Computing Performance Task: Summary, Status, and Future Updates

Julia Yarba

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Geant4 Computing Performance Task (I)

- Purpose
  - Monitor Geant4 CPU & memory through the development cycle
  - Identify issues (if any)
  - Identify opportunities for code improvement
  - Provide feedback to the working group leaders
  - Close all open issues before the next release

Geant4 Computing Performance Task (II)

- Ongoing activities
  - Regular profiling/benchmarking of Geant4 development and public release, specific development tags as needed
  - Maintenance and evolution of the profiling infrastructure
    - Geant4 by default builds in MT mode and operates on Tasking RM
    - Operations on SerialOnly RM preserved as needed
- Migration 2021
  - Resources
    - WC-IC at FNAL, CPU nodes IntelXeonCPUE52650v2@2.60GHzS
  - Compiler: gcc8.3.0
  - Profiling Tools
    - OpenlSpeedShop 2.4.1
    - IgProf 5.9.16
- Ongoing migration: gcc11 or gcc12

Overview of the 11.0.rXX Profiling Campaign (https://g4cpt.fnal.gov)

Geant4 Profiling and Benchmarking

Geant4 CPU Performance by Version (Geant4.10.x-series and Geant4-11.0)

1) The Current profiling activity is a part of Geant4 Computing Performance Task

2) Profiling Results

Since January 2021 and release 10.7.r01 migrated to IntelXeonCPUE52650v2@2.60GHzS
(releases 10.5.p01, 10.6.p03, 10.7 re-profiled on the new resources)
(cyan: gcc 8.3.0 -O3)

Geant4 Version	Application	Performance		Summary	
11.0.p03	SimplifiedCalo	OpenISpeedshop	IgProf(Memory)	CPU	MEM
11.0.p03	cmsExp	OpenISpeedshop	IgProf(Memory)	CPU	MEM
11.0.p03	cmsExpVecGeom	OpenISpeedshop	IgProf(Memory)	CPU	MEM
10.7.p04	SimplifiedCalo	OpenISpeedshop	IgProf(Memory)	CPU	MEM
10.7.p04	cmsExp	OpenISpeedshop	IgProf(Memory)	CPU	MEM
10.7.p04	cmsExpVecGeom	OpenISpeedshop	IgProf(Memory)	CPU	MEM
11.0.r07	SimplifiedCalo	OpenISpeedshop	IgProf(Memory)	CPU	MEM
11.0.r07	cmsExp	OpenISpeedshop	IgProf(Memory)	CPU	MEM
11.0.r07	cmsExpVecGeom	OpenISpeedshop	IgProf(Memory)	CPU	MEM
11.0.r06	SimplifiedCalo	OpenISpeedshop	IgProf(Memory)	CPU	MEM
11.0.r06	cmsExp	OpenISpeedshop	IgProf(Memory)	CPU	MEM
11.0.r06	cmsExpVecGeom	OpenISpeedshop	IgProf(Memory)	CPU	MEM
11.1.b01.c00	cmsExp	OpenISpeedshop	IgProf(Memory)	CPU	MEM
11.0.r05	SimplifiedCalo	OpenISpeedshop	IgProf(Memory)	CPU	MEM
11.0.r05	cmsExp	OpenISpeedshop	IgProf(Memory)	CPU	MEM
11.0.r05	cmsExpVecGeom	OpenISpeedshop	IgProf(Memory)	CPU	MEM
11.0.p02	SimplifiedCalo	OpenISpeedshop	IgProf(Memory)	CPU	MEM
11.0.p02	cmsExp	OpenISpeedshop	IgProf(Memory)	CPU	MEM
11.0.p02	cmsExpVecGeom	OpenISpeedshop	IgProf(Memory)	CPU	MEM
11.0.r04	SimplifiedCalo	OpenISpeedshop	IgProf(Memory)	CPU	MEM
11.0.r04	cmsExp	OpenISpeedshop	IgProf(Memory)	CPU	MEM
11.0.r04	cmsExpVecGeom	OpenISpeedshop	IgProf(Memory)	CPU	MEM
11.0.r03	SimplifiedCalo	OpenISpeedshop	IgProf(Memory)	CPU	MEM
11.0.r03	cmsExp	OpenISpeedshop	IgProf(Memory)	CPU	MEM
11.0.r03	cmsExpVecGeom	OpenISpeedshop	IgProf(Memory)	CPU	MEM
11.0.p01	SimplifiedCalo	OpenISpeedshop	IgProf(Memory)	CPU	MEM
11.0.p01	cmsExp	OpenISpeedshop	IgProf(Memory)	CPU	MEM
11.0.p01	cmsExpVecGeom	OpenISpeedshop	IgProf(Memory)	CPU	MEM
11.0.r02+MR2622	cmsExp	OpenISpeedshop	IgProf(Memory)	CPU	MEM
11.0.r02	SimplifiedCalo	OpenISpeedshop	IgProf(Memory)	CPU	MEM
11.0.r02	cmsExp	OpenISpeedshop	IgProf(Memory)	CPU	MEM
11.0.r02	cmsExpVecGeom	OpenISpeedshop	IgProf(Memory)	CPU	MEM
11.0.r01	SimplifiedCalo	OpenISpeedshop	IgProf(Memory)	CPU	MEM

OpenISpeedShop

Geant4.11.0.r07 SimplifiedCalo

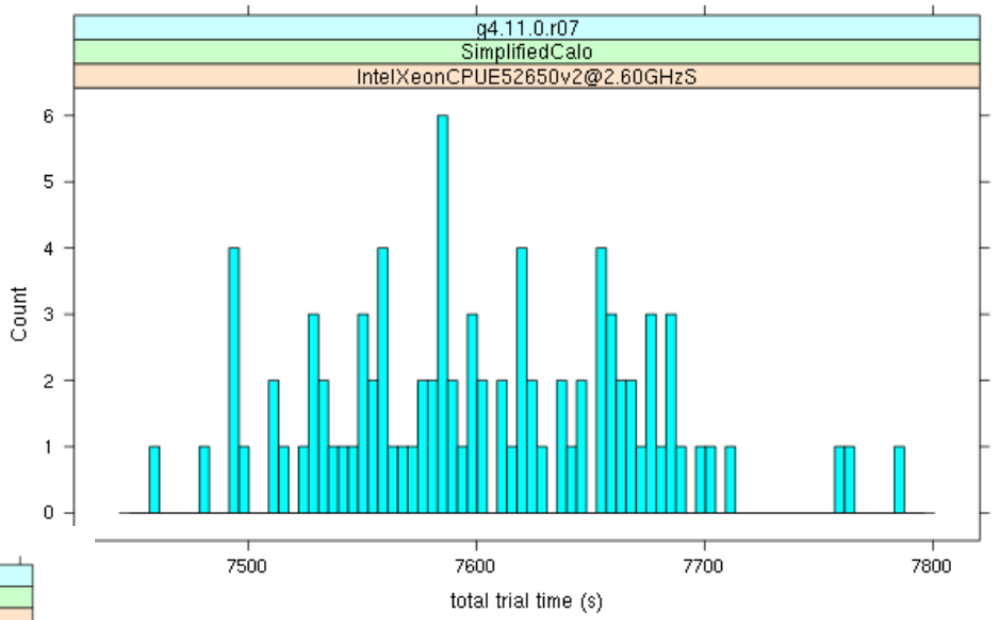
Sample	Physics List	B-Field	Energy
Higgs->ZZ	FTFP_BERT	ON (4.0T)	14 TeV PYTHIA
		OFF (0.0T)	14 TeV PYTHIA
100 MeV e- (5K e-/event)	FTFP_BERT	ON (4.0T)	100 MeV
	Shielding	ON (4.0T)	100 MeV
	Shielding_EMZ	ON (4.0T)	100 MeV
Electrons	FTFP_BERT	ON (4.0T)	1 GeV 5 GeV 10 GeV 50 GeV
		OFF (0 T)	1 GeV 5 GeV 10 GeV 50 GeV
Pions-	FTFP_BERT	ON (4.0T)	1 GeV 5 GeV 10 GeV 50 GeV
		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
	Shielding	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

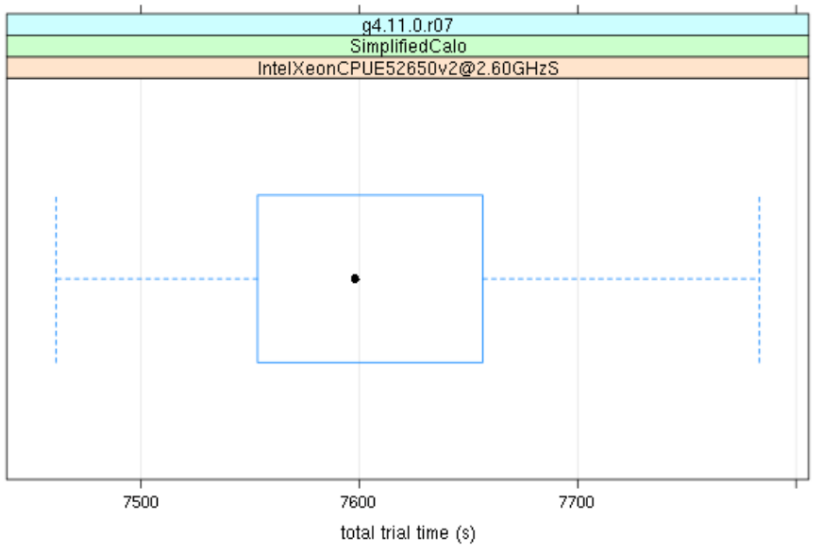
We believe that, in general, we reasonably cover all aspects that can be critical for the Geant4 development.

However, since representatives of various experiments and projects are presenting their vision, we would like to use the opportunity and to inquire if we miss something important.

Measurements are done on statistical basis

Example: CPU estimate e.g. for Higgs input sample processed through SimplifiedCalo geometry is repeated multiple times which allows to reliably determine mean and error

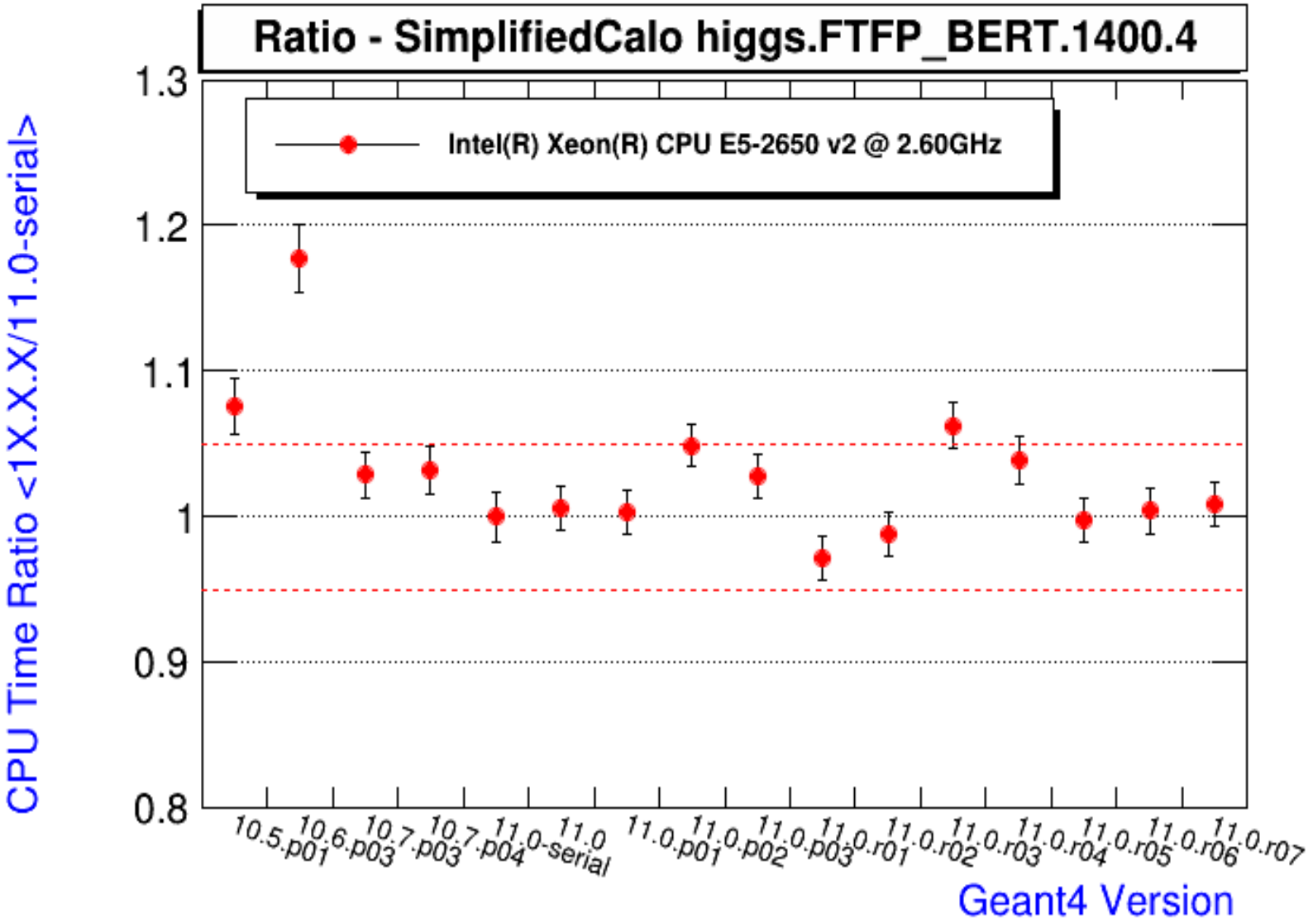




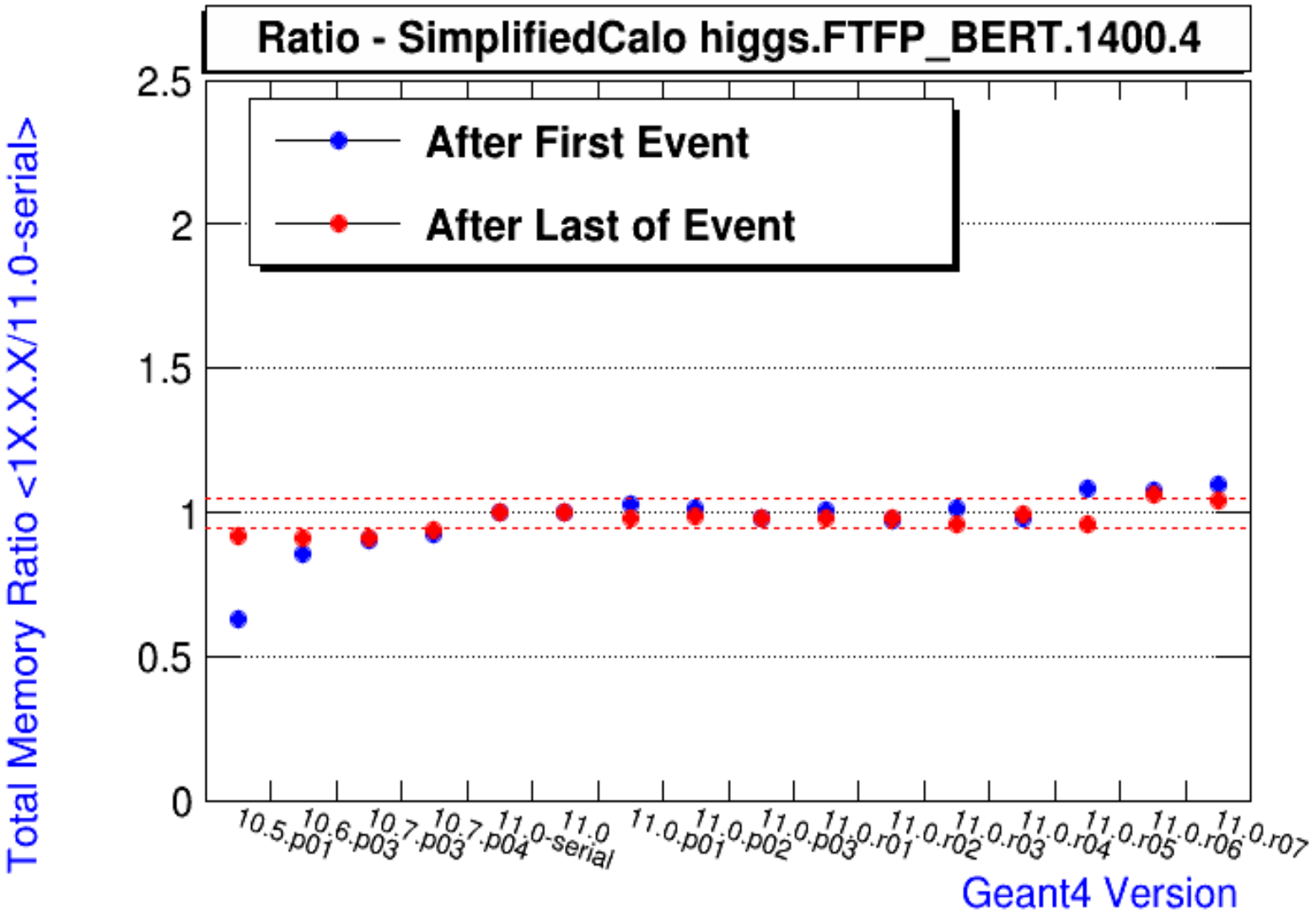
The same measurements are presented as box and whisker plot

Fermilab

CPU Trends in Geant4



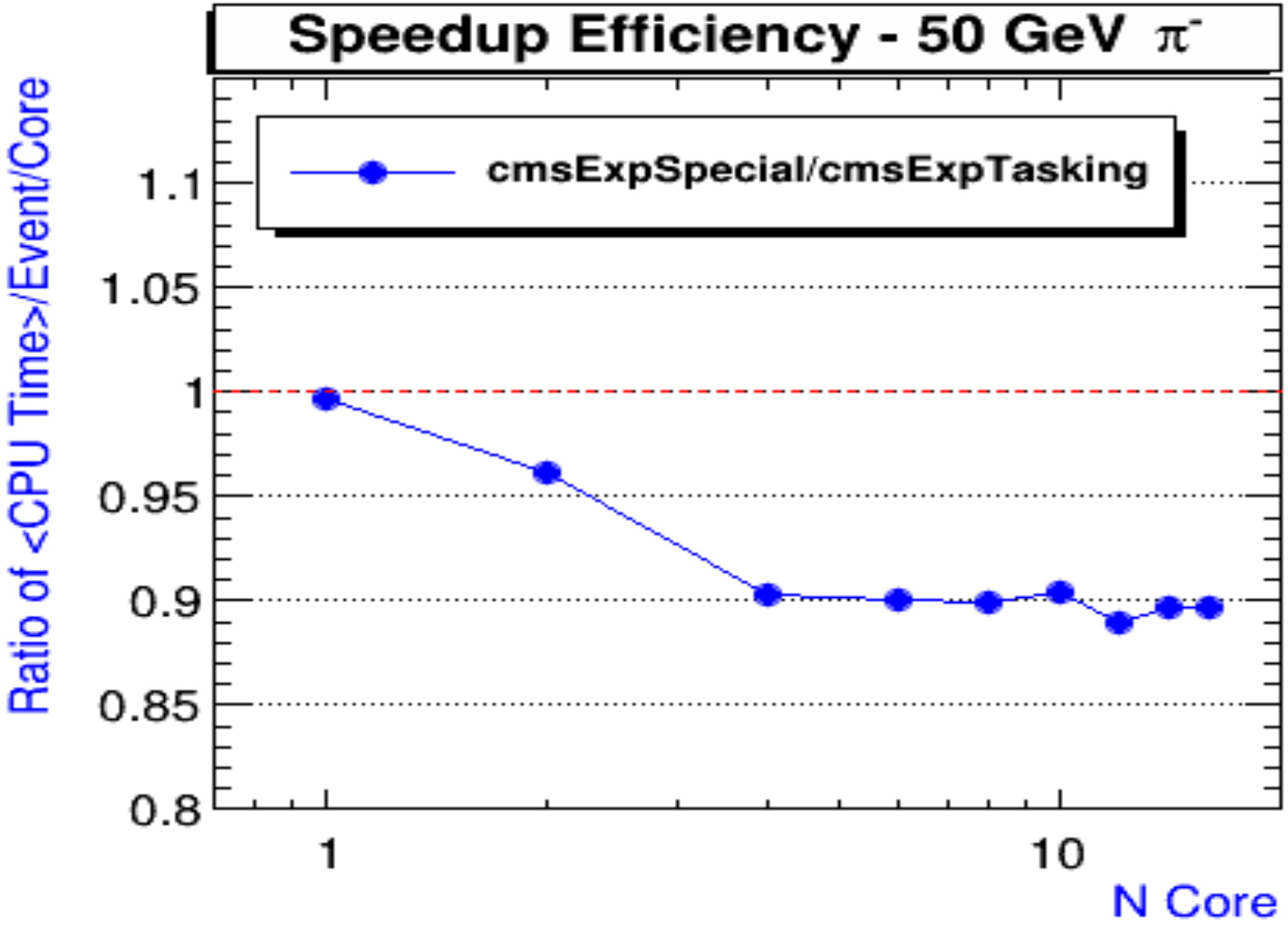
Memory Trends in Geant4



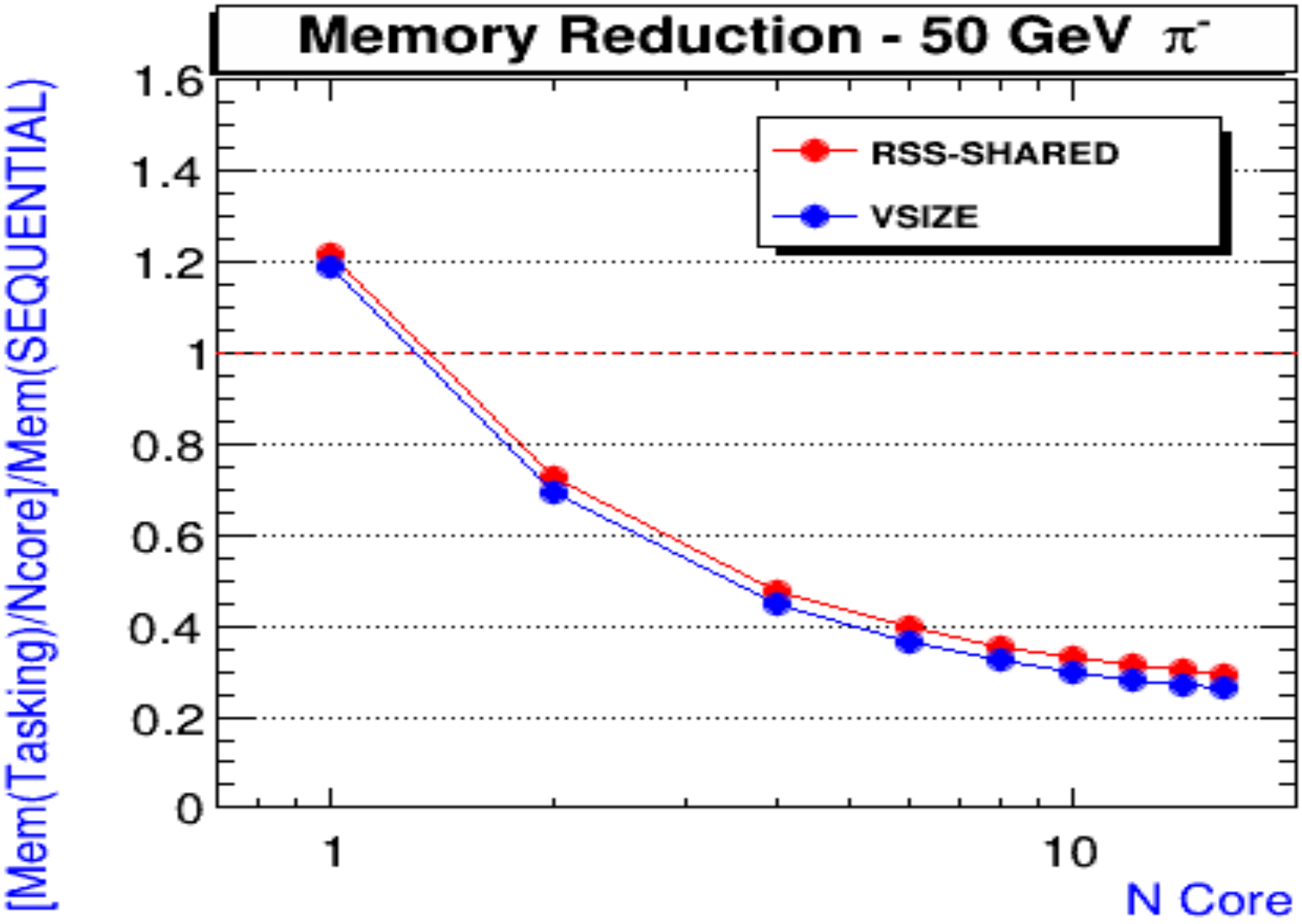
Example of measured physics observables

Particle	Mean	Sigma	Low	1/4Quad	Median	3/4Quad	High
Nstep e-	1.8569e+07	5.6469e+05	1.7141e+07	1.8245e+07	1.8618e+07	1.8936e+07	1.9875e+07
Nstep e+	2.5147e+06	1.2314e+05	2.2458e+06	2.4346e+06	2.5196e+06	2.5824e+06	2.8240e+06
Nstep gamma	1.7717e+07	4.9999e+05	1.6436e+07	1.7396e+07	1.7780e+07	1.8057e+07	1.8863e+07
Nstep N	7.8831e+06	7.8890e+05	5.7678e+06	7.5095e+06	7.9879e+06	8.3231e+06	9.4254e+06
Nstep other	4.1847e+05	4.2988e+04	3.0033e+05	3.9716e+05	4.2341e+05	4.4328e+05	5.1027e+05
Nstep p	3.3610e+05	3.4225e+04	2.4258e+05	3.2064e+05	3.4072e+05	3.5593e+05	4.0348e+05
Nstep pi-	4.1075e+04	4.4140e+03	2.9226e+04	3.8642e+04	4.1185e+04	4.3945e+04	4.9739e+04
Nstep pi+	4.3246e+04	4.5117e+03	3.1411e+04	4.0238e+04	4.3112e+04	4.6420e+04	5.2571e+04
Ntrack e-	1.4559e+07	4.0663e+05	1.3511e+07	1.4299e+07	1.4611e+07	1.4833e+07	1.5480e+07
Ntrack e+	3.5197e+05	1.4352e+04	3.1892e+05	3.4314e+05	3.5198e+05	3.6028e+05	3.8750e+05
Ntrack gamma	4.5273e+06	1.4461e+05	4.1678e+06	4.4461e+06	4.5372e+06	4.6204e+06	4.8670e+06
Ntrack N	1.8784e+05	1.8999e+04	1.3645e+05	1.7857e+05	1.9028e+05	1.9880e+05	2.2425e+05
Ntrack other	2.5500e+05	2.5516e+04	1.8528e+05	2.4264e+05	2.5799e+05	2.6958e+05	3.0444e+05
Ntrack p	1.0702e+05	1.0786e+04	7.7724e+04	1.0201e+05	1.0844e+05	1.1345e+05	1.2806e+05
Ntrack pi-	2.9245e+03	3.0692e+02	2.1110e+03	2.7850e+03	2.9455e+03	3.1270e+03	3.5370e+03
Ntrack pi+	3.1984e+03	3.3022e+02	2.3200e+03	3.0460e+03	3.1990e+03	3.4060e+03	3.8690e+03

CPU/Event : Geant4-Serial over Geant4-Tasking



Memory/Core : Geant4-Tasking over Geant4-Serial



Summary

- Performed CPU and memory profiling for development and public releases, and for specific candidates (dev. tags)
  - Measurements are done on substantial statistical basis
- Reported results to the working group leaders
- Regularly presented (S.Y. Jun) results and issues of computing performance at the Steering Board meetings
- Planned migration to gcc11 (or perhaps gcc12) is in progress
- Many thanks to the FNAL HPC team for support !

BACKUP SLIDES

https://g4cpt.fnal.gov/g4p/oss_11.0.r07_SimplifiedCalo_01/compare_vs_11.0.r06.html

Table-A) Average (CPU Time)/Event: 11.0.r07 vs 11.0.r06

110r06 mean	110r06 error	110r07 mean	110r07 error	100*(r07-r06)/r06 %diff	100*(r07-r06)/r06 error	sample
151.3000	1.5770	152.0600	1.3503	0.5	1.4	higgs.FTFP_BERT.1400.4
123.2800	1.4663	122.0400	1.0771	-1.0	1.5	higgs.FTFP_BERT.1400.0
8.6447	0.1005	8.7619	0.0750	1.4	1.5	e-100MeV.FTFP_BERT.100MeV.4
18.4150	0.2004	19.0110	0.1714	3.2	1.5	e-100MeV.Shielding.100MeV.4
52.3860	0.7493	55.2150	0.6686	5.4	2.0	e-100MeV.Shielding_EMZ.100MeV.4
0.0078	0.0001	0.0078	0.0001	0.0	1.8	e-.FTFP_BERT.1.0
0.0392	0.0005	0.0388	0.0004	-1.0	1.6	e-.FTFP_BERT.5.0
0.0779	0.0010	0.0777	0.0010	-0.3	1.8	e-.FTFP_BERT.10.0
0.3834	0.0053	0.3811	0.0040	-0.6	1.7	e-.FTFP_BERT.50.0
0.0102	0.0001	0.0103	0.0001	1.0	1.4	e-.FTFP_BERT.1.4
0.0510	0.0007	0.0520	0.0005	2.0	1.7	e-.FTFP_BERT.5.4
0.1027	0.0015	0.1033	0.0012	0.6	1.9	e-.FTFP_BERT.10.4
0.5040	0.0066	0.5111	0.0047	1.4	1.6	e-.FTFP_BERT.50.4
0.0144	0.0002	0.0143	0.0002	-0.7	2.0	pi-.FTFP_BERT.1.0
0.0575	0.0007	0.0567	0.0007	-1.4	1.7	pi-.FTFP_BERT.5.0
0.1071	0.0013	0.1062	0.0012	-0.8	1.6	pi-.FTFP_BERT.10.0
0.4891	0.0053	0.4854	0.0054	-0.8	1.5	pi-.FTFP_BERT.50.0
0.0162	0.0002	0.0161	0.0002	-0.6	1.7	pi-.FTFP_BERT.1.4
0.0654	0.0007	0.0655	0.0008	0.2	1.6	pi-.FTFP_BERT.5.4
0.1242	0.0014	0.1250	0.0015	0.6	1.7	pi-.FTFP_BERT.10.4
0.5765	0.0055	0.5812	0.0067	0.8	1.5	pi-.FTFP_BERT.50.4
0.0162	0.0002	0.0161	0.0002	-0.6	1.7	pi-.QGSP_BERT.1.4
0.0654	0.0008	0.0659	0.0008	0.8	1.7	pi-.QGSP_BERT.5.4
0.1243	0.0013	0.1253	0.0014	0.8	1.5	pi-.QGSP_BERT.10.4
0.5744	0.0068	0.5806	0.0058	1.1	1.6	pi-.QGSP_BERT.50.4
0.0149	0.0001	0.0149	0.0001	0.0	0.9	pi-.QGSP_BIC.1.4
0.0625	0.0007	0.0630	0.0005	0.8	1.4	pi-.QGSP_BIC.5.4
0.1184	0.0012	0.1203	0.0010	1.6	1.3	pi-.QGSP_BIC.10.4
0.5601	0.0051	0.5630	0.0043	0.5	1.2	pi-.QGSP_BIC.50.4
0.0364	0.0005	0.0365	0.0004	0.3	1.8	anti_proton.FTFP_BERT.1.4
0.0867	0.0009	0.0869	0.0011	0.2	1.6	anti_proton.FTFP_BERT.5.4
0.1480	0.0016	0.1474	0.0017	-0.4	1.6	anti_proton.FTFP_BERT.10.4
0.6056	0.0066	0.6099	0.0071	0.7	1.6	anti_proton.FTFP_BERT.50.4
0.0109	0.0001	0.0108	0.0001	-0.9	1.3	proton.FTFP_BERT.1.4
0.0649	0.0007	0.0646	0.0009	-0.5	1.8	proton.FTFP_BERT.5.4
0.1277	0.0014	0.1276	0.0016	-0.1	1.7	proton.FTFP_BERT.10.4
0.5920	0.0060	0.5936	0.0059	0.3	1.4	proton.FTFP_BERT.50.4
0.0625	0.0006	0.0620	0.0005	-0.8	1.2	pi-.FTFP_INCLXX.1.4
0.2136	0.0017	0.2132	0.0017	-0.2	1.1	pi-.FTFP_INCLXX.5.4
0.3832	0.0027	0.3877	0.0031	1.2	1.1	pi-.FTFP_INCLXX.10.4
0.5461	0.0040	0.5495	0.0046	0.6	1.1	pi-.FTFP_INCLXX.15.4
0.0500	0.0004	0.0495	0.0004	-1.0	1.1	proton.FTFP_INCLXX.1.4
0.2425	0.0018	0.2417	0.0021	-0.3	1.1	proton.FTFP_INCLXX.5.4
0.4354	0.0029	0.4398	0.0037	1.0	1.1	proton.FTFP_INCLXX.10.4
0.6188	0.0053	0.6195	0.0055	0.1	1.2	proton.FTFP_INCLXX.15.4
0.0774	0.0005	0.0767	0.0005	-0.9	0.9	proton.FTFP_BERT_HP.1.4
0.4146	0.0030	0.4162	0.0029	0.4	1.0	proton.FTFP_BERT_HP.5.4
0.0775	0.0006	0.0771	0.0004	-0.5	0.9	proton.Shielding.1.4
0.4198	0.0030	0.4201	0.0029	0.1	1.0	proton.Shielding.5.4
0.0837	0.0013	0.0865	0.0012	3.3	2.2	gamma.FTFP_BERT_EMZ_AugerOff.250MeV
0.1192	0.0015	0.1240	0.0012	4.0	1.7	gamma.FTFP_BERT_EMZ_AugerOn.250MeV.
0.0325	0.0004	0.0337	0.0005	3.7	2.0	gamma.FTFP_BERT_EMZ_AugerOff.1.0
0.0466	0.0006	0.0486	0.0006	4.3	1.9	gamma.FTFP_BERT_EMZ_AugerOn.1.0

Table-B) Total Memory : 11.0.r07 vs 11.0.r06

total 110r06	memory 110r07	100*(r07-r06)/r06 %diff	sample
4719.1100	4640.1700	-1.7	higgs.FTFP_BERT.1400.4
4587.6500	4626.4400	0.8	higgs.FTFP_BERT.1400.0
191.4890	190.5440	-0.5	e-100MeV.FTFP_BERT.100MeV.4
54087.4000	54107.1000	0.0	e-100MeV.Shielding.100MeV.4
95751.5000	97628.0000	2.0	e-100MeV.Shielding_EMZ.100MeV.4
121.8600	120.7960	-0.9	e-.FTFP_BERT.1.0
122.7260	121.6060	-0.9	e-.FTFP_BERT.5.0
123.6020	122.5730	-0.8	e-.FTFP_BERT.10.0
131.3000	130.1160	-0.9	e-.FTFP_BERT.50.0
121.8860	120.8500	-0.8	e-.FTFP_BERT.1.4
122.7360	121.5930	-0.9	e-.FTFP_BERT.5.4
123.6590	122.6520	-0.8	e-.FTFP_BERT.10.4
131.4030	130.2080	-0.9	e-.FTFP_BERT.50.4
142.5090	140.8780	-1.1	pi-.FTFP_BERT.1.0
194.9840	193.9760	-0.5	pi-.FTFP_BERT.5.0
246.4290	239.3110	-2.9	pi-.FTFP_BERT.10.0
611.1280	624.9220	2.3	pi-.FTFP_BERT.50.0
141.3870	138.6280	-2.0	pi-.FTFP_BERT.1.4
195.2590	197.0960	0.9	pi-.FTFP_BERT.5.4
242.9770	241.1800	-0.7	pi-.FTFP_BERT.10.4
601.2970	611.0500	1.6	pi-.FTFP_BERT.50.4
141.7670	138.9620	-2.0	pi-.QGSP_BERT.1.4
195.5530	197.2900	0.9	pi-.QGSP_BERT.5.4
243.1740	241.3390	-0.8	pi-.QGSP_BERT.10.4
667.5310	651.4240	-2.4	pi-.QGSP_BERT.50.4
894.4340	894.9720	0.1	pi-.QGSP_BIC.1.4
2807.7200	2870.0000	2.2	pi-.QGSP_BIC.5.4
4536.8400	4679.1400	3.1	pi-.QGSP_BIC.10.4
16957.5000	16381.7000	-3.4	pi-.QGSP_BIC.50.4
163.1320	162.2880	-0.5	anti_proton.FTFP_BERT.1.4
218.9500	216.4100	-1.2	anti_proton.FTFP_BERT.5.4
279.8730	277.3670	-0.9	anti_proton.FTFP_BERT.10.4
705.0410	677.7160	-3.9	anti_proton.FTFP_BERT.50.4
138.4860	136.9830	-1.1	proton.FTFP_BERT.1.4
212.2610	213.7970	0.7	proton.FTFP_BERT.5.4
288.2930	276.9860	-3.9	proton.FTFP_BERT.10.4
714.5540	708.6620	-0.8	proton.FTFP_BERT.50.4
2184.4800	2257.6100	3.3	pi-.FTFP_INCLXX.1.4
6874.5300	6834.5500	-0.6	pi-.FTFP_INCLXX.5.4
12070.6000	12032.3000	-0.3	pi-.FTFP_INCLXX.10.4
17169.7000	16719.2000	-2.6	pi-.FTFP_INCLXX.15.4
1831.3700	1785.4100	-2.5	proton.FTFP_INCLXX.1.4
8181.4700	8072.0100	-1.3	proton.FTFP_INCLXX.5.4
14220.8000	14211.3000	-0.1	proton.FTFP_INCLXX.10.4
19675.6000	19705.4000	0.2	proton.FTFP_INCLXX.15.4
12874.8000	12890.5000	0.1	proton.FTFP_BERT_HP.1.4
20982.8000	21045.9000	0.3	proton.FTFP_BERT_HP.5.4
12870.9000	12875.2000	0.0	proton.Shielding.1.4
21022.0000	21041.4000	0.1	proton.Shielding.5.4
436.9390	439.9940	0.7	gamma.FTFP_BERT_EMZ_AugerOff.250MeV.0
717.3790	726.0590	1.2	gamma.FTFP_BERT_EMZ_AugerOn.250MeV.0
971.3680	990.1740	1.9	gamma.FTFP_BERT_EMZ_AugerOff.1.0
2101.0900	2136.1600	1.7	gamma.FTFP_BERT_EMZ_AugerOn.1.0