# Validation of Geant4 for CMS Simulation

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Sunanda Banerjee
Vladimir Ivantchenko

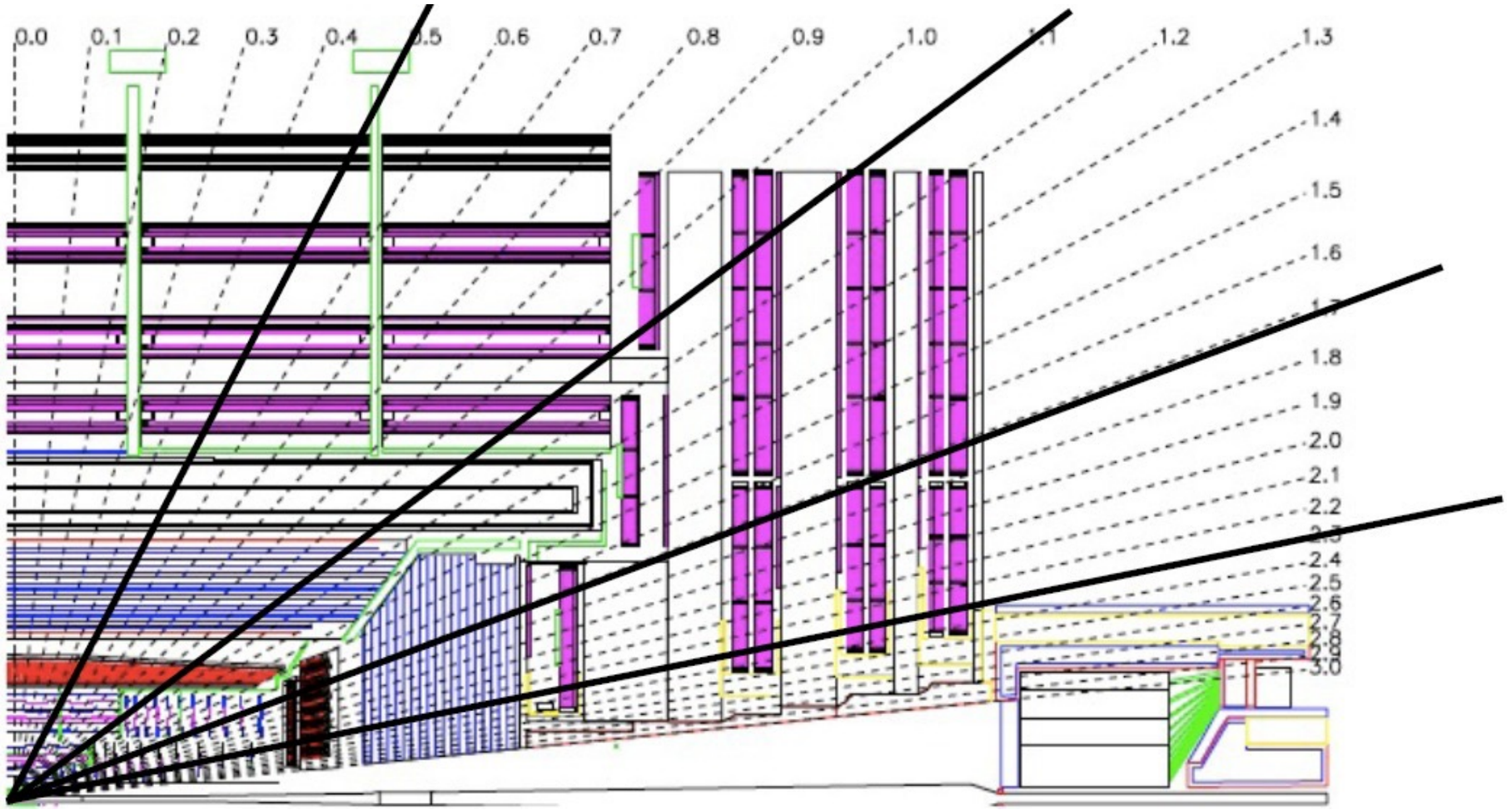
# New Geant4 Version

- Geant4 came with a new version 10.4 on December 8, 2017
- This version is of interest to CMS mainly because of extension of the Geometry part:
  - Possibility to be interfaced with the VecGeom Unified Solids Library to replace the original Geant4 solids. This will require an additional external (VecGeom library of version v00.05.00)
- Some of these new features are tested in special CMSSW builds and compared with earlier default in CMS for
  - Computing performance
  - Physics performance
  - Robustness during execution

# What is Done for Physics Validation

- Compare ratio of calorimeter energy measurement to beam or track momentum between data and MC. Data come from
  - test beam studies with identified particle type
  - isolated charged hadron sample in collision data
- Source of Data:
  - 2006 test beam set up in the SPS H2 beam line with HB prototype and one EB supermodule
  - Low luminosity runs taken during 2016B run period using Zero Bias and Minimum Bias triggers
- For Monte Carlo, events are generated using FTFP_BERT_EMM Physics List for Geant4 versions 10.2.p02, 10.3.p03 (, 10.4.beta) and 10.4 with CMSSW_9_2_5_patch1 and CMSW_10_0_0_pre3. All the non-standard Geant4 versions are custom made with the same same CLHEP (except the effect of the version 2.8.0 is also tried):
  - Generate 50k events at each beam energy for the said type and for calibration generate 50k electron events in setups with and without EB
  - Generate 100k single particle event sample using a flat energy distribution between 1 and 20 GeV with a given admixture of pions, kaons and protons and anti-protons (as expected in minimum bias sample)

# Energy Measurements




- Select good charged tracks using standard cuts
- Propagate them to calorimeter surface and select those which are well isolated from other charged or neutral particles in the calorimeter surface
- Measure energy by combining energy measurements from a matrix of NxN cells around the cell hit by the extrapolated track to the calorimeter surface in four regions (two in the barrel, one in the endcap and one in transition region)

# Collision Data

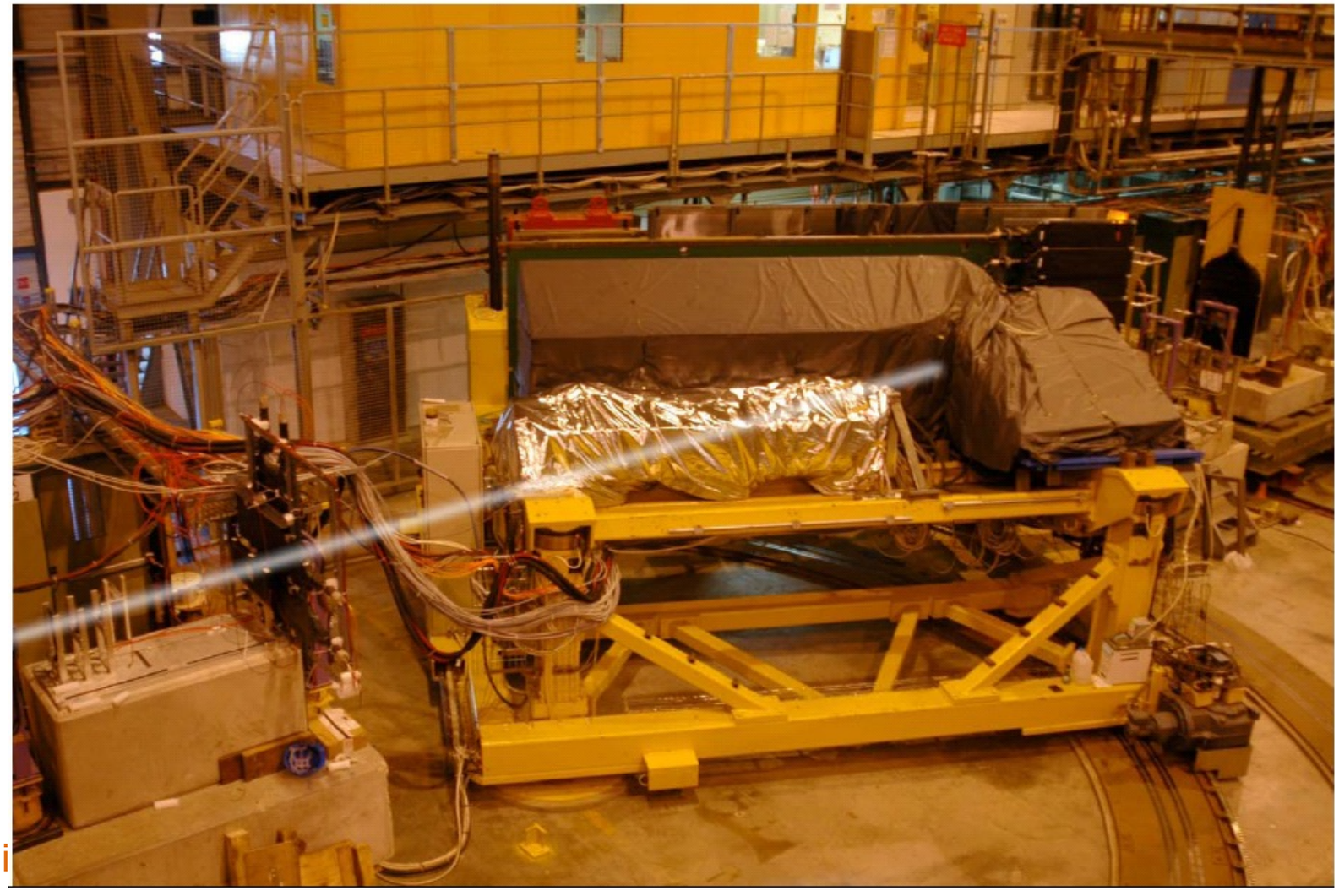
- The level of disagreement between data and MC is between 2.0% to 5.5% for the Geant4 version 10.4 depending on the region of the detector

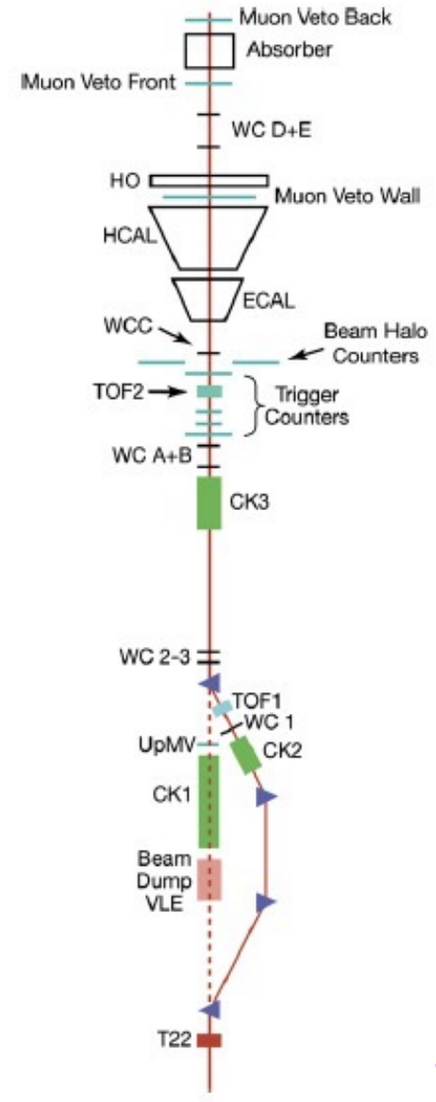
Mean level of disagreement between MC and data

| | $(E_{7x7}+H_{3x3})/p$ 10.2.p02 | $(E_{7x7}+H_{3x3})/p$ 10.4.beta | $(E_{7x7}+H_{3x3})/p$ 10.4 | $(E_{11x11}+H_{5x5})/p$ 10.2.p02 | $(E_{11x11}+H_{5x5})/p$ 10.4.beta | $(E_{11x11}+H_{5x5})/p$ 10.4 |
|---|---|---|---|---|---|---|
| **Barrel 1** | (2.3±0.4)% | (1.9±0.4)% | (2.1±0.4)% | (2.6±0.4)% | (1.9±0.4)% | (2.7±0.4)% |
| **Barrel 2** | (3.6±0.4)% | (5.0±0.4)% | (3.6±0.4)% | (2.2±0.4)% | (2.6±0.4)% | (2.0±0.4)% |
| **Transition** | (4.9±0.5)% | (7.2±0.5)% | (5.5±0.5)% | (2.2±0.5)% | (4.8±0.5)% | (2.8±0.5)% |
| **Endcap** | (3.1±0.3)% | (5.9±0.5)% | (5.0±0.5)% | (1.5±0.5)% | (3.9±0.5)% | (3.0±0.5)% |

# 2006 TestBeam Data

- The data correspond to energy response due to well identified single particles over a large momentum range (2 to 350 GeV)
- The results consist of the energy distributions for well identified particles at a fixed momentum, mean response and energy resolution as a function of beam momentum and fraction of events not interacting in the ECAL
  - Particle identification is rather good for beam momenta at or below 9 GeV
- Use the setup described within CMSSW to simulate events with single particles.





# Test Beam Data

## Mean level of disagreement between MC and data

| | Negative pions | Positive Pions | Negative Kaons | Positive Kaons | Protons | Anti-protons |
|---|---|---|---|---|---|---|
| 10.2.p02 | (1.6±0.7)% | (1.2±0.6)% | (12.8±1.2)% | (12.8±1.2)% | (2.3±1.0)% | (3.3±0.9)% |
| 10.3.p03 | (1.5±0.7)% | (0.9±0.6)% | (13.6±1.2)% | (13.8±1.2)% | (2.4±1.1)% | (3.9±0.9)% |
| 10.4 | (1.3±0.7)% | (0.8±0.6)% | (14.2±1.2)% | (13.7±1.2)% | (2.6±1.1)% | (3.4±0.9)% |

- The level of disagreement between pion data and MC is below 1.6% for all Geant4 version and there is some improvement in the version 10.4
- For proton and anti-protons, the level of disagreement stays below 2.6% and 3.9% and the best agreement was in 10.2.p02
- The level of disagreement is the largest for kaons (of either charge) for all the Geant4 versions tested here

# Integration of Geant4+VecGeom with CMSSW

- CMS is interested in using the improved geometry classes from VecGeom integrated with Geant4 in CMS simulation software. Almost all the shapes required by CMS come from VecGeom
- There have been a series of developments of VecGeom which have been tested using the CMSSW framework
  - The first results were reported using the 10.4.beta version integrated with the VecGeom version (v.00.04.00)
    - There was an issue due to segmentation violations after tracks with direction along z-axis getting stuck
      - This was due to inadequacy in one of the methods of finding distance to in/out
  - The first fix using the VecGeom branch raman/vecgeom-450 was tested also with 10.4.beta version of Geant4
    - There was no crash but several reports of stuck tracks for 2016 and 2018 geometries
      - Larger statistics of events are generated (3000 minimum bias and 1500 t-tbar) to see the type of volumes which cause this
      - The volumes concerned were only Polycone's and Polyhedra's
        - At least one of the concerned volume (mother or daughter) has one z-value where $R_{In} = R_{Out}$
  - A second set of corrections taken from the main branch (November 2) was tested with 10.3.Ref10 version of Geant4
    - This cured the stuck track issues for Polyhedra's
  - The branch raman/vecgeom-453 was tested with 10.3.Ref11 version of Geant4
    - This branch caused more stuck tracks and also segmentation violation due to lack of recovery from stuck tracks
  - The next set of corrections were taken from the main branch (November 29) and was tested with 10.4.Cand01 version of Geant4
  - The tagged version v00.05.00 is tested with the release version of Geant4.10.4

# Tests Performed

- Two different CMS geometries are used for testing CMSSW with Geant4-VecGeom
  - 2016 Geometry with 100k single particles (mixture of π/K/p) and their anti-particles with momentum between 1-20 GeV
  - 2018 Geometry for 8 different data sets
    - 3000 events of single muons in the barrel and similar number in the endcap
    - 3000 events of single electrons in the barrel and the same in the endcap
    - 3000 events of single pions in the barrel and the same in the endcap
    - 3000 minimum bias events at center-of-mass energy of 14 TeV
    - 1500 t-tbar events at 14 TeV

Summary of Stuck Tracks in different versions

| | v00.04.00 | raman450 | Nov 2 | raman453 | Nov 29 | v00.05.00 |
|---|---|---|---|---|---|---|
| Barrel μ | 0/3000 | 0/3000 | 0/3000 | 65/3000 | 0/3000 | 0/3000 |
| Endcap μ | 0/3000 | 0/3000 | 0/3000 | 66/3000 | 0/3000 | 0/3000 |
| Barrel e | 0/3000 | 0/3000 | 0/3000 | 41/88 | 0/3000 | 0/3000 |
| Endcap e | 1/3000 | 1/3000 | 1/3000 | 151/3000 | 0/3000 | 0/3000 |
| Barrel π | 0/3000 | 0/3000 | 0/3000 | 733/3000 | 0/3000 | 0/3000 |
| Endcap π | 1/3000 | 1/3000 | 1/3000 | 54/1828 | 0/3000 | 0/3000 |
| MinBias | 29/500 | 194/3000 | 177/3000 | 78/7 | 1/3000 | 0/3000 |
| t-tbar | 39/110 | 413/1500 | 408/1500 | 53/1 | 0/1500 | 0/1500 |
| single had | 585/173k | 306/100k | 334/100k | 485/912 | 0/100k | 0/100k |

# Comparison between Native/VecGeom Versions

- "Stuck Track" warnings are not fatal if Geant4 can recover with a small push
- Both "Native" and "VecGeom" versions report "stuck track". The most recent "VecGeom" version provides acceptable rate.
  - "Single particle" sample uses 2016 Geometry while all others come from 2018 Geometry

| Version Used | Single Particle | 50 GeV pions in the barrel | Top Pair |
|---|---|---|---|
| Native | 1/100000 | 1/3000 | 2/1500 |
| VecGeom | 0/100000 | 0/3000 | 0/1500 |

- Volumes giving rise to "Stuck Track" warnings
  - Native version in 2018 Geometry:
    - PixelBarrelLayer0CoolantHalf: Tubs
    - PixelBarrelLayer3CoolantHalf: Tubs
    - ESPM: Subtraction Solid
  - Native version in 2016 Geometry:
    - ESPM: Subtraction Solid

# Performance of the Scalar Version

- The CPU and memory performance of CMSSW 10.0.0.pre3 with Geant4.10.4 using “native” and “VecGeom” geometry versions:

| | RSS (Native) (GB) | CPU (VecGeom) (wrt Native) | RSS (VecGeom) (GB) |
|---|---|---|---|
| Muon (Barrel) | 0.55 | 0.926 | 0.60 |
| Muon (Endcap) | 0.55 | 0.953 | 0.60 |
| Pion (Barrel) | 0.59 | 0.930 | 0.63 |
| Pion (Endcap) | 0.58 | 0.903 | 0.63 |
| Elec (Barrel) | 0.52 | 0.974 | 0.53 |
| Elec (Endcap) | 0.57 | 0.944 | 0.61 |
| Minimum Bias | 0.65 | 0.870 | 0.67 |
| t-tbar | 0.69 | 0.926 | 0.69 |
| Single Hadrons | 0.61 | 0.872 | 0.71 |

- 7-13% improvement in CPU performance with similar memory usage
- Usage of CLHEP version 2.8.0 does not change the CPU performance

# Quality of Collision

- The level of disagreement between data and MC is between 1.8% and 5.4% in the Geant4 version 10.4 with VecGeom (v0.5) depending on the region of the detector

Mean level of disagreement between MC and data

| | $(E_{7x7}+H_{3x3})/p$ 10.2.p02 | $(E_{7x7}+H_{3x3})/p$ 10.4 | $(E_{7x7}+H_{3x3})/p$ VecGeom | $(E_{11x11}+H_{5x5})/p$ 10.2.p02 | $(E_{11x11}+H_{5x5})/p$ 10.4 | $(E_{11x11}+H_{5x5})/p$ VecGeom |
|---|---|---|---|---|---|---|
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| **Barrel 2** | (3.6±0.4)% | (3.6±0.4)% | (3.9±0.4)% | (2.2±0.4)% | (2.0±0.4)% | (2.3±0.4)% |
| **Transition** | (4.9±0.5)% | (5.5±0.5)% | (5.2±0.5)% | (2.2±0.5)% | (2.8±0.5)% | (2.7±0.5)% |
| **Endcap** | (3.1±0.3)% | (5.0±0.5)% | (5.4±0.5)% | (1.5±0.5)% | (3.0±0.5)% | (3.3±0.5)% |

Also examined track reconstruction efficiency and colorimeter quantities

→ No difference from native G4 version

# Summary

- Predictions from the physics list FTFP_BERT_EMM from Geant4 versions 10.2.p02, 10.3.p03 and 10.4 are compared with the data
- The level of agreement between data and Monte Carlo for the version 10.4 of Geant4 is quite good for collision data and similar to earlier comparisons for test beam data (pion data at low energies show slightly wider energy distributions than MC predictions; also small differences for mean response of kaons and antiprotons)
- Geant4.10.4 is an acceptable candidate for the next CMSSW version

- CMS has been following several versions of “VecGeom” replacing the “Native” geometry routines of Geant4
- The initial issues are resolved in the most recent version of VecGeom which is tested with CMSSW, the initial issues being
  - Tracks getting stuck and is recovered after small push
  - Segmentation fault for track getting stuck even after the push
- Quality of the simulation is tested for
  - Calorimetric observables in ECAL/HCAL
  - Track reconstruction efficiency of isolated charged hadrons
  - Energy response measurement (comparison with the data)
- All tests give acceptable performance
- The “VecGeom” version gives an enhancement between 5-8% in CPU time with no additional memory requirement
- The current VecGeom version is good for production release of CMSSW