

Geant4 Performance Profiling and Monitoring

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J. Yarba (Fermilab)

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Overview

1. Geant4 Computing Performance Task (G4CPT) at Fermilab
2. Geant4 built-in profiling with Timemory
3. Geant4 performance regression testing and monitoring

Geant4 Computing Performance Task

Geant4 Computing Performance Task (G4CPT)

▶ Purpose

- Monitor Geant4 CPU & memory through the development cycle
 - ▷ Currently using tools such as IgProf 5.9.12 and Open|SpeedShop 2.3
 - ▷ Willing to consider newer emerging tools as well
- Identify issues (if any) and opportunities for code improvement
- Provide feedback to the working group leaders
- Close all open issues before the next release

▶ Ongoing Activities

- Regular profiling/benchmarking of Geant4 development tags and public releases
- Addition of new profiling applications as needed (if possible)
- Maintenance and evolution of the profiling infrastructure
 - ▷ Adapt in response to changing computing environment

Current G4CPT Resources at FNAL

- ▶ Central web server — <https://g4cpt.fnal.gov>
- ▶ FY2020 members and contributions
 - J. Yarba, S. Y. Jun, K. Genser, D. Elvira, P. Canal
- ▶ FNAL Wilson Cluster — <https://wilsonweb.fnal.gov>

Test Type(s)	Nodes	Cores	Node Hours	Core Hours
Sequential (amd32_g4perf)	21	32	~144	~4600
Sequential (intel12)	25	12	~50	~600
Multi-threaded (amd32)	2	up to 32	~14	~150
Multi-threaded (intel12)	2	up to 12	~10	~50
Memory (tevnfsg4)	1	1	~12	~12
Total	51			~5412

- ▶ Transition to Fermilab IC and LQ clusters planned in the near future

Overview of the Profiling Campaign for Geant4 10.6.rXX

Regular profiling of SimplifiedCalo, cmsExp, and cmsExp+VecGeom Geant4 applications.

Various primaries, energies, and physics lists.

Profiled on the Wilson CPU cluster using AMD 6128HE Opteron 2GHz
(green: gcc 7.1.0 -O3), (pink: gcc 6.3.0 -O2), (yellow: gcc 4.9.2 -O2)

Geant4 Version	Application	Performance	Summary
10.6.r08	SimplifiedCalo	OpenSpeedshop IgProf(Memory)	CPU MEM
10.6.r08	cmsExp	OpenSpeedshop IgProf(Memory)	CPU MEM
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10.6	cmsExp	OpenSpeedshop IgProf(Memory) - N/A	CPU MEM - N/A
10.5.p01	SimplifiedCalo	OpenSpeedshop IgProf(Memory)	CPU MEM
10.4.p03	SimplifiedCalo	OpenSpeedshop IgProf(Memory)	CPU MEM
10.3.p03	SimplifiedCalo	OpenSpeedshop IgProf(Memory)	CPU MEM
10.2.p03	SimplifiedCalo	OpenSpeedshop IgProf(Memory)	CPU MEM
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Open SpeedShop			
Geant4.10.6.r08 SimplifiedCalo			
Sample	Physics List	B-Field	Energy
Higgs->ZZ	FTFP_BERT	ON (4.0T)	14 TeV PYTHIA
		OFF (0.0T)	14 TeV PYTHIA
100 MeV e- (5K e-levent)	FTFP_BERT	ON (4.0T)	100 MeV
		ON (4.0T)	100 MeV
Electrons	FTFP_BERT	ON (4.0T)	1 GeV, 5 GeV, 10 GeV, 50 GeV
		OFF (0 T)	1 GeV, 5 GeV, 10 GeV, 50 GeV
Pions-	FTFP_BERT	ON (4.0T)	1 GeV, 5 GeV, 10 GeV, 50 GeV
		OFF (0 T)	1 GeV, 5 GeV, 10 GeV, 50 GeV
		ON (4.0T)	1 GeV, 5 GeV, 10 GeV, 50 GeV
		ON (4.0T)	1 GeV, 5 GeV, 10 GeV, 50 GeV
Protons	FTFP_BERT	ON (4.0T)	1 GeV, 5 GeV, 10 GeV, 15 GeV
		ON (4.0T)	1 GeV, 5 GeV, 10 GeV, 15 GeV
		ON (4.0T)	1 GeV, 5 GeV, 10 GeV, 15 GeV
		ON (4.0T)	1 GeV, 5 GeV, 10 GeV, 15 GeV
Anti-Protons	FTFP_BERT	ON (4.0T)	1 GeV, 5 GeV, 10 GeV, 50 GeV
		ON (4.0T)	1 GeV, 5 GeV, 10 GeV, 50 GeV
Gamma	FTFP_BERT_EMZ_AugerOff	ON (0 T)	250 MeV, 1 GeV
		OFF (0 T)	250 MeV, 1 GeV

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Regular profiling of SimplifiedCalo, cmsExp, and cmsExp+VecGeom Geant4 applications.

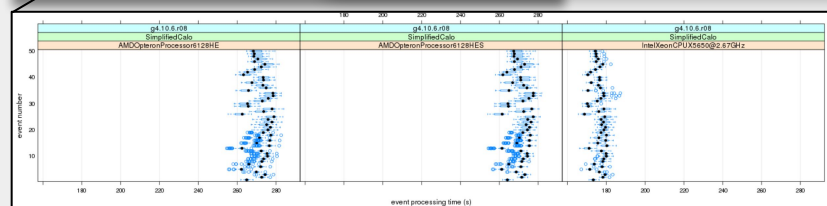
Various primaries, energies, and physics lists.

Profiled on the [Wilson](#) CPU cluster using AMD 6128HE Optron 2GHz (green: gcc 7.1.0 -O3), (pink: gcc 6.3.0 -O2), (yellow: gcc 4.9.2 -O2)

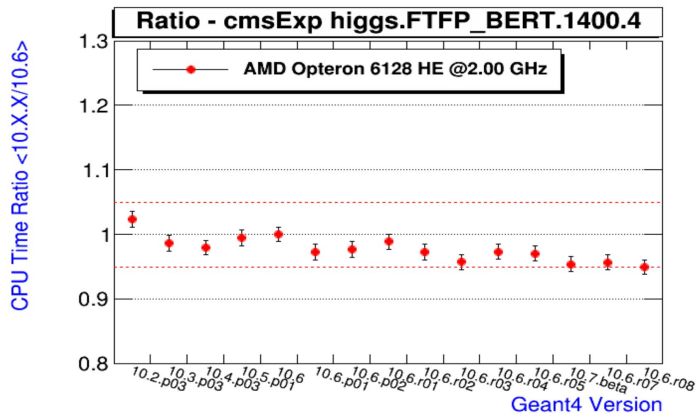
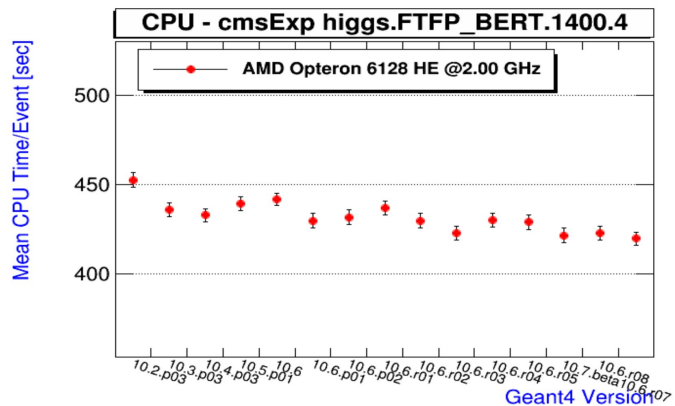
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Open|SpeedShop
Geant4.10.6.r08 SimplifiedCalo

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	Shielding	ON (4.0T)	100 MeV
	Shielding_EMZ	ON (4.0T)	100 MeV
Electrons	FTFP_BERT	ON (4.0T)	1 GeV, 5 GeV, 10 GeV, 50 GeV
		OFF (0 T)	1 GeV, 5 GeV, 10 GeV, 50 GeV
Pions-	FTFP_BERT	OFF (0 T)	1 GeV, 5 GeV, 10 GeV, 50 GeV
	QGSP_BERT	ON (4.0T)	1 GeV, 5 GeV, 10 GeV, 50 GeV
	QGSP_BIC	ON (4.0T)	1 GeV, 5 GeV, 10 GeV, 50 GeV
	FTFP_INCLXX	ON (4.0T)	1 GeV, 5 GeV, 10 GeV, 15 GeV
Protons	FTFP_BERT	ON (4.0T)	1 GeV, 5 GeV, 10 GeV, 50 GeV
	FTFP_INCLXX	ON (4.0T)	1 GeV, 5 GeV, 10 GeV, 15 GeV
	FTFP_BERT_HP	ON (4.0T)	1 GeV, 5 GeV
Anti-Protons	FTFP_BERT	ON (4.0T)	1 GeV, 5 GeV, 10 GeV, 50 GeV
Gamma	FTFP_BERT_EMZ_AugerOff	OFF (0 T)	250 MeV, 1 GeV
Gamma	FTFP_BERT_EMZ_AugerOn	OFF (0 T)	250 MeV, 1 GeV



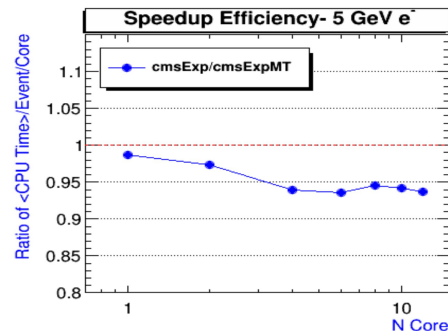
Examples of Performance Trends in Geant4 10.6.x



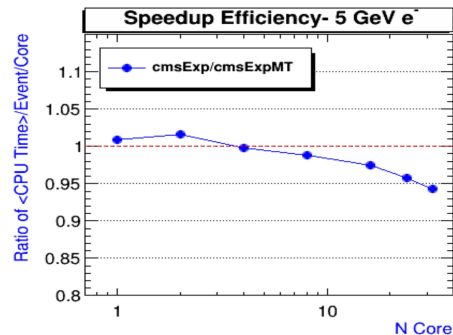
Geant4 MT (10.6.r08) Performance - Single Electrons/Pions

cmsExpMT: PhysicsList = FTFP_BERT, Magnetic Field = 3.8T

Processor: AMD Opteron(tm) Processor 6128 : 32 cores (4 CPU sockets x 8 cores)



Processor: Intel(R) Xeon(R) X5650 : 12 cores (2 CPU sockets x 6 cores)



G4CPT Summary

- ▶ Performed CPU and memory profiling for development and public releases, and for specific candidates (dev. tags)
- ▶ Identified a number of “hot spots” through the release cycle
- ▶ Reported results to the working group leaders and, if needed, to developers
- ▶ Modified the profiling protocol to include newly added applications
- ▶ Plan to migrate benchmark/profiling measurements to new hardware clusters (Fermilab IC and LQ)

Geant4 Built-in Profiling with Timemory

Timemory

Timemory is designed, first and foremost, to be a portable, modular, and fully customizable toolkit for performance measurement and analysis of serial and parallel programs written in C, C++, Fortran, Python, and CUDA.

▶ Repository on GitHub

- <https://github.com/nersc/timemory>

▶ Documentation

- <https://timemory.readthedocs.io>
- <https://timemory.readthedocs.io/en/latest/doxygen-docs/>

▶ Tutorials

- <https://github.com/NERSC/timemory-tutorials>

Basics of Timemory in Geant4

► Five profiling categories

- Run → `G4ProfilerConfig<G4ProfileType::Run>`
- Event → `G4ProfilerConfig<G4ProfileType::Event>`
- Track → `G4ProfilerConfig<G4ProfileType::Track>`
- Step → `G4ProfilerConfig<G4ProfileType::Step>`
- User → `G4ProfilerConfig<G4ProfileType::User>`

► Corresponding managers for first four categories all create instances in/around the primary section which processes simulation stage

► Callbacks are used to define

- Whether profiling is enabled
- What profiling data is collected
- How the entry is labeled

Basics of Timemory in Geant4 (cont.)

▶ Callbacks enable:

- Creating custom labels
 - ▷ Example: electrons in certain energy range
- Creating custom filters for specific conditions
 - ▷ Example: particle name + creator process name
- Modifying collection types and scoping
 - ▷ Example: add additional measurement type(s) to `G4Track`
 - ▷ Example: profile steps as a nested hierarchy vs. flat profile

▶ Timemory enables:

- Integration with external profilers
- Creating custom measurements as needed
- Direct access to data for testing → pass/fail status based on relative change

Sample Timemory Geant4 Profiling Report

```
>>> BeamOn@G4RunManager.cc:266           :      9.184619 sec wall,      2 laps, depth 0 (exclusive: 71.2%)
>>> |_RunInitialization@G4RunManagerKernel.cc:660 :      2.034925 sec wall,      2 laps, depth 1 (exclusive:  0.1%)
...
>>> neutron                               :      37.867025 sec wall, 13333 laps, depth 0
>>> proton                                 :     116.327824 sec wall, 23122 laps, depth 0
>>> deuteron                               :       0.662813 sec wall,  2471 laps, depth 0
>>> gamma                                  :       3.645594 sec wall, 12885 laps, depth 0
>>> e-                                      :     18.665260 sec wall,  91821 laps, depth 0
>>> alpha                                  :       0.487940 sec wall,   999 laps, depth 0
>>> C13                                     :       0.262488 sec wall,   903 laps, depth 0
>>> Al27                                    :     13.273209 sec wall,  4310 laps, depth 0
>>> Mg27                                    :       0.045587 sec wall,   165 laps, depth 0
>>> Al27[843.760]                          :       0.022125 sec wall,   114 laps, depth 0
>>> anti_nu_e                              :       0.102242 sec wall,   812 laps, depth 0
>>> O16                                     :     18.509317 sec wall,  6149 laps, depth 0
>>> Al28                                     :       0.084983 sec wall,   552 laps, depth 0
>>> Si28[1779.030]                        :       0.114113 sec wall,   552 laps, depth 0
>>> Si28                                     :       0.223719 sec wall,   552 laps, depth 0
>>> Na24                                    :       0.057237 sec wall,    94 laps, depth 0
>>> Mg24[4122.889]                        :       0.021973 sec wall,    94 laps, depth 0
>>> Mg24[1368.672]                        :       0.039716 sec wall,    94 laps, depth 0
>>> e+                                      :       0.054599 sec wall,   340 laps, depth 0
>>> Mg24                                    :       0.027572 sec wall,    94 laps, depth 0
>>> Al27[1014.560]                        :       0.009520 sec wall,    52 laps, depth 0
>>> O18                                     :       0.056089 sec wall,    19 laps, depth 0
>>> O17                                     :       0.028313 sec wall,     6 laps, depth 0
>>> C14                                     :       0.008031 sec wall,     1 laps, depth 0
>>> N14                                     :       0.000065 sec wall,     1 laps, depth 0
```

Features

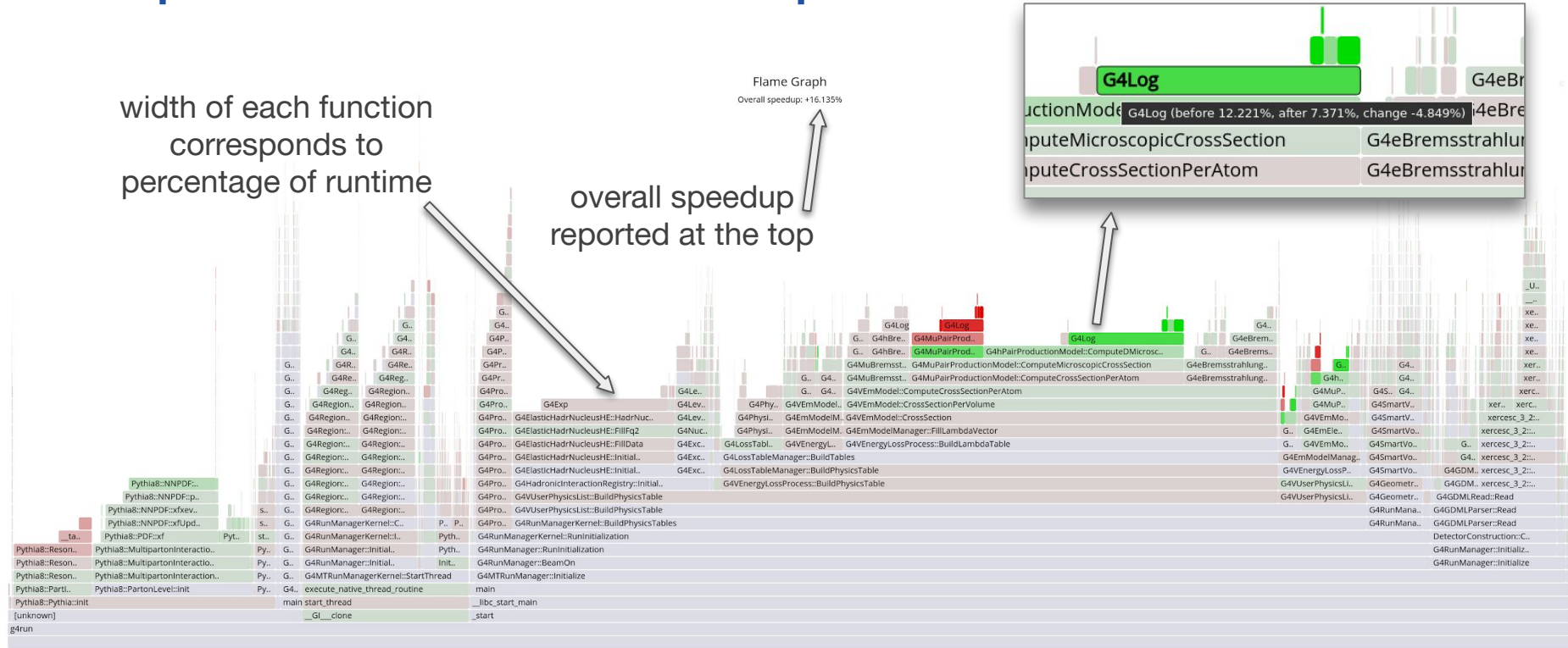
- ▶ Support for **G4Messenger** interface
 - `/profiler/run/components wall_clock cpu_clock peak_rss`
 - `/profiler/per_thread false`
 - `/profiler/output/json true`
- ▶ Metrics collected in each category are independent
 - Run can collect wall-clock, cpu-clock, hardware-counters, etc.
 - Event can collect wall-clock, cpu-clock
 - Track can collect wall-clock
- ▶ Default functors defined in extern “C” `void G4RunProfilerInit()`
 - Change profiling behavior via `LD_PRELOAD`

Geant4 Performance Regression Testing

Goals

- ▶ Quickly identify cause of performance regressions in Geant4
 - Compare Geant4 performance before and after changes from a merge request
 - Automated performance report generated for each merge request as part of CI
 - ▷ Easy to interpret visualization of performance changes based on <https://github.com/brendangregg/FlameGraph> with some customizations
 - Exchange the breadth of analysis done by G4CPT with configurability
 - ▷ Launch performance report with appropriate configuration for merge request
- ▶ Make it easy for developers to assess performance impact of their changes
 - Run performance report as part of development or to search for performance issues

Sample Performance Report



Legend: green = better (less cycles), red = worse (more cycles)

Saturation is proportional to relative change

Sample Performance Report (cont.)

Visual report complemented with more detailed information in text reports

```
Performance changes: hot spots

Overall speedups: +18.89% (time), +13.77% (cycles), +1.63% (instructions)

Prev: overhead for the baseline          Diff: Curr - Prev
Curr: overhead for the changes being tested Ratio: Curr / Prev

  CPU Cycles      |      Instructions
-----|-----
Prev  Curr  Diff  Ratio  Prev  Curr  Diff  Ratio  Symbol
-----|-----
22.054% 0.007% -22.047% 0.00 11.197% 0.004% -11.193% 0.00 G4hPairProductionModel::ComputeDMicroscopicCrossSection
7.686% 4.965% -2.721% 0.56 3.933% 3.622% -0.311% 0.91 G4MuPairProductionModel::ComputeDMicroscopicCrossSection
0.442% 0.539% 0.097% 1.05 0.758% 0.855% 0.097% 1.11 Pythia8::SigmaMultiparton::sigma
0.502% 0.622% 0.120% 1.07 0.646% 0.635% -0.011% 0.97 __strcmp_avx2
0.554% 0.676% 0.122% 1.05 0.676% 0.753% 0.077% 1.10 __dynamic_cast
0.912% 1.212% 0.300% 1.15 1.532% 1.695% 0.163% 1.09 G4ProductionCutsTable::ScanAndSetCouple

Performance changes: L1 cache

Overall speedups: +17.49% (time) +1.61% (instructions)

  L1 Data Cache Misses |      L1 Instruction Cache Misses
-----|-----
Prev  Curr  Diff  Ratio  Prev  Curr  Diff  Ratio  Symbol
-----|-----
4.285% 4.935% 0.650% 1.15 0.308% 0.224% -0.083% 0.73 Pythia8::SigmaMultiparton::sigma
4.103% 4.775% 0.672% 1.16 0.497% 0.338% -0.159% 0.68 G4ProductionCutsTable::ScanAndSetCouple
2.542% 2.890% 0.349% 1.14 0.745% 0.414% -0.330% 0.56 Pythia8::Rndm::flat
2.136% 2.444% 0.308% 1.14 0.756% 0.617% -0.139% 0.82 Pythia8::MultipartonInteractions::sigmaPT2scatter
0.198% 0.157% -0.041% 0.79 0.327% 0.430% 0.103% 1.32 G4eBremsstrahlungRelModel::ComputeXSectionPerAtom
0.057% 0.079% 0.022% 1.38 1.377% 1.554% 0.177% 1.13 G4LossTableBuilder::BuildRangeTable
0.003% 0.002% -0.001% 0.72 0.096% 0.214% 0.118% 2.22 __tan_fma

Performance report: hot spots

Cycles  Instr.  IPC  IPB  Branch  Stalls  Stalls  Symbol
-----  -----  -----  -----  -----  -----  -----  -----
8.961%  6.396%  1.313  24.680  0.092%  0.023%  86.339%  G4ElasticHadrNucleusHE::HadrNucDifferCrSec
8.640%  12.693%  2.702  6.205  0.441%  0.265%  44.638%  Pythia8::NNPDF::polint
7.064%  9.608%  2.502  5.996  0.218%  0.134%  51.135%  G4Region::BelongsTo
4.965%  3.622%  1.342  14.514  4.670%  0.473%  71.111%  G4MuPairProductionModel::ComputeDMicroscopicCrossSection
...
```

Report for [merge request 1158](#) “Optimizations for G4MuPairProduction initialization”

Current Status

▶ Standalone Geant4 application

- Configurable parameters
 - ▷ GDML geometry file
 - ▷ Reference physics list
 - ▷ Particle gun or Pythia events
 - ▷ Number of threads and events

▶ Integration with CDash, Jenkins and GitLab CI under development

- Basic reports include flamegraph and metrics like IPC and L1 cache statistics per function
- Further reports to be added soon (TLB usage, stalls caused by divisions/sqrt, etc)
- Standard performance test is CMS geometry with FTFP_BERT physics list and ttbar events
- Scripts can be reused to create similar reports for runs within a full framework, like CMSSW

Summary and Plans

- ▶ Created Geant4 application to run and profile simulations
 - Simple to run, single script runs the full build + performance reports
 - Easy to interpret view of performance changes to be run in continuous integration tests
 - Currently using only **perf**, but reports based on VTune also planned for near future
 - Would like to integrate also the magnetic field map, main difference with CMSSW
- ▶ Integration with GitLab CI, Jenkins, and CDash under development
 - Pilot builds functional, but still need better integration with CI systems
 - ▶ Suggestion: **Do:performance** command in GitLab, similar to **Do:stage**, etc
 - Configurability to allow checking for specific areas of Geant4 if needed
 - ▶ Specific physics list, particle, energy range, initialization vs event loop, etc
 - Two new planned reports for Intel hardware: div/sqrt and microarchitecture usage
 - Consider addition of extra reports based on integration with Timemory and user actions