Gaussian G03 Scaling Benchmarks

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Systems:

Clusters	CPUs/node	RAM/node	OS	Interconnect
Bull	4 (quad core), Opteron @ 2.4 GHz	32.0 GB	HP Linux XC 3.1	Quadrics Elan4
Narwhal	4 (2 dual-core), Opteron @ 2.2 GHz	8.0 GB	HP Linux XC 3.1	Myrinet 2g (gm)
Saw	8 (2 quad-core), Xeon @ 3.0 GHz	16.0 GB	HP Linux XC4	InfiniBand

Molecules and Methods/Models:

	Molecule\Module	B3LYP	MP2	CISD	CCSD
		Opt + Freq	Opt + Freq	Opt + Freq	Opt +Freq
I	**C4H14Cl2P2Pd** (test job 445)	BS on card	BS on card		
II	**C10H10**	6-311g(2df,p)	6-311g		
III	**CH3OH** (test job 58)			6-31g*, 6-311g*, 6-311g(2df,p)	
IV	**CH3CH2** (test job 684)				6-31g*, 6-311g*

Notes:
Molecule-I is a reasonable size for scaling tests.
Molecule-II is a smaller molecule, which may not be good for scaling tests, however, it reproduced the same trend as for molecule-I.

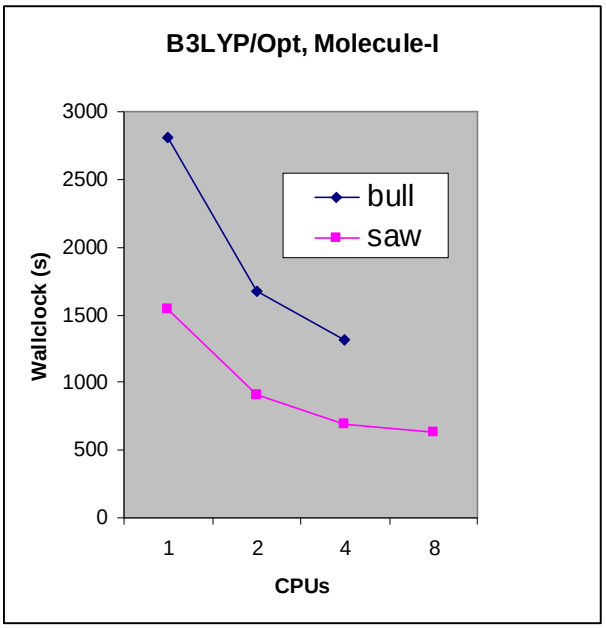
Gaussian versions:

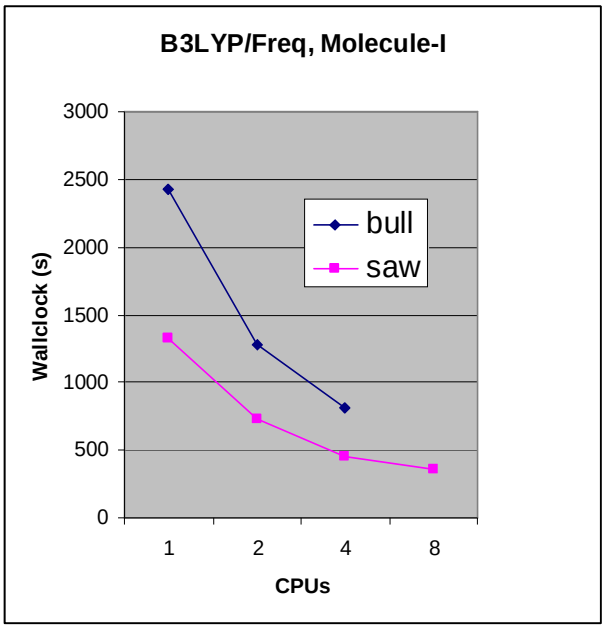
G03 versions		
C.02 (C.02-b)	Binary from Gaussian Inc	
D.01 (D.01-s)	Compiled from source on XC cluster	
E.01 (-b, -s)	E.01-b, x86_64 Linux binary from Gaussian Inc	E.01-s compiled (amd64 on bull, em64t on saw) from source

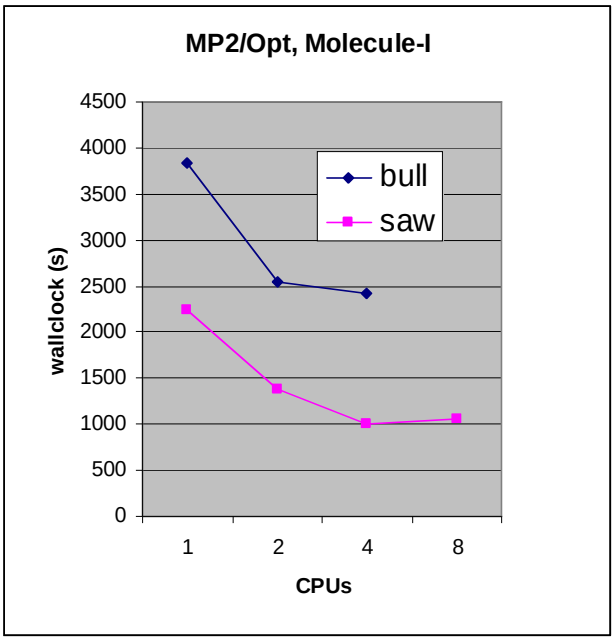
Target goals:

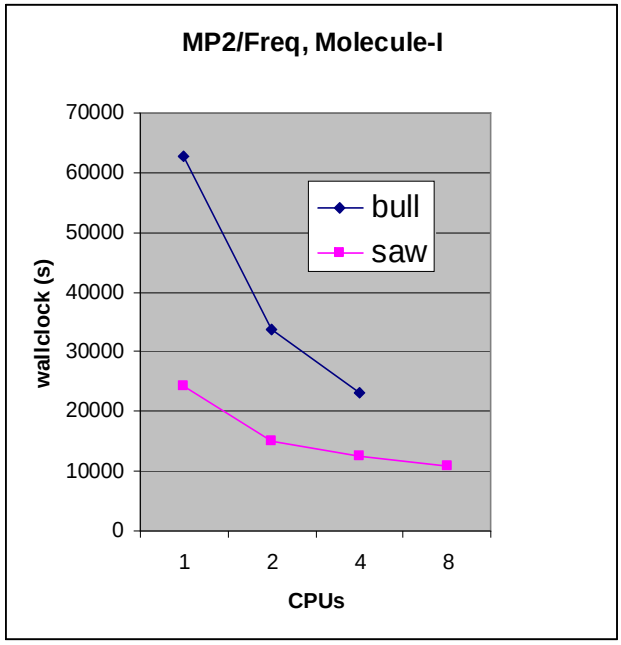
[1] scaling results for typical models/methods in Gaussian 03
[2] clusters (bull, saw, narwhal) performance comparison: same G03 version E.01
[3] g03 version comparison: G03-C.02, G03-D.01, G03-E.01, and binary vs. source

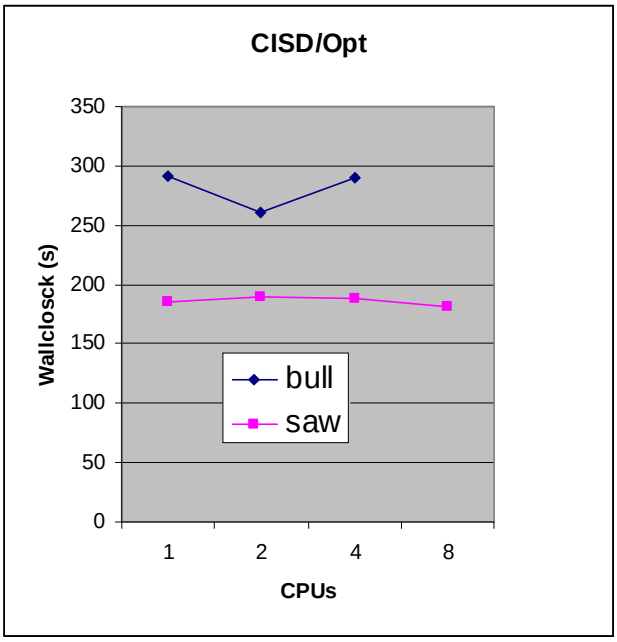
Results in graphics (scaling, bull and saw)

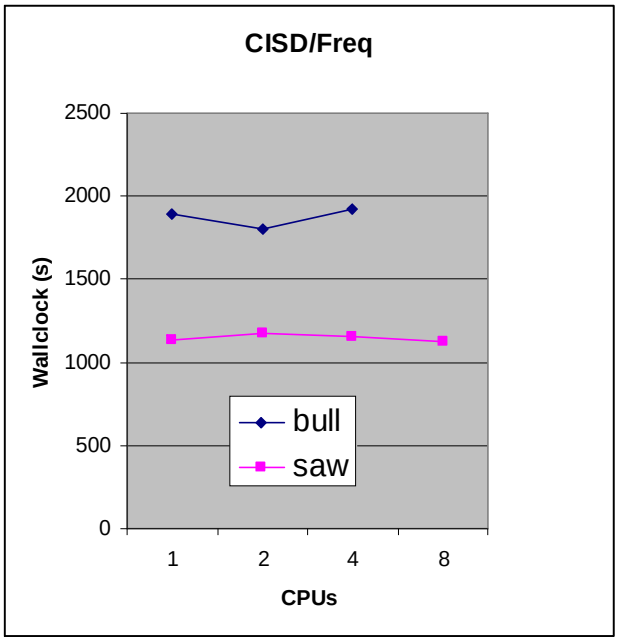


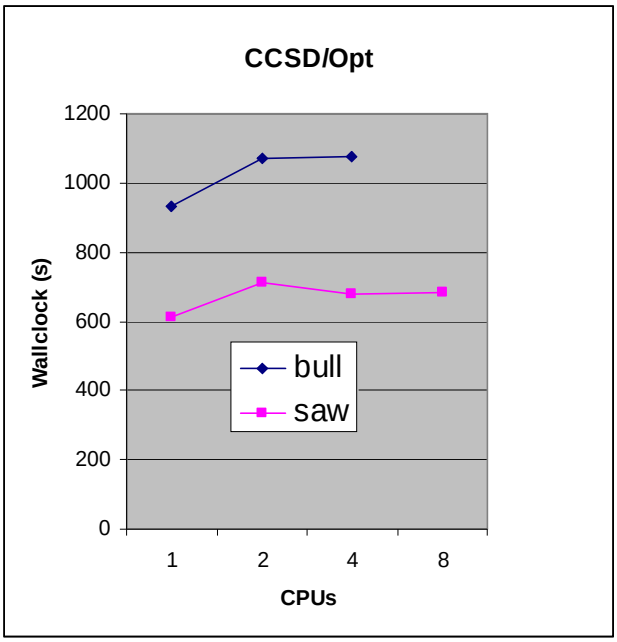


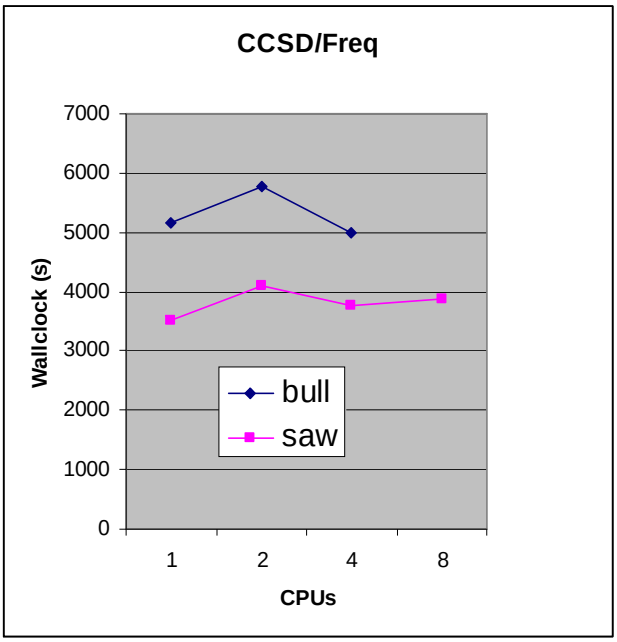












General conclusions:

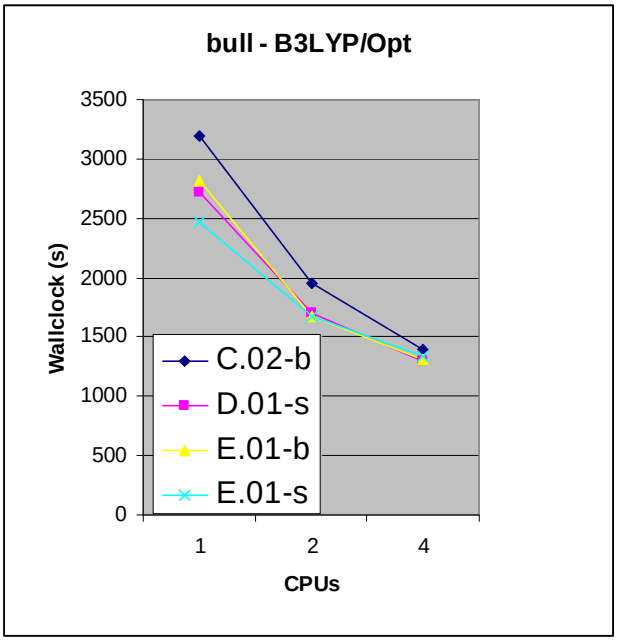
[1] No. of CPUs recommended to use for a Gaussian-03 job

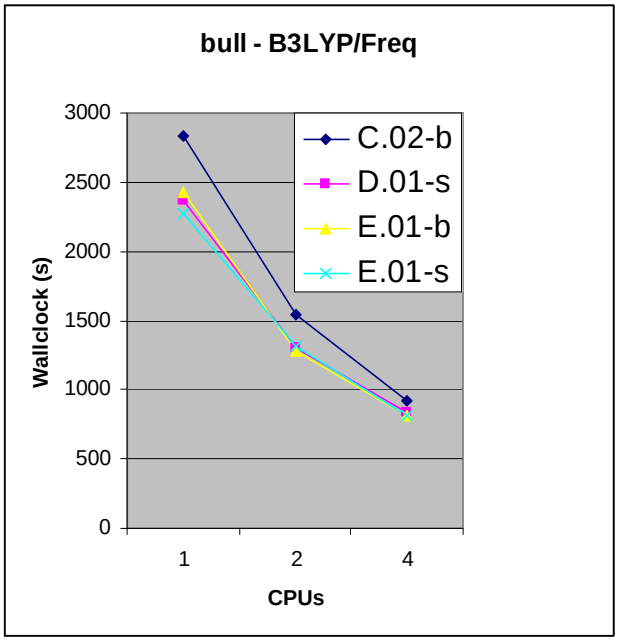
Methods/Modules	**Opt**	**Freq**	**Energy**
HF	4	4	4
DFT (B3LYP, etc)	4	4	4
MP(2, 3, 4)	4	4	4
CISD (cis, cid, cisd, qcisd)	1	1	1
CCSD (ccd, ccsd, ccsd(t))	1	1	1

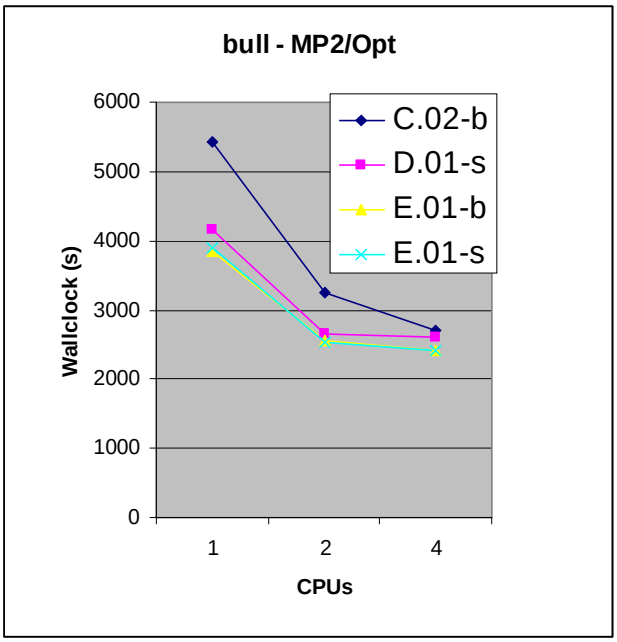
Some other methods such as **Oniom, G2, G3** are a combination of HF, MP2 and CISD (QCISD), the scale will be somewhere between 1-4.

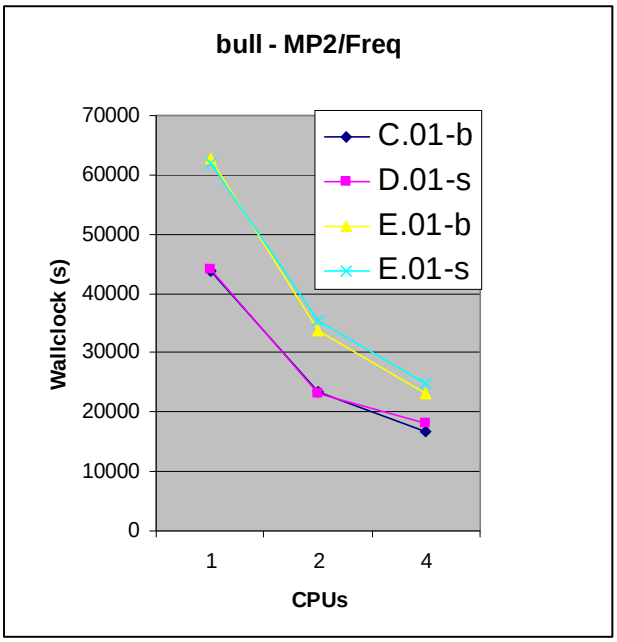
[2] **saw** is 50%-100% faster than **bull** for G03 jobs.

Results in graphics (bull for diff. G03 versions)





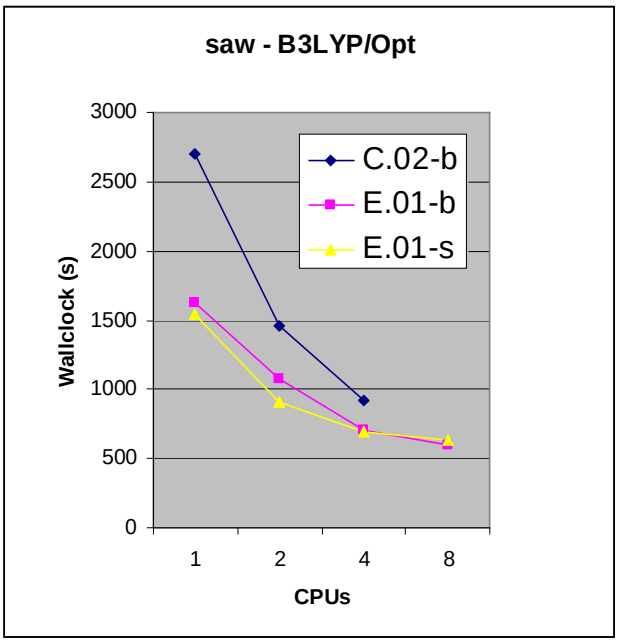


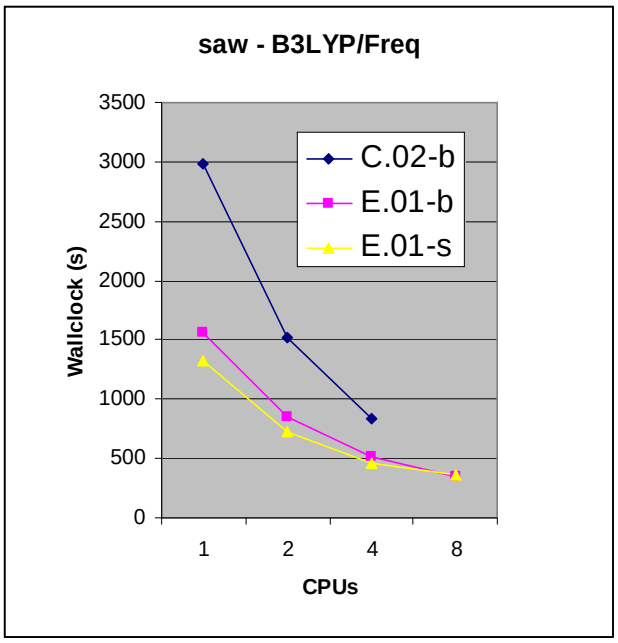


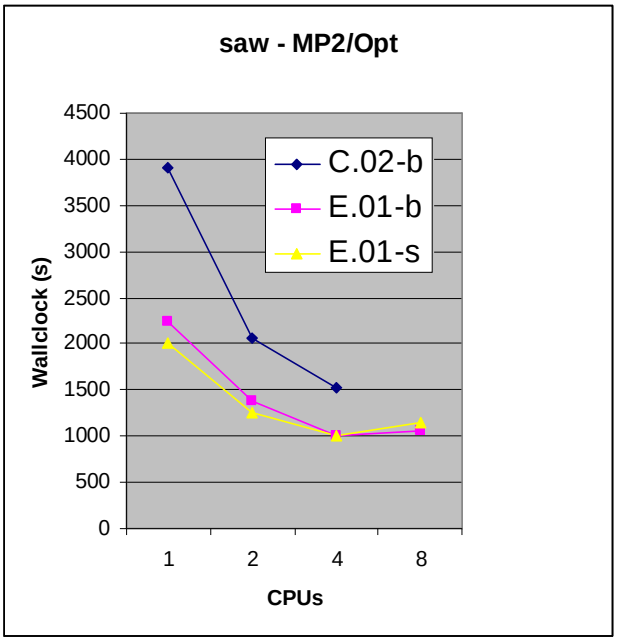
Conclusions:

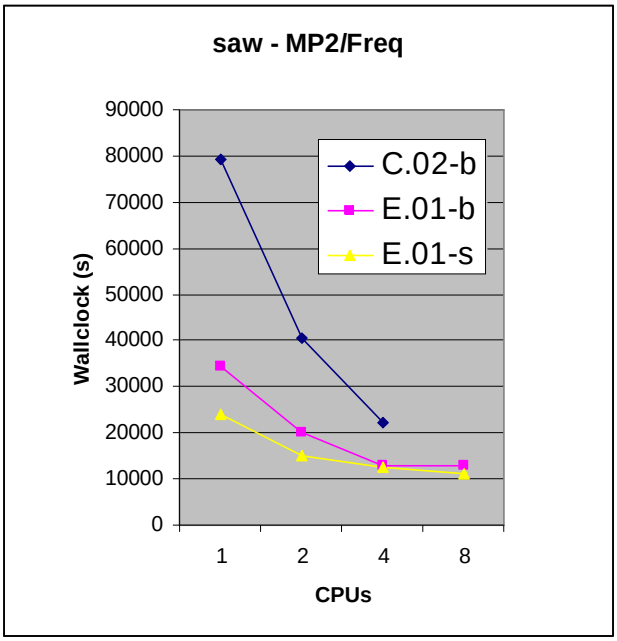
[1] All G03 versions have good scaling to 4 CPUs.
[2] Compiled code has very similar, or a bit better, performance than the binary versions.
[3] Newer versions have better performance than the older one except for MP2/Freq where G03-E.01 has worse performance. The same results have been reproduced on narwhal but not on saw. It's a bit odd for the AMD Opteron servers (either quad-core or dual-core).

Results in graphics (saw for diff. G03 versions)





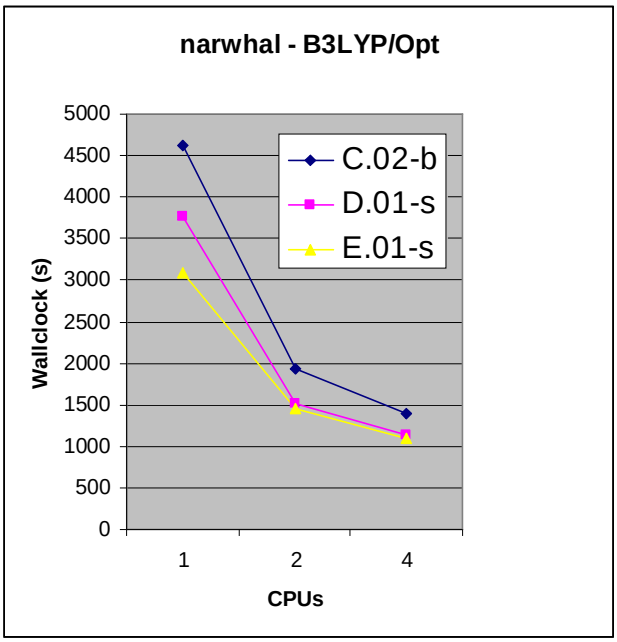


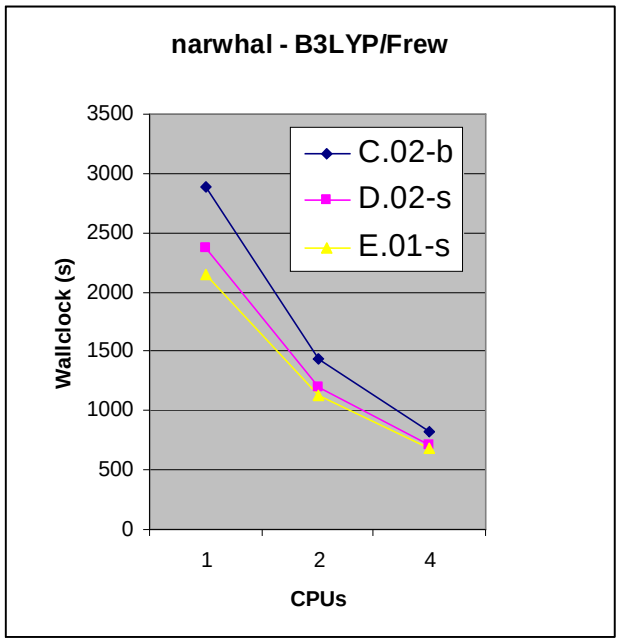


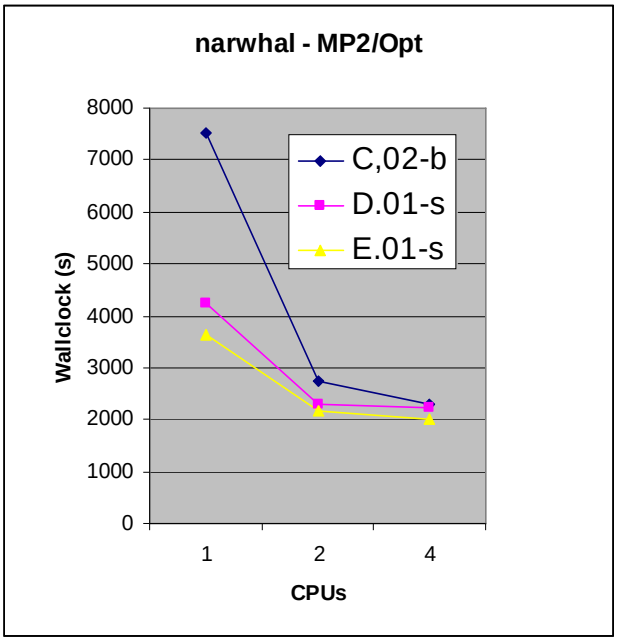
Conclusions:

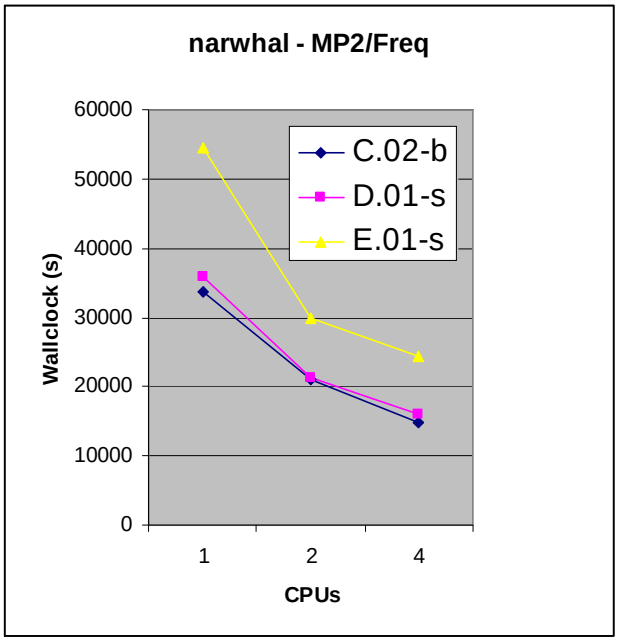
[1] All G03 versions have good scaling to 4 CPUs, very small speedup from 4 to 8 CPUs.
[2] Compiled code has very similar, or a bit better, performance than the binary versions.
[3] Newer versions have better performance than the older one, no exceptions for MP2/Freq in G03-E.01, as observed on bull and narwhal.

Results in graphics (narwhal for diff. G03 versions)









Conclusions:

[1] All G03 versions have good scaling to 4 CPUs.
[2] The same results as obtained on bull, i.e., the G03-E.01 has worse performance for MP2/Freq.

Results: **scaling results, cluster performance comparison**
Version: G03-E.01, Molecule - I

B3LYP / Opt

	bull		saw		bull/saw	narwhal	
	Runtime(s)	**speedup**			**speedup**		
1	2810 (46m50s)	1	1537 (25m37s)	1	1.83	3097 (51m37s)	1
2	1672 (27m52s)	1.68	914 (15m14s)	1.68	1.83	1451 (24m11s)	2.13
4	1314 (21m54s)	2.14	697 (11m37s)	2.21	1.89	1092 (18m12)	2.84
8			631 (10m31s)	2.44			

B3LYP / Freq

	bull		saw		bull/saw	narwhal	
	Runtime(s)	**speedup**			**speedup**		
1	2427 (40m27s)	1	1323 (22m3s)	1	1.83	2144 (35m44s)	1
2	1273 (21m13s)	1.91	731 (12m11s)	1.81	1.74	1125 (18m45s)	1.91
4	816 (13m36s)	2.97	460 (7m40s)	2.88	1.77	683 (11m23s)	3.14
8			362 (6m2s)	3.65			

MP2 / Opt

	bull		saw		bull/saw	narwhal	
	Runtime(s)	**speedup**			**speedup**		
1	3840 (1h4m)	1	2246 (37m26s)	1	1.71	3629 (1h29s)	1
2	2554 (42m34s)	1.50	1377 (22m57s)	1.63	1.85	2157 (35m57s)	1.68
4	2418 (40m18s)	1.59	997 (16m37s)	2.25	2.43	2006 (33m26s)	1.81
8			1051 (17m31s)	2.14			

MP2 / Freq

	bull		saw		bull/saw	narwhal	
	Runtime(s)	**speedup**			**speedup**		
1	62687 (17h24m47s)	1	24171 (6h42m51s)	1	2.59	54521 (15h8m41s)	1
2	33687 (9h21m27s)	1.86	15010 (4h10m10s)	1.61	2.24	29931 (8h18m51s)	1.82
4	23233 (6h27m13s)	2.70	12548 (3h29m8s)	1.93	1.85	24402 (6h46m42s)	2.23
8			10997 (3h3m17s)	2.20			

Results: cluster performance comparison
Version: G03-E.01, Molecule - II

B3LYP / Opt

	bull		**saw**		**bull/saw**	**narwhal**	
	Runtime(s)	**speedup**			speedup		
1	3446 (57m26s)	1	1592 (26m32s)	1	2.16	3222 (53m42s)	1
2	2115 (35m15s)	1.63	896 (14m56s)	1.78	2.36	1779 (29m39s)	1.81
4	1308 (21m48s)	2.63	566 (9m26s)	2.81	2.31	1129 (18m49s)	2.85
8			704 (11m44s)	2.26			

B3LYP / Freq

	bull		**saw**		**bull/saw**	**narwhal**	
	Runtime(s)	**speedup**			**speedup**		
1	7056 (1h57m36s)	1	3229 (53m49s)	1	2.19	6349 (1h45m49s)	1
2	3969 (1h6m9s)	1.78	1659 (27m39s)	1.95	2.39	3355 (55m55s)	1.89
4	2419 (40m19s)	2.92	942 (15m42s)	3.43	2.57	2096 (34m56s)	3.03
8			877 (14m37s)	3.68			

MP2 / Opt

	bull		**saw**		**bull/saw**	**narwhal**	
	Runtime(s)	**speedup**			**speedup**		
1	651 (10m51s)	1	360 (6m)	1	1.81	446 (7m26s)	1
2	510 (8m30s)	1.28	278 (4m38s)	1.30	1.83	408 (6m48s)	1.09
4	501 (8m21s)	1.30	256 (4m16s)	1.41	1.96	386 (6m26s)	1.16
8			276 (4m36s)	1.30			

MP2 / Freq

	bull		**saw**		**bull/saw**	**narwhal**	
	Runtime(s)	**speedup**			**speedup**		
1	6247 (1h44m7s)	1	3266 (54m26s)	1	1.91	5170 (1h26m10s)	1
2	4111 (1h8m31s)	1.52	2092 (34m52s)	1.56	1.97	3600 (1h)	1.44
4	3443 (57m23s)	1.81	1720 (28m40s)	1.90	2.0	2883 (48m3s)	1.79
8			1626 (27m6s)	2.01			

Results: CISD

Version: G03-E.01, Molecule-III

Cluster: bull, Basis sets: 6-311g*

	OPT		**bull/saw**	**Freq**		**bull/saw**
	Runtimes(s)	**speedup**	**speedup**			**speedup**
1	291 (4m51s)	1	1.57	1891 (31m31s)	1	1.66
2	261 (4m21s)	1.11	1.40	1806 (30m6s)	1.05	1.54
4	290 (4m50s)	1.0	1.54	1927 (32m7s)	0.98	1.66

Cluster: saw

	Opt+Freq		**Opt**		**Freq**		**Opt**		**Freq**	
	6-31g*		**6-311g***		**6-311g***		**6-311g(2df,p)**		**6-311g(2df,p)**	
	Run time	Speed up								
1	18m46s	1	3m5s	1	1136 (18m56s)	1	626 (10m26s)	1	5303 (1h28m23s)	1
2	18m43s	1	3m9s	1	1171 (19m31s)	0.97	507 (8m27s)	1.23	3732 (1h2m12s)	1.42
4	18m43s	1	3m8s	1	1159 (19m19s)	0.98	762 (12m42s)	0.82	5504 (1h31m44s)	0.96
8	18m48s	1	3m1s	1	1124 (18m44s)	1.01	780 (13m)	0.80	5220 (1h27m)	1.02

Results: CCSD

Version: G03-E.01, Molecule-IV

Cluster: bull, 6-311g*

	OPT		**bull/saw**	**Freq**		**bull/saw**
	Runtimes(s)	**speedup**	**speedup**			**speedup**
1	934 (15m34s)	1	1.53	5147 (1h25m47s)	1	1.46
2	1071 (17m51s)	0.87	1.50	5768 (1h36m8s)	0.89	1.41
4	1078 (17m58s)	0.87	1.58	4980 (1h23m)	1.03	1.32

Cluster: saw

	Opt+Freq		**Opt**		**Freq**	
	6-31g*		**6-311g***		**6-311g***	
	Run time	**Speed up**				
1	34m45s	1	610 (10m10s)	1	3518 (58m38s)	1
2	34m16s	1	711 (11m51s)	0.86	4096 (1h8m16s)	0.86
4	34m11s	1	681 (11m21s)	0.90	3759 (1h2m39s)	0.94
8	failed	1	682 (11m22s)	0.89	3864 (1h4m24s)	0.91

Results: version comparison (C.02, D.01, E.01), clusters: bull, saw, narwhal

Cluster: bull, Molecule - I

B3LYP / opt

	C.02-b		**D.01-s**		**E-01-b**		**E-01-s**	
	Runtime(s)	**speedup**						
1	3199 (53m19s)	1	2722 (45m22s)	1	2810 (46m50s)	1	2469 (41m9s)	1
2	1952 (32m32s)	1.64	1697 (28m17s)	1.60	1672 (27m52s)	1.68	1674 (27m54s)	1.48
4	1397 (23m17s)	2.29	1292 (21m32s)	2.11	1314 (21m54s)	2.14	1338 (22m18s)	1.85

B3LYP / freq

	C.02-b		**D.01-s**		**E-01-b**		**E-01-s**	
	Runtime(s)	**speedup**						
1	2827 (47m7s)	1	2367 (39m27s)	1	2427 (40m27s)	1	2276 (37m56s)	1
2	1540 (25m40s)	1.84	1297 (21m37s)	1.82	1273 (21m13s)	1.91	1310 (21m50s)	1.74
4	917 (15m17s)	3.08	838 (13m58s)	2.82	816 (13m36s)	2.97	815 (13m35s)	2.79

MP2 / opt

	C.02-b		**D.01-s**		**E.01-b**		**E-01-s**	
	Runtime(s)	**speedup**						
1	5422 (1h30m22s)	1	4151 (1h9m11s)	1	3840 (1h4m)	1	3888 (1h4m48s)	1
2	3254 (54m14s)	1.67	2651 (44m11s)	1.57	2554 (42m34s)	1.50	2539 (42m19s)	1.53
4	2706 (45m6s)	2.00	2616 (43m36s)	1.59	2418 (40m18s)	1.59	2409 (40m9s)	1.66

MP2 / freq

	C.02-b		**D.01-s**		**E.01-b**		**E-01-s**	
	Runtime(s)	**speedup**						
1	43688 (12h8m8s)	1	43962 (12h12m42s)	1	62687 (17h24m47s)	1	61927 (17h12m7s)	1
2	23473 (6h31m13s)	1.86	23110 (6h25m10s)	1.90	33687 (9h21m27s)	1.86	35353 (9h49m13s)	1.75
4	16735 (4h38m55s)	2.61	18000 (5h)	2.44	23233 (6h27m13s)	2.70	24801 (6h53m21s)	2.50

Cluster: bull, Molecule - II

MP2 / opt

	C.02-b		D.01-s		E-01-b		E-01-s	
	Runtime(s)	**speedup**						
1	764 (12m44s)	1	605 (10m5s)	1	651 (10m51s)	1	715 (11m55s)	1
2	539 (8m59s)	1.42	481 (8m1s)	1.26	510 (8m30s)	1.28	512 (8m32s)	1.40
4	466 (7m46s)	1.64	445 (7m25s)	1.40	501 (8m21s)	1.30	488 (8m8s)	1.47

MP2 / freq

	C.02-b		D.01-s		E-01-b		E-01-s	
	Runtime(s)	**speedup**						
1	5184 (1h26m24s)	1	4242 (1h10m42s)	1	6247 (1h44m7s)	1	6650 (1h50m50s)	1
2	3280 (54m40s)	1.58	3032 (50m32s)	1.40	4111 (1h8m31s)	1.52	4325 (1h12m5s)	1.54
4	2867 (47m47s)	1.81	2392 (39m52s)	1.77	3443 (57m23s)	1.81	3476 (57m56s)	1.91

B3LYP / opt (6-311g)

	C.02-b		D.01-s		E-01-b		E-01-s	
	Runtime(s)	**speedup**						
1	353 (5m53s)	1	296 (4m54s)	1	512 (8m32s)	1	399 (6m39s)	1
2	253 (4m13s)	1.40	233 (3m53s)	1.27	240 (4m)	2.13	248 (4m8s)	1.62
4	217 (3m37s)	1.63	207 (3m27s)	1.43	234 (3m54s)	2.19	227 (3m47s)	1.76

B3LYP / freq (6-311g)

	C.02-b		D.01-s		E-01-b		E-01-s	
	Runtime(s)	**speedup**						
1	455 (7m35s)	1	372 (6m12s)	1	409 (6m49s)	1	441 (7m21s)	1
2	264 (4m24s)	1.72	228 (3m48s)	1.63	218 (3m38s)	1.88	286 (4m26s)	1.54
4	182 (3m2s)	2.5	160 (2m40s)	2.33	156 (2m36s)	2.62	168 (2m48s)	2.63

B3LYP, 6-311g(2df,p) –G03-E.01-b

	Opt		Freq	
	Runtime(s)	**speedup**		
1	3446 (57m26s)	1	7056 (1h57m36s)	1
2	2115 (35m15s)	1.63	3969 (1h6m9s)	1.78
4	1308 (21m48s)	2.63	2419 (40m19s)	2.92

Cluster: saw, Molecule - I

B3lyp / opt

	C.02-b		E.01-b		E.01-s	
	Runtime(s)	**speedup**				
1	2700 (45m)	1	1621 (27m1s)	1	1537 (25m37s)	1
2	1463 (24m23s)	1.85	1071 (17m51s)	1.51	914 (15m14s)	1.68
4	920 (15m20s)	2.93	700 (11m40s)	2.32	697 (11m37s)	2.21
8			597 (9m57s)	2.72	631 (10m31s)	2.44

B3LYP / Freq

	C.02-b		E.01-b		E.01-s	
	Runtime(s)	**speedup**				
1	2986 (49m46s)	1	1561 (26m1s)	1	1323 (22m3s)	1
2	1523 (25m23s)	1.93	847 (14m7s)	1.84	731 (12m11s)	1.81
4	840 (14m19s)	3.55	513 (8m33s)	3.04	460 (7m40s)	2.88
8			345 (5m45s)	4.52	362 (6m2s)	3.65

MP2 / opt

	C.02-b		E.01-b		E.01-s	
	Runtime(s)	**speedup**				
1	3903 (1h5m3s)	1	2246 (37m26s)	1	2015 (33m35s)	1
2	2058 (34m18s)	1.90	1377 (22m57s)	1.63	1259 (20m59s)	1.60
4	1523 (25m23s)	2.56	997 (16m37s)	2.25	1012 (16m52s)	1.99
8*			1051 (17m31s)	2.14	1154 (19m14s)	1.75

MP2 / Freq

	C.02-b		E.01-b		E.01-s	
	Runtime(s)	**speedup**				
1	79115 (21h58m35s)	1	34517 (9h35m17s)	1	24171 (6h42m51s)	1
2	40684 (11h18m4s)	1.94	20192 (5h36m32s)	1.71	15010 (4h10m10s)	1.61
4	22239 (6h10m39s)	3.56	13054 (3h37m34s)	2.64	12548 (3h29m8s)	1.93
8*			12849 (3h34m9s)	2.69	10997 (3h3m17s)	2.20

Cluster: saw, Molecule - II

B3LYP – 6-311g(2df,p) /OPT

	C.02-b		E.01-b		E.01-s	
	Runtime(s)	**speedup**				
1	3022 (52m22s)	1	1959 (32m39s)	1	1592 (26m32s)	1
2	1659 (27m39s)	1.82	1125 (18m45s)	1.74	896 (14m56s)	1.78
4	916 (15m16s)	3.3	655 (10m55s)	2.99	566 (9m26s)	2.81
8*			491 (8m11s)	3.99	704 (11m44s)	2.26

B3LYP – 6-311g(2df,p) /Freq

	C.02-b		E.01b		E.01-s	
	Runtime(s)	**speedup**				
1	7201 (2h01s)	1	3971 (1h6m11s)	1	3229 (53m49s)	1
2	3709 (1h1m49s)	1.94	2003 (33m23s)	1.98	1659 (27m39s)	1.95
4	2018 (33m38s)	3.57	1073 (17m53s)	3.70	942 (15m42s)	3.43
8			692 (11m32s)	5.74	877 (14m37s)	3.68

MP2 – 6-311g / OPT

	C.02-b		E.01-b		E.01-s	
	Runtime(s)	**speedup**				
1	625 (10m25s)	1	365 (6m5s)	1	360 (6m)	1
2	346 (5m46s)	1.81	304 (5m4s)	1.20	278 (4m38s)	1.30
4	289 (4m49s)	2.16	258 (4m18s)	1.41	256 (4m16s)	1.41
8*			260 (4m20s)	1.40	276 (4m36s)	1.30

MP2 – 6-311g / Freq

	C.02-b		E.01-b		E.01-s	
	Runtime(s)	**speedup**				
1	9903 (2h45m3s)	1	4550 (1h15m50s)	1	3266 (54m26s)	1
2	5005 (1h23m25s)	1.98	3134 (52m14s)	1.45	2092 (34m52s)	1.56
4	2821 (47m1s)	3.51	1921 (32m1s)	2.37	1720 (28m40s)	1.90
8*			1750 (29m10s)	2.60	1626 (27m6s)	2.01

Cluster: narwhal, Molecule - I

MP2 / Opt

	C.02-b		D.01-s		E.01-s	
	Runtimes(s)	**speedup**				
1	7522 (2h5m22s)	1	4231 (1h10m31s)	1	3629 (1h29s)	1
2	2744 (45m44s)	2.74	2300 (38m20s)	1.84	2157 (35m57s)	1.68
4	2285 (38m5s)	3.29	2236 (37m16s)	1.89	2006 (33m26s)	1.81

MP2 / Freq

	C.02-b		D.01-s		E.01-s	
	Runtimes(s)	**speedup**				
1	33799 (9h23m19s)	1	35904 (9h58m24s)	1	54521 (15h8m41s)	1
2	20962 (5h49m22s)	1.61	21218 (5h53m38s)	1.69	29931 (8h18m51s)	1.82
4	14751 (4h5m51s)	2.29	15936 (4h25m36s)	2.25	24402 (6h46m42s)	2.23

B3LYP / OPT

	C.02-b		D.01-s		E.01-s	
	Runtimes(s)	**speedup**				
1	4614 (1h16m54s)	1	3769 (1h2m49s)	1	3097 (51m37s)	1
2	1925 (32m05s)	2.40	1522 (25m22s)	2.48	1451 (24m11s)	2.13
4	1403 (23m23s)	3.29	1126 (18m46s)	3.35	1092 (18m12)	2.84

B3LYP / Freq

	C.02-b		D.01-s		E.01-s	
	Runtimes(s)	**speedup**				
1	2880 (48m)	1	2370 (39m30s)	1	2144 (35m44s)	1
2	1435 (23m55s)	2.0	1201 (20m1s)	1.97	1125 (18m45s)	1.91
4	829 (13m49s)	3.47	708 (11m48s)	3.35	683 (11m23s)	3.14

Cluster: narwhal, Molecule II

B3LYP -6-311g(2df,p) / opt

	C.02-b		D.01-s		E.01-s	
	Runtimes(s)	**speedup**				
1	3973 (1h6m13s)	1	3713 (1h1m53s)	1	3222 (53m42s)	1
2	2231 (37m11s)	1.78	1825 (30m25s)	2.03	1779 (29m39s)	1.81
4	1291 (21m31s)	3.08	1131 (18m51s)	3.28	1129 (18m49s)	2.85

B3LYP -6-311g(2df,p) / Freq

	C.02-b		D.01-s		E.01-s	
	Runtimes(s)	**speedup**				
1	8043 (2h14m03s)	1	6909 (1h55m9s)	1	6349 (1h45m49s)	1
2	4384 (1h13m04s)	1.83	3505 (58m25s)	1.97	3355 (55m55s)	1.89
4	2545 (42m25s)	3.16	2117 (35m17s)	3.26	2096 (34m56s)	3.03

MP2 – 6-311g / opt

	C.02-b		D.01-s		E.01-s	
	Runtimes(s)	**speedup**				
1	523 (8m43s)	1	536 (8m56s)	1	446 (7m26s)	1
2	383 (6m23s)	1.37	338 (5m38s)	1.59	408 (6m48s)	1.09
4	324 (5m24s)	1.61	319 (5m19s)	1.68	386 (6m26s)	1.16

MP2 – 6-311g / freq

	C.02-b		D.01-s		E.01-s	
	Runtimes(s)	**speedup**				
1	4220 (1h10m20s)	1	4080 (1h8m39s)	1	5170 (1h26m10s)	1
2	2520 (42m)	1.67	2301 (38m21s)	1.77	3600 (1h)	1.44
4	1840 (30m40s)	2.29	1900 (31m40s)	2.15	2883 (48m3s)	1.79

Input files

%mem = 2GB for B3LYP and MP2 computations
%mem = 2GB or 4GB for CISD and CCSD computations

%nproc varies for 1, 2, 4 and/or 8 threads/cpus

Molecule – I, for B3LYP and MP2

It is from Gaussian test job 445, the geom. and basis sets can found in test445.com in the directory
/opt/sharcnet/local/gaussian/g03/tests/com
or
/opt/sharcnet/gaussian/g03/tests/com

The following leading lines have been added above the geom. inputs
(%nproc varies for 1, 2, 4 and 8 threads/cpus)

%nosave
%mem=2GB
%chk=benchmark-b3lyp-1
%nproc=1
#p b3lyp/gen 6d opt freq (for B3LYP computations)
[#p mp2/gen 6d opt freq (for MP2 computations)]

Gaussian Test Job 445:
(H2PCH2CH2PH2)PdCl2(CH3)2 benchmark optimization

0 1

……

Molecule – II, for B3LYP and MP2

%NoSave
%chk=naph_b3lyp-2
%mem=2GB
%nproc=2
#p b3lyp/6-311g(2df,p) opt freq [#p mp2/6-311g opt freq for MP2]

B3lyp_naph Geometry Optimization and Freq computation

0 1
C
C 1 R2
C 1 R3 2 A3
C 2 R4 1 A4 3 D4 0
C 3 R5 1 A5 2 D5 0
C 4 R6 2 A6 1 D6 0
C 5 R7 3 A7 1 D7 0
C 6 R8 4 A8 2 D8 0
C 7 R9 5 A9 3 D9 0
C 8 R10 6 A10 4 D10 0
H 1 R11 2 A11 3 D11 0

H	2	R12	3	A12	1	D12	0
H	3	R13	1	A13	2	D13	0
H	4	R14	2	A14	1	D14	0
H	7	R15	5	A15	3	D15	0
H	8	R16	6	A16	4	D16	0
H	9	R17	7	A17	5	D17	0
H	10	R18	8	A18	6	D18	0

Variables:

R2	1.337
R3	1.337
R4	1.337
R5	1.337
R6	1.337
R7	1.337
R8	1.337
R9	1.337
R10	1.337
R11	1.1
R12	1.1
R13	1.1
R14	1.1
R15	1.1
R16	1.1
R17	1.1
R18	1.1
A3	120.
A4	120.
A5	120.
A6	120.
A7	120.
A8	120.
A9	120.
A10	120.
A11	120.
A12	150.
A13	120.
A14	120.
A15	120.
A16	120.
A17	120.
A18	120.
D4	0.
D5	0.
D6	0.
D7	-180.
D8	180.
D9	180.
D10	-180.
D11	180.
D12	0.
D13	180.
D14	180.
D15	0.
D16	0.
D17	-180.
D18	-180.

Molecule – III for CISD Opt and Freq

```
%NoSave
%chk=ch3oh_cisd-4
%mem=2GB
%nproc=4
#p cisd/6-311g(2df,p) opt freq

Gaussian Test Job 58:
MEOH opt, freq STD MOD cisd

0 1
C
O 1 CO
H 1 CH 2 T
H 1 CH 2 T 3 T 1
H 1 CH 2 T 3 T -1
H 2 OH 1 T 3 180.

CO 1.43
CH 1.09
OH 0.96
T 109.471221
```

Molecule –IV, for CCSD Opt and Freq

```
%NoSave
%chk=ch3ch2_ccsd-8
%mem=4GB
%nproc=8
#p ccsd/6-311g* opt freq

Gaussian Test Job 684:
Ethyl radical CCSD opt+freq

0 2
C1
C2 C1 CC
H1 C1 CH C2 T
H2 C1 CH C2 T H1 T 1
H3 C2 CH C1 T H1 180.
H4 C2 CH C1 T H3 120.
H5 C2 CH C1 T H3 240.

CC 1.54
CH 1.09
T 109.471221
```