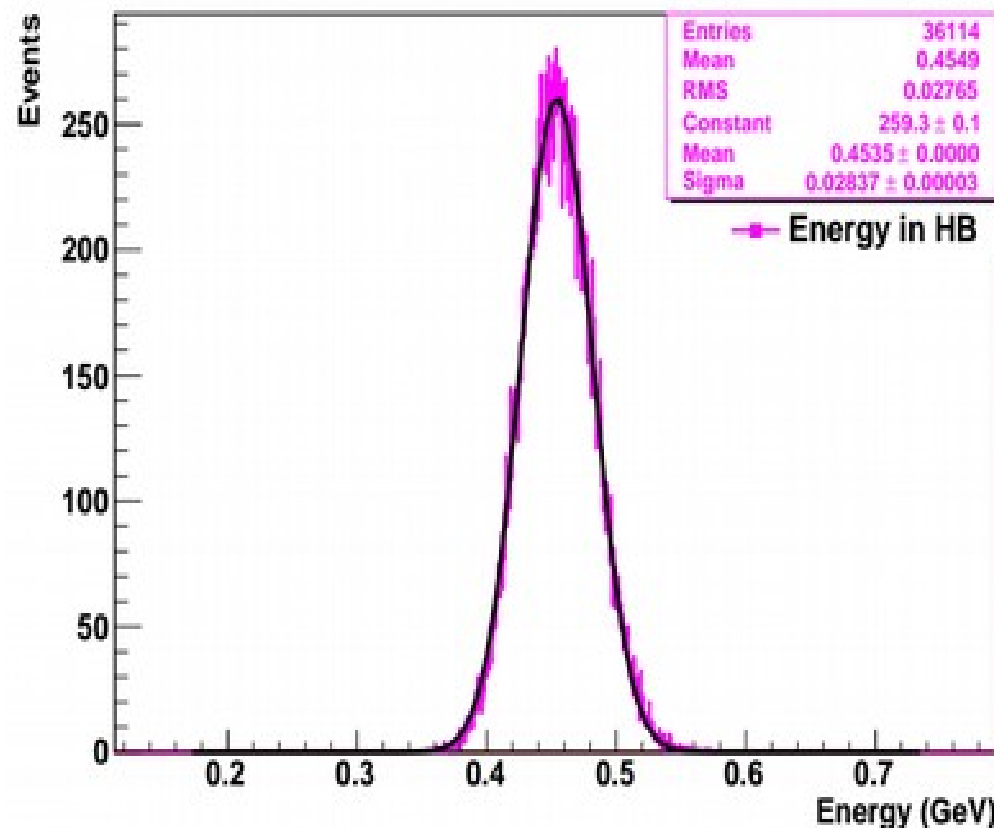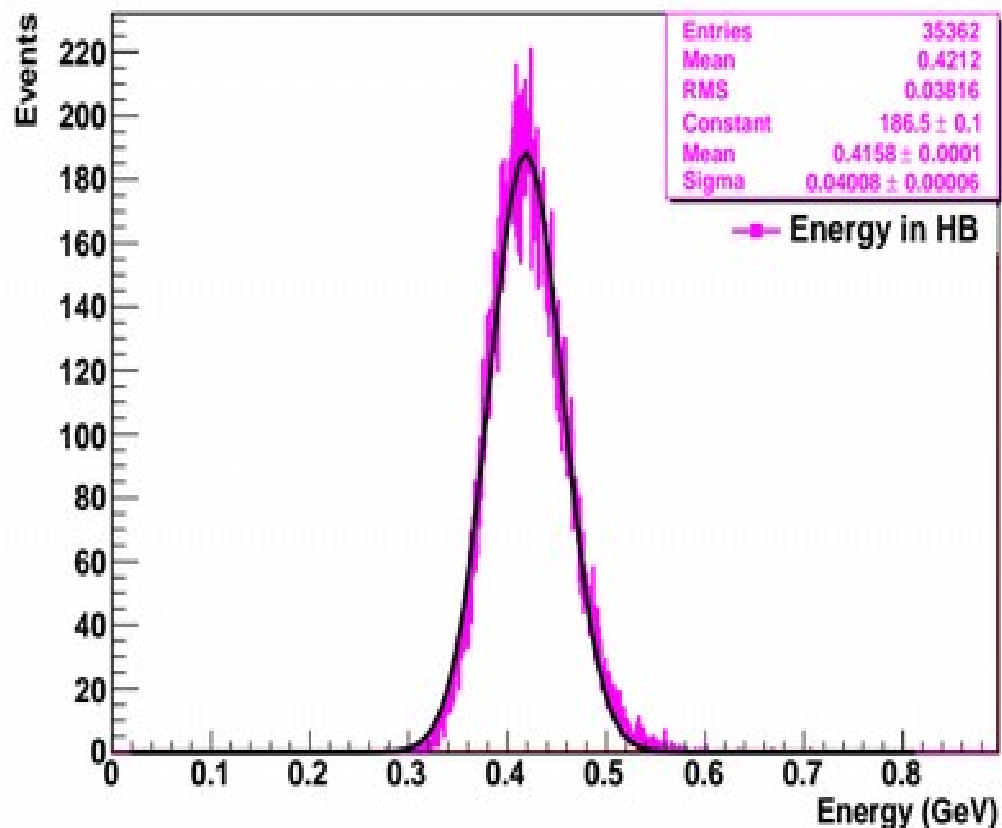
χ2/N for 2006 test beam MC/Data comparison

Geant4 version	π+	π̄	p	pbar	K+	Ḱ
10.4.3	0.96	0.54	0.61	1.93	25.0	24.5
10.7.2	0.89	0.31	0.54	3.28	15.5	19.3
11.0.1	2.58	0.63	0.61	2.07	16.8	21.3

Degradation of π+ results connected with problem of calibration of HCAL signal, which is shifted for ~2%. Smaller problem is seen for other particles

Isolated Charged Particles

- Compare ratio of calorimeter energy measurement to track momentum for isolated charged hadrons between data and MC

- Select good charged tracks reaching the calorimeter surface

- Impose isolation of these charged particles
  - propagate track to calorimeter surface and study momentum of tracks (selected with looser criteria) reaching ECAL (HCAL) within a matrix of 31x31 (7x7) around the impact point of the selected track for charge isolation
  - study energy deposited in an annular region in ECAL (HCAL) between 15x15 and 11x11 (7x7 and 5x5) matrices for neutral isolation

- Two versions of NxN matrix are defined for ECAL and HCAL
  - ECAL uses 7x7 or 11x11 matrix
  - HCAL uses 3x3 or 5x5 matrix

- Comparisons are made in 4 different regions of the calorimeter
  - Two in the barrel, one in the endcap, one in the transition region

Mean Level of Disagreement for FTFP_BERT_EMM

- The level of disagreement between data and MC for FTFP_BERT_EMM is (0.7 - 2.7)% for the Geant4 version 11.0.p01, (1.4 - 2.0)% for the version 11.0.ref01, and (1.4 - 2.3)% for the version 11.0.ref02. Adjusting transition region between FTF and Bertini is crucial to get reasonable agreement for the new versions.

Mean level of disagreement between MC and data

	$(E_{7x7}+H_{3x3})/p$ 10.4.p03	$(E_{7x7}+H_{3x3})/p$ 11.0.p01	$(E_{11x11}+H_{5x5})/p$ 10.4.p03	$(E_{11x11}+H_{5x5})/p$ 11.0.p01
Barrel 1	(1.6±0.4)%	(1.9±0.4)%	(2.1±0.4)%	(2.2±0.4)%
Barrel 2	(4.0±0.4)%	(2.2±0.4)%	(2.8±0.4)%	(1.6±0.4)%
Transition	(5.3±0.5)%	(2.7±0.5)%	(3.6±0.5)%	(2.3±0.5)%
Endcap	(5.5±0.5)%	(0.9±0.5)%	(5.0±0.5)%	(0.7±0.5)%

	$(E_{7x7}+H_{3x3})/p$ 11.0.ref01	$(E_{7x7}+H_{3x3})/p$ 11.0.ref02	$(E_{11x11}+H_{5x5})/p$ 11.0.ref01	$(E_{11x11}+H_{5x5})/p$ 11.0.ref02
Barrel 1	(1.6±0.4)%	(2.0±0.4)%	(1.8±0.4)%	(2.3±0.4)%
Barrel 2	(1.8±0.4)%	(1.6±0.4)%	(1.5±0.4)%	(1.4±0.4)%
Transition	(1.9±0.5)%	(2.1±0.5)%	(1.4±0.5)%	(1.9±0.5)%
Endcap	(2.0±0.5)%	(1.7±0.5)%	(1.6±0.5)%	(1.9±0.5)%

Summary

- Predictions from the new Geant4 versions 11.0, 11.0.p01, 11.0.ref01 and 11.0.ref02 using several physics lists from FTFP_BERT and QGSP_FTFP_BERT families are compared with the test beam 2006 and detector data

- The predictions for the 2006 test beam as well as collision data from these versions are comparable with those from earlier versions like 10.7.p02
  - There is a problem (~2%) with the scale in HCAL

- Tests with the Run3 and the latest Phase2 scenarios reveal several warnings (mostly for the version with VecGeom) and also premature termination or indefinite looping (again for the version with VecGeom)

Backups

Warnings and Errors

- Several warning messages used to appear in some recent versions:

  - Warnings about possible overlaps:

  - Warnings during tracking in B-field where some tracks are killed:

  - Error message from hadronic physics and decays:

  - The EMZ physics lists run till end for the phase2 geometry but goes in infinite loop for the run2 geometry

  - Two warnings from track propagation
    - Difficulty in the convergence during estimation of intersection point
    - Negative step length during track propagation

- In addition, there used to be failures due to two possible sources

  - Miscalculation of step length during propagation (a)

  - Tracks cannot be propagated after 25 attempts (b)

    - One failure and reduced number of old warnings in the current version

Energy Measurements
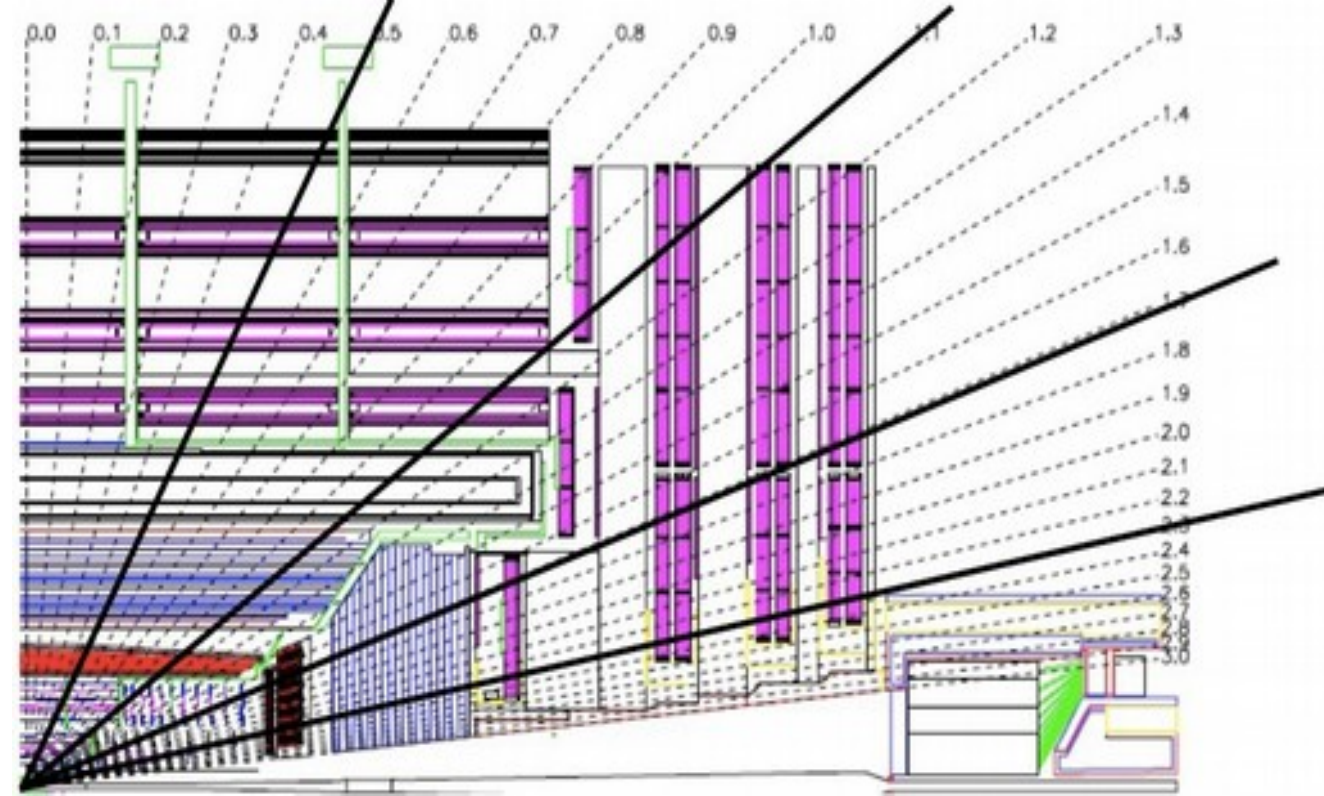
- Look at tracks in 4 different regions: two in the barrel, one in the endcap and one in the transition region
- Measure energy by combining energy measurements from a matrix of NxN cells around the cell hit by the extrapolated track to the calorimeter surface. Two versions of NxN matrix used:
  - 7x7 matrix for ECAL and 3x3 matrix for HCAL (better purity)
  - 11x11 matrix for ECAL and 5x5 matrix for HCAL (better containment)
- For the data use two low luminosity data sets from the 2016B run period
  - Distributions from Zero Bias and Minimum Bias triggers agree quite well
  - Combine these two data sets and compare that with Monte Carlo