

G16 benchmark

(Updated November 2022)

Galileo100

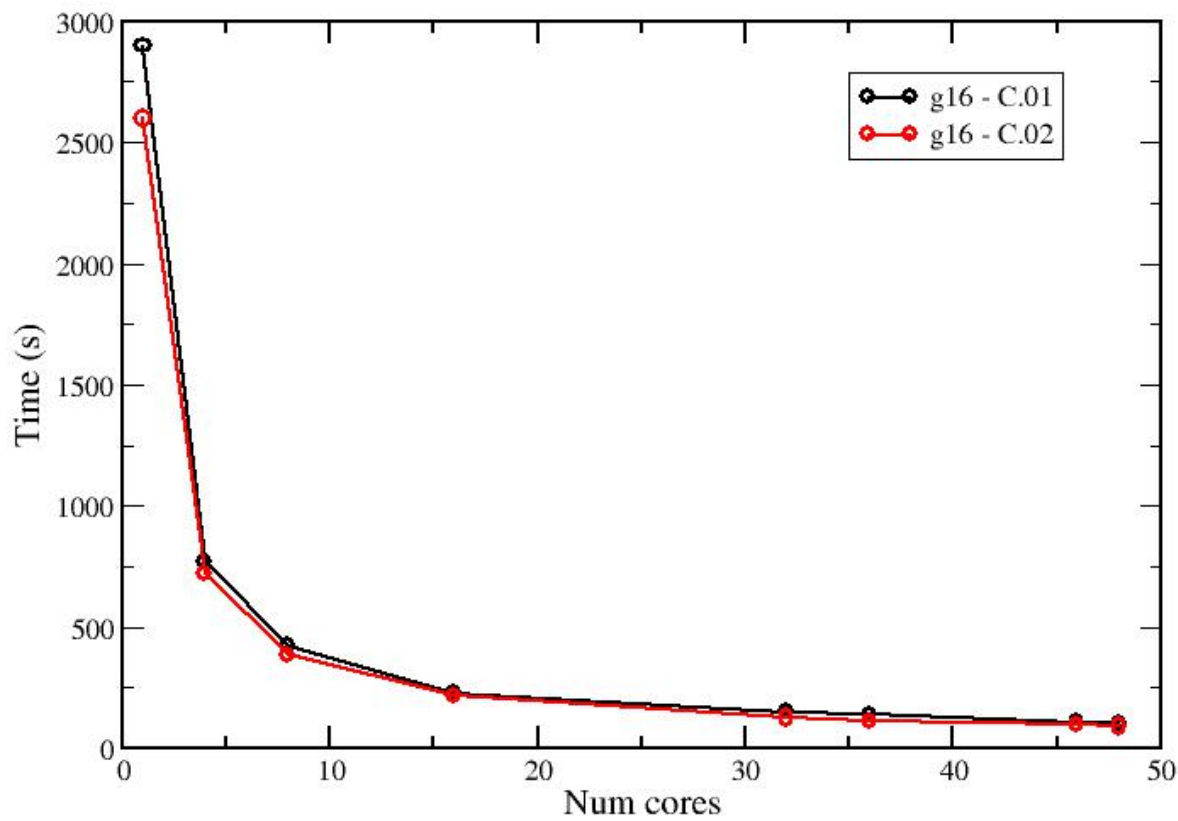
G16 (relC.01, relC.02)

Benchmark performed in production time. One replica per job.

The picture shows the elapsed-time trend (in seconds) varying the number of cores (on 1 Node)

Test0397

(DFT / 3-21G) + Force on Valinomycin
#p rb3lyp/3-21g force test scf=novaracc (mem=Default)



Parallelism (number cores)	Elapsed-time (s) (C.01)	Elapsed-time (s) (C.02)
1	2890	2600

4	770	721
8	423	385
16	228	215
32	150	127
36	138	111
46	106	97
48	105	92

Marconi A3 (intel SKL)

- node exclusive,
- 48 core/node,
- 182.000 MB memory/node (usable)

Test0397

(DFT / 3-21G) + Force on Valinomicyn
 #p rb3lyp/3-21g force test scf=novaracc (mem=86.000MB)

Parallelism	Cpu-time	Elapsed-time
serial	0:58:24	0:58:35
4 procs	0:59:30	0:14:57
8 procs	1:02:41	0:07:53
16 procs	1:07:53	0:04:17
32 procs	1:20:24	0:02:33
46 procs	1:30:31	0:02:30
48 procs	1:33:49	0:02:30
Ref (4 cores)	1:3:xx	0:16:00

Test0590

(Local Spin Density Approx
 #p lsda/gen/auto opt=(modred,expert) test (mem=200MB)

Parallelism	Cpu-time	Elapsed-time
serial small_M	0:54:35	0:54:48
serial large_M	0:54:40	0:54:53
4 procs	1:01:29	0:16:03
8 procs	1:09:41	0:09:28
16 procs	1:29:15	0:06:24

32 procs	2:14:25	0:05:00
46 procs	3:16:03	0:05:06
48 procs	3:25:18	0:05:08
Ref (4 cores)	1:02:26	0:16:30