Bastion timing benchmark on (small) bigmem nodes on Saga

September 19, 2021

Table 1: acetamide aug-cc-pVDZ

Task	cc2		cc3		ccs		ccsd	
	cpu	wall	cpu	wall	cpu	wall	cpu	wall
SCF solver	–	–	–	–	–	–	–	–
Cholesky decomposition of ERIs	34.23 s	1.20 s	33.64 s	1.15 s	34.24 s	1.15 s	33.81 s	1.27 s
CC GS solver time	16.55 s	0.42 s	78.95 min	2.00 min	3.81 s	0.10 s	5.79 min	10.18 s
multipliers	35.39 s	0.89 s	2.66 h	4.09 min	2.95 s	0.07 s	6.29 min	12.47 s
excited state (right)	–	–	–	–	5.54 s	0.14 s	11.01 min	26.84 s
excited state (left)	–	–	–	–	2.12 s	0.05 s	3.67 min	6.56 s
Time to calculate EOM properties	–	–	–	–	–	–	–	–

Table 2: acetamide aug-cc-pVTZ

Task	cc2		cc3		ccs		ccsd	
	cpu	wall	cpu	wall	cpu	wall	cpu	wall
SCF solver	–	–	–	–	–	–	–	–
Cholesky decomposition of ERIs	4.31 min	7.55 s	3.75 min	6.70 s	3.89 min	6.94 s	3.90 min	6.94 s
CC GS solver time	2.09 min	3.18 s	26.88 h	41.17 min	24.05 s	0.62 s	98.90 min	3.18 min
multipliers	8.97 min	13.58 s	53.38 h	81.86 min	16.52 s	0.44 s	58.62 min	2.06 min
excited state (right)	31.55 min	108.21 s	124.82 h	3.18 h	24.06 s	0.64 s	117.36 min	4.63 min
excited state (left)	8.05 min	18.01 s	121.65 h	3.12 h	11.53 s	0.31 s	36.12 min	71.92 s
Time to calculate EOM properties	–	–	–	–	–	–	–	–

Table 3: thymine aug-cc-pVDZ

Task	cc2		cc3		ccs		ccsd	
	cpu	wall	cpu	wall	cpu	wall	cpu	wall
SCF solver	–	–	–	–	–	–	–	–
Cholesky decomposition of ERIs	2.93 min	5.84 s	2.74 min	5.54 s	2.71 min	5.49 s	3.25 min	6.32 s
CC GS solver time	3.88 min	6.19 s	130.36 h	3.29 h	28.84 s	0.74 s	86.46 min	2.83 min
multipliers	11.68 min	17.65 s	283.34 h	7.15 h	40.32 s	1.05 s	102.57 min	4.04 min
excited state (right)	44.39 min	5.12 min	673.23 h	16.98 h	33.11 s	0.89 s	3.18 h	8.80 min
excited state (left)	12.78 min	37.26 s	628.34 h	15.88 h	29.67 s	0.78 s	59.57 min	2.08 min
Time to calculate EOM properties	–	–	–	–	–	–	–	–

Table 4: formaldehyde aug-cc-pVDZ

Task	cc2		cc3		ccs		ccsd	
	cpu	wall	cpu	wall	cpu	wall	cpu	wall
SCF solver	–	–	–	–	–	–	–	–
Cholesky decomposition of ERIs	8.35 s	0.26 s	8.79 s	0.27 s	9.27 s	0.31 s	8.95 s	0.30 s
CC GS solver time	3.24 s	0.09 s	111.92 s	2.90 s	1.34 s	0.05 s	23.11 s	0.62 s
multipliers	3.79 s	0.10 s	3.87 min	5.92 s	0.67 s	0.02 s	35.62 s	0.98 s
excited state (right)	15.83 s	0.44 s	6.59 min	10.01 s	3.45 s	0.09 s	41.49 s	1.14 s
excited state (left)	6.73 s	0.22 s	6.33 min	9.97 s	0.65 s	0.02 s	26.33 s	2.59 s
Time to calculate EOM properties	–	–	–	–	–	–	–	–

Table 5: formaldehyde aug-cc-pVTZ

Task	cc2		cc3		ccs		ccsd	
	cpu	wall	cpu	wall	cpu	wall	cpu	wall
SCF solver	–	–	–	–	–	–	–	–
Cholesky decomposition of ERIs	41.64 s	1.49 s	39.37 s	1.42 s	38.38 s	1.49 s	40.14 s	1.54 s
CC GS solver time	13.08 s	0.33 s	16.55 min	25.50 s	3.99 s	0.10 s	4.39 min	7.41 s
multipliers	34.24 s	0.86 s	29.26 min	46.52 s	1.12 s	0.03 s	3.27 min	5.55 s
excited state (right)	89.99 s	4.29 s	51.80 min	79.85 s	4.44 s	0.11 s	4.61 min	8.15 s
excited state (left)	28.60 s	0.81 s	53.38 min	84.07 s	0.89 s	0.02 s	2.20 min	5.43 s
Time to calculate EOM properties	–	–	–	–	–	–	–	–

Table 6: furan aug-cc-pVDZ

Task	cc2		cc3		ccs		ccsd	
	cpu	wall	cpu	wall	cpu	wall	cpu	wall
SCF solver	–	–	–	–	–	–	–	–
Cholesky decomposition of ERIs	44.80 s	1.81 s	48.02 s	1.81 s	48.84 s	2.30 s	46.07 s	1.83 s
CC GS solver time	21.39 s	0.61 s	2.58 h	3.92 min	4.65 s	0.12 s	8.15 min	14.82 s
multipliers	47.70 s	1.20 s	4.96 h	7.60 min	4.64 s	0.12 s	9.47 min	19.94 s
excited state (right)	2.02 min	6.74 s	7.20 h	10.95 min	6.01 s	0.15 s	8.20 min	17.32 s
excited state (left)	51.02 s	1.93 s	7.44 h	11.41 min	3.73 s	0.39 s	4.74 min	8.75 s
Time to calculate EOM properties	–	–	–	–	–	–	–	–

Table 7: furan aug-cc-pVTZ

Task	cc2		cc3		ccs		ccsd	
	cpu	wall	cpu	wall	cpu	wall	cpu	wall
SCF solver	–	–	–	–	–	–	–	–
Cholesky decomposition of ERIs	4.64 min	8.19 s	4.68 min	8.24 s	5.01 min	8.70 s	4.58 min	7.99 s
CC GS solver time	2.68 min	4.10 s	43.36 h	65.51 min	28.86 s	0.74 s	107.63 min	2.93 min
multipliers	13.05 min	20.13 s	99.46 h	2.53 h	23.69 s	0.64 s	2.83 h	4.93 min
excited state (right)	17.89 min	49.34 s	135.04 h	3.42 h	28.23 s	0.74 s	2.43 h	4.28 min
excited state (left)	8.23 min	17.87 s	142.76 h	3.63 h	14.17 s	0.37 s	94.80 min	2.63 min
Time to calculate EOM properties	–	–	–	–	–	–	–	–

Table 8: betaine aug-cc-pVDZ

Task	ccs		lowmem-cc2	
	cpu	wall	cpu	wall
SCF solver	–	–	–	–
Cholesky decomposition of ERIs	6.10 h	9.89 min	5.98 h	9.97 min
CC GS solver time	105.21 min	9.50 min	193.51 h	5.82 h
multipliers	–	–	–	–
excited state (right)	2.81 h	7.56 min	1465.10 h	42.97 h
excited state (left)	–	–	–	–
Time to calculate EOM properties	–	–	–	–

Table 9: ATP aug-cc-pVDZ

Task	ccs		lowmem-cc2	
	cpu	wall	cpu	wall
SCF solver	–	–	–	–
Cholesky decomposition of ERIs	2.08 h	3.39 min	2.04 h	3.30 min
CC GS solver time	38.75 min	58.78 s	34.54 h	55.00 min
multipliers	–	–	–	–
excited state (right)	64.54 min	100.29 s	903.19 h	23.16 h
excited state (left)	–	–	–	–
Time to calculate EOM properties	–	–	–	–

Table 10: cytosine aug-cc-pVDZ

Task	cc2		cc3		ccs		ccsd	
	cpu	wall	cpu	wall	cpu	wall	cpu	wall
SCF solver	–	–	–	–	–	–	–	–
Cholesky decomposition of ERIs	2.26 min	4.38 s	2.32 min	4.45 s	2.70 min	5.02 s	115.64 s	3.90 s
CC GS solver time	2.43 min	3.82 s	48.81 h	73.77 min	30.40 s	0.79 s	51.28 min	100.94 s
multipliers	7.37 min	11.14 s	98.90 h	2.50 h	39.93 s	1.06 s	58.15 min	2.30 min
excited state (right)	38.37 min	4.79 min	324.20 h	8.22 h	52.57 s	1.41 s	64.00 min	2.69 min
excited state (left)	6.52 min	19.97 s	344.38 h	8.75 h	32.13 s	0.83 s	33.26 min	70.27 s
Time to calculate EOM properties	–	–	–	–	–	–	–	–

Table 11: tryptophane aug-cc-pVDZ

Task	cc2		ccs		ccsd	
	cpu	wall	cpu	wall	cpu	wall
SCF solver	–	–	–	–	–	–
Cholesky decomposition of ERIs	12.64 min	22.02 s	12.43 min	21.67 s	12.87 min	22.42 s
CC GS solver time	28.41 min	44.11 s	105.22 s	2.68 s	16.82 h	28.64 min
multipliers	106.75 min	2.74 min	4.30 min	6.48 s	34.86 h	65.11 min
excited state (right)	3.60 h	17.15 min	3.16 min	4.91 s	36.94 h	70.92 min
excited state (left)	73.81 min	3.67 min	2.84 min	4.29 s	20.60 h	36.13 min
Time to calculate EOM properties	–	–	–	–	–	–

Table 12: lsd aug-cc-pVDZ

Task	cc2		ccs		ccsd	
	cpu	wall	cpu	wall	cpu	wall
SCF solver	–	–	–	–	–	–
Cholesky decomposition of ERIs	74.53 min	118.24 s	70.73 min	112.55 s	70.59 min	111.95 s
CC GS solver time	4.31 h	6.88 min	12.23 min	18.77 s	296.47 h	8.17 h
multipliers	20.87 h	32.37 min	59.52 min	90.11 s	588.62 h	17.21 h
excited state (right)	93.10 h	16.90 h	23.42 min	36.77 s	1671.32 h	66.63 h
excited state (left)	19.51 h	58.97 min	29.18 min	44.18 s	442.88 h	12.93 h
Time to calculate EOM properties	–	–	–	–	–	–