Current and Future Performance of the CMS Simulation

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Overview

- CMS full simulation uses Geant4
- Sim is 40% of total CPU time used by CMS
 → most expensive "step" in MC production
 (vs. generation, digitization, reconstruction)
- Largest contributors to CPU usage in Geant4: geometry, magnetic field, EM physics
- CMS has implemented numerous technical options and approximations to improve CPU usage in the simulation
- Continue to explore new options and improvements
- Including GeantV, vectorized transport engine (currently in development)



The CMS Detector





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The CMS Detector



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The CMS Detector



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Challenges of Phase 2

- CMS Phase 0 and Phase 1 simulation geometries have 2.1 million elements
- Phase 2 geometry has 21.9 million elements: 10×(Phase 1)
- This translates to an increase in CPU time for simulation





- Simulate more events to keep up with HL-LHC data volumes: 10×(Phase1)
- May also need to improve accuracy of physics lists to simulate HGCal
- Reconstruction will take longer due to high pileup and granular detectors
- Need more events, more accuracy, in more complicated geometry... w/ relatively smaller fraction of total CPU usage

Existing Improvements

- **Static library**: avoid calls to procedure linkage table (PLT) for dynamic loading of libraries
- **Production cuts**: 0.01mm (pixel), 0.1mm (strip tracker), 1 mm (ECAL/HCAL), 0.002 mm (muon systems), 1 cm (support structure)
- **Tracking cut**: 2 MeV (within beampipe) \rightarrow avoid looping electrons
- **Time cut**: 500 ns
- Shower library: use pre-generated showers in forward region (HF, ZDC, Castor)
- **Russian roulette**: discard N-1 neutrons < 10 MeV or gammas < 5 MeV (in calorimeters), retain Nth particle and assign it a weight of N
- **FTFP_BERT_EMM**: modified physics list, simplified multiple scattering model for most regions (default used for HCAL, HGCal)
- > When all optimizations applied together, CMS achieves $\sim 3-5 \times$ speedup!

Results of Existing Improvements

	Relative CPU usage	
Configuration	MinBias	ttbar
No optimizations	1.00	1.00
Static library	0.95	0.93
Production cuts	0.93	0.97
Tracking cut	0.69	0.88
Time cut	0.95	0.97
Shower library	0.60	0.74
Russian roulette	0.75	0.71
FTFP_BERT_EMM	0.87	0.83
All optimizations	0.21	0.29

• From HEP Software Foundation Community White Paper

o CMS Phase 0 detector, Geant4 10.2

- HF shower library, Russian Roulette have largest impacts
- Cumulative effects: with all improvements, simulation is 4.7× (3.4×) faster for MinBias (ttbar)
- CMS simulation takes 4.3 sec[†]/event (24.6 sec[†]/event) for MinBias (ttbar)

^{\dagger}1 sec = 11 HS06 for test machine

Multithreading



Num Workers

- Geant4 includes event-level multithreading
- Nearly perfect scaling with physical cores, further 30% gain from hyperthreading
- Memory reduced by factor of 10 (vs. multiprocessing approach) CHEP 2018

- CMSSW framework supports multithreading
- Similar gains in throughput observed, memory usage remains under 2GB
- More efficient use of grid resources (included in CMS production releases)

New Improvements: Geometry

VecGeom: new library for detector geometry

- Supports vectorization and new architectures
- Code rewritten to be more modern and efficient (vs. Geant4, ROOT, USolids)
- Can be used in scalar mode with Geant4
- CMS observes 7–13% speedup with similar memory usage
 - \rightarrow Just from code improvements, no vectorization!
- Included in latest CMS production releases
 - o First mainstream use of vectorized library by experiment

	Relative CPU usage	
Geometry library	MinBias	ttbar
Native	1.00	1.00
VecGeom	0.87	0.93

New Improvements: Magnetic Field

• Faster stepper (G4DormandPrince745) for tracking in magnetic field

o Also a more robust algorithm

- Smart tracking: energy-dependent propagation through EM fields
- CMS observes 8–10% speedup with these optimizations (preliminary)
 - o Enabled by migration to latest Geant4 version 10.4

	Relative CPU usage	
Stepper	MinBias	ttbar
G4ClassicalRK4	1.00	1.00
G4DormandPrince745	0.93	0.98
G4DormandPrince745 + smart tracking	0.92	0.90

(tested w/ gcc 7.0 and 16 threads)

Potential Improvements: GeantV

- CMS has already achieved significant speedups in Geant4 and enabled eventlevel multithreading for more efficient use of resources
- However, even this will not suffice for the demands of Phase 2
- Enter GeantV: Vectorized Transport Engine
 - Track-level parallelism: process multiple events simultaneously
 - Exploit single instruction, multiple data (SIMD) vectorization
 - Group similar tracks into *basket* (based on particle type, geometry/material)
 - Send entire basket to algorithm: process particles in parallel



Early Testing of GeantV in CMSSW

- Started with integration into toy-mt-framework → included in alpha release
 O Used for CMS multithreading R&D (Intel Thread Building Blocks)
- > Now have a working example compatible w/ CMSSW development release
- Run GeantV in "external loop" mode using CMSSW ExternalWork feature:

Asynchronous task-based processing



Co-development approach: test consistency of threading models, interfaces
 Provide feedback to prevent divergence between CMS and GeantV

Elements of GeantV Integration

- ✓ Generate events in CMSSW framework, convert HepMC to GeantV format
- ✓ Build CMSSW geometry natively and pass to GeantV engine
- Using constant magnetic field, limited EM-only physics list
- Sensitive detectors and scoring not yet adapted to new interfaces
- Production cuts also not yet included
- First integration of GeantV into experimental software framework
 - o Run with elements specified above
 - Integration with downstream steps (e.g. digitization):
 longer timescale, requires more development for thread-safe scoring
- CMS will test GeantV beta release, targeting demonstration of speedup
 - Community decision to support GeantV engine as part of Geant4 on timescale of HL-LHC

Conclusions

- CMS has substantially reduced CPU usage of Geant4 full simulation
 - $\circ \sim 3-5 \times$ speedup using various technical improvements and physicspreserving approximations
 - Continue to find ~10% improvements, e.g. from VecGeom and magnetic field stepper/tracking optimizations
- HL-LHC and Phase 2 upgrades bring significant challenges:
 - Need more events, more accuracy, in more complicated geometry... w/ relatively smaller fraction of total CPU usage
- GeantV is one promising approach to speed up full simulation even further
 Track-level parallelism (rather than event-level), vectorized components
 - <u>Alpha release</u> is available, beta release planned for 2019
 - Successful early integration in CMS software framework!
 - \circ Aim for 2–5× speedup with final version

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 - o CMS Simulation Group
 - o CMS Core Software Group
 - o HEP Software Foundation
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References

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- D. Elvira et al., "CMS Simulation in the HL-LHC Era", <u>HSF-CWP-011</u>, January 2017.
- D. Elvira, "VecGeom in CMS, Mu2e, Muon g-2". Joint WLCG & HSF Workshop, Napoli, March 2018.
- J. Apostolakis et al., "Towards a high performance geometry library for particle-detector simulations", *J. Phys. Conf. Ser.* 608 (2015) 012023, doi:10.1088/1742-6596/608/1/012023.
- K. Pedro, "Tests of GeantV in CMS Software Framework". Joint WLCG & <u>HSF Workshop</u>, Napoli, March 2018.

Repositories

- CMSSW (<u>GitHub/cms-sw</u>)
 CMS Offline Software, ~6 million LOC
- VecCore (<u>GitHub/root-project</u>)

 SIMD abstraction library
 Supports backends: Vc, UME::SIMD, CUDA
- VecMath (<u>GitHub/root-project</u>)

 Vectorized math utilities
 Built on top of VecCore
- VecGeom (<u>CERN/GitLab</u>)

o Vectorized geometry and navigation, multi-particle interface

- GeantV (<u>CERN/GitLab</u>)
 - o <u>Alpha release</u> now available!
 - o <u>cmsToyGV example</u>
- toy-mt-framework (<u>GitHub/Dr15Jones</u>)
 Original toy framework for CMS multithreading development
- install-geant (<u>GitHub/kpedro88</u>), SimGVCore (<u>GitHub/kpedro88</u>)
 o Test repositories to install and integrate GeantV in CMSSW

Backup

CMS & LHC Upgrade Schedule

- Phase 1 upgrades began during Run 2 and will be in operation through the end of Run 3 (installation finishes during Long Shutdown 2)
- Phase 2 upgrades will be in operation during Runs 4, 5 (installation during Long Shutdown 3)



Simulation Test Details

- Machine: olhswep16.cern.ch (CERN OpenLab)
- Single-threaded runs
- Compiler: gcc 6.3.0
- Geant4: version 10.2
- FTFP_BERT physics list
- Pythia event generation: $\sqrt{s} = 13$ TeV, 300 events, $|\eta| < 5.5$ (minimum bias, ttbar)
- Particle gun event generation: 50 GeV electrons, muons, pions flat distribution in $\eta = [-0.8, 0.8], \eta = [2.0, 2.7], \varphi = [0, 2\pi]$
- Geometry: 2016 detector version (default)

Multithreading





External Work in CMSSW (1)

Setup:

- TBB controls running modules
- Concurrent processing of multiple events
- Separate helper thread to control external
- Can wait until enough work is buffered before running external process

External Controlling Thread		
Running		
Waiting To Run	MODULE A MODULE B MODULE C	MODULE A MODULE B MODULE C
	Event Loop 1	Event Loop 2

External Work in CMSSW (2)

Acquire:

- Module *acquire()* method called
- Pulls data from event
- Copies data to buffer
- Buffer includes callback to start next phase of module running



External Work in CMSSW (3)

Work starts:

- External process runs
- Data pulled from buffer
- Next waiting modules can run (concurrently)

External Controlling Thread	1	2
Running	MODULE B	MODULE B
Waiting To Run	MODULE	MODULE
	Event Loop 1	Event Loop 2

External Work in CMSSW (4)

Work finishes:

- Results copied to buffer
- Callback puts module back into queue



External Work in CMSSW (5)

Produce:

- Module *produce()* method is called
- Pulls results from buffer
- Data used to create objects to put into event

