Disco timing benchmark on (small) bigmem nodes on Saga

September 19, 2021

Table 1: ATP aug-cc-pVDZ

Task	ccs		lowmem-cc2	
	cpu	wall	cpu	wall
SCF solver	24.64 h	37.06 min	24.66 h	37.08 min
Cholesky decomposition of ERIs	2.30 h	3.94 min	2.38 h	4.10 min
CC GS solver time	45.99 min	70.49 s	36.35 h	57.67 min
multipliers	–	–	–	–
excited state (right)	70.33 min	109.74 s	941.26 h	24.14 h
excited state (left)	–	–	–	–
Time to calculate EOM properties	–	–	–	–

Table 2: acetamide aug-cc-pVDZ

Task	cc2		cc3		ccs		ccsd	
	cpu	wall	cpu	wall	cpu	wall	cpu	wall
SCF solver	2.89 min	4.43 s	3.36 min	5.16 s	2.81 min	4.38 s	2.92 min	4.48 s
Cholesky decomposition of ERIs	41.55 s	1.41 s	48.23 s	1.53 s	40.42 s	1.38 s	42.41 s	1.44 s
CC GS solver time	20.95 s	0.53 s	80.56 min	2.04 min	4.60 s	0.12 s	5.38 min	9.58 s
multipliers	36.91 s	0.94 s	2.51 h	3.86 min	2.69 s	0.07 s	5.63 min	11.20 s
excited state (right)	3.44 min	14.08 s	5.43 h	8.33 min	5.59 s	0.14 s	10.81 min	26.72 s
excited state (left)	57.04 s	2.14 s	5.50 h	8.53 min	2.48 s	0.06 s	3.65 min	6.57 s
Time to calculate EOM properties	5.06 s	0.15 s	44.36 min	75.29 s	0.18 s	0.01 s	1.83 s	0.07 s

Table 3: acetamide aug-cc-pVTZ

Task	cc2		cc3		ccs		ccsd	
	cpu	wall	cpu	wall	cpu	wall	cpu	wall
SCF solver	30.68 min	46.72 s	30.67 min	46.70 s	30.79 min	46.92 s	30.55 min	46.52 s
Cholesky decomposition of ERIs	4.91 min	8.86 s	5.18 min	9.43 s	4.78 min	8.68 s	4.75 min	8.61 s
CC GS solver time	2.17 min	3.29 s	26.00 h	39.86 min	25.69 s	0.66 s	100.06 min	3.19 min
multipliers	8.80 min	13.34 s	51.72 h	79.17 min	16.92 s	0.45 s	56.30 min	2.01 min
excited state (right)	27.83 min	102.11 s	118.05 h	3.00 h	25.10 s	0.66 s	115.26 min	4.56 min
excited state (left)	7.47 min	17.04 s	117.17 h	3.00 h	12.53 s	0.33 s	36.32 min	73.03 s
Time to calculate EOM properties	56.32 s	1.58 s	17.75 h	28.68 min	0.24 s	0.01 s	10.96 s	0.45 s

Table 4: betaine aug-cc-pVDZ

Task	ccs		lowmem-cc2	
	cpu	wall	cpu	wall
SCF solver	91.47 h	2.29 h	91.42 h	2.29 h
Cholesky decomposition of ERIs	7.03 h	12.15 min	6.48 h	10.77 min
CC GS solver time	2.08 h	9.85 min	203.80 h	6.05 h
multipliers	–	–	–	–
excited state (right)	3.09 h	7.91 min	1531.66 h	44.90 h
excited state (left)	–	–	–	–
Time to calculate EOM properties	–	–	–	–

Table 5: cytosine aug-cc-pVDZ

Task	cc2		cc3		ccs		ccsd	
	cpu	wall	cpu	wall	cpu	wall	cpu	wall
SCF solver	18.36 min	27.73 s	18.27 min	27.60 s	18.27 min	27.66 s	18.28 min	27.61 s
Cholesky decomposition of ERIs	2.26 min	4.70 s	2.26 min	4.67 s	2.44 min	4.99 s	2.40 min	4.90 s
CC GS solver time	2.66 min	4.18 s	46.86 h	70.86 min	21.32 s	0.55 s	51.31 min	100.98 s
multipliers	6.86 min	10.42 s	94.99 h	2.40 h	22.19 s	0.58 s	53.21 min	2.12 min
excited state (right)	37.12 min	4.68 min	301.27 h	7.65 h	20.99 s	0.56 s	62.96 min	2.62 min
excited state (left)	6.27 min	19.09 s	331.85 h	8.43 h	18.90 s	0.49 s	31.54 min	66.11 s
Time to calculate EOM properties	46.79 s	1.49 s	28.72 h	47.55 min	0.20 s	0.01 s	17.82 s	0.76 s

Table 6: formaldehyde aug-cc-pVDZ

Task	cc2		cc3		ccs		ccsd	
	cpu	wall	cpu	wall	cpu	wall	cpu	wall
SCF solver	14.84 s	0.43 s	14.94 s	0.44 s	17.09 s	1.10 s	14.80 s	0.43 s
Cholesky decomposition of ERIs	9.81 s	0.31 s	12.47 s	0.38 s	10.23 s	0.36 s	10.06 s	0.31 s
CC GS solver time	3.44 s	0.09 s	111.90 s	2.82 s	1.08 s	0.03 s	25.37 s	0.65 s
multipliers	3.48 s	0.09 s	3.61 min	5.44 s	0.51 s	0.01 s	33.66 s	0.86 s
excited state (right)	14.62 s	0.41 s	6.07 min	9.20 s	2.20 s	0.06 s	38.72 s	1.00 s
excited state (left)	4.69 s	0.12 s	6.24 min	9.51 s	0.51 s	0.01 s	26.08 s	2.39 s
Time to calculate EOM properties	0.52 s	0.02 s	64.17 s	1.90 s	0.17 s	0.01 s	0.33 s	0.01 s

Table 7: formaldehyde aug-cc-pVTZ

Task	cc2		cc3		ccs		ccsd	
	cpu	wall	cpu	wall	cpu	wall	cpu	wall
SCF solver	95.18 s	2.61 s	95.36 s	2.62 s	94.74 s	2.60 s	95.50 s	2.62 s
Cholesky decomposition of ERIs	48.93 s	1.74 s	51.92 s	1.80 s	50.75 s	1.78 s	55.30 s	1.89 s
CC GS solver time	14.14 s	0.36 s	17.05 min	26.27 s	4.18 s	0.11 s	4.47 min	7.45 s
multipliers	32.49 s	0.82 s	29.02 min	45.92 s	0.89 s	0.02 s	3.98 min	27.76 s
excited state (right)	81.03 s	2.28 s	49.95 min	77.17 s	3.99 s	0.10 s	5.08 min	15.79 s
excited state (left)	26.61 s	0.68 s	54.26 min	85.29 s	0.84 s	0.02 s	2.14 min	3.39 s
Time to calculate EOM properties	3.68 s	0.10 s	9.51 min	16.58 s	0.16 s	0.01 s	0.90 s	0.03 s

Table 8: furan aug-cc-pVDZ

Task	cc2		cc3		ccs		ccsd	
	cpu	wall	cpu	wall	cpu	wall	cpu	wall
SCF solver	4.73 min	7.20 s	4.63 min	7.05 s	4.71 min	7.18 s	4.54 min	6.91 s
Cholesky decomposition of ERIs	60.95 s	2.25 s	58.94 s	2.19 s	59.20 s	2.24 s	59.68 s	2.23 s
CC GS solver time	29.35 s	0.74 s	2.61 h	3.96 min	5.46 s	0.14 s	8.18 min	14.67 s
multipliers	57.54 s	1.54 s	5.06 h	7.74 min	3.53 s	0.09 s	8.76 min	18.32 s
excited state (right)	119.51 s	6.25 s	6.53 h	9.94 min	6.14 s	0.15 s	7.94 min	16.82 s
excited state (left)	50.69 s	1.79 s	7.01 h	10.74 min	3.38 s	0.08 s	4.57 min	8.43 s
Time to calculate EOM properties	8.33 s	0.24 s	96.26 min	2.75 min	0.19 s	0.01 s	2.99 s	0.12 s

Table 9: furan aug-cc-pVTZ

Task	cc2		cc3		ccs		ccsd	
	cpu	wall	cpu	wall	cpu	wall	cpu	wall
SCF solver	42.32 min	64.40 s	42.34 min	64.41 s	42.24 min	64.27 s	42.27 min	64.32 s
Cholesky decomposition of ERIs	6.10 min	11.48 s	6.90 min	12.66 s	5.87 min	11.00 s	6.40 min	11.95 s
CC GS solver time	3.31 min	5.08 s	44.81 h	67.75 min	30.74 s	0.78 s	97.88 min	2.69 min
multipliers	14.98 min	23.08 s	88.73 h	2.26 h	23.10 s	0.63 s	2.68 h	4.69 min
excited state (right)	17.36 min	47.39 s	125.13 h	3.16 h	30.49 s	0.81 s	2.31 h	4.08 min
excited state (left)	8.07 min	16.80 s	133.11 h	3.39 h	17.16 s	0.47 s	91.76 min	2.55 min
Time to calculate EOM properties	88.51 s	2.58 s	34.99 h	56.54 min	1.57 s	0.04 s	14.80 s	0.59 s

Table 10: lsd aug-cc-pVDZ

Task	cc2		ccs		ccsd	
	cpu	wall	cpu	wall	cpu	wall
SCF solver	18.98 h	28.54 min	18.96 h	28.52 min	18.80 h	28.28 min
Cholesky decomposition of ERIs	76.15 min	2.03 min	82.07 min	2.22 min	77.52 min	2.06 min
CC GS solver time	4.38 h	6.97 min	16.43 min	25.27 s	297.07 h	8.28 h
multipliers	20.83 h	32.79 min	59.66 min	90.32 s	588.77 h	17.51 h
excited state (right)	96.19 h	15.43 h	25.67 min	40.20 s	1670.70 h	65.18 h
excited state (left)	19.58 h	59.44 min	31.29 min	47.46 s	443.33 h	12.80 h
Time to calculate EOM properties	118.06 min	3.96 min	1.92 s	0.05 s	37.57 min	106.36 s

Table 11: thymine aug-cc-pVDZ

Task	cc2		cc3		ccs		ccsd	
	cpu	wall	cpu	wall	cpu	wall	cpu	wall
SCF solver	29.99 min	45.20 s	29.37 min	44.28 s	30.14 min	45.46 s	29.95 min	45.12 s
Cholesky decomposition of ERIs	3.66 min	7.35 s	3.80 min	7.50 s	3.37 min	6.79 s	3.68 min	7.26 s
CC GS solver time	4.10 min	6.63 s	125.87 h	3.17 h	33.12 s	0.86 s	84.23 min	2.76 min
multipliers	11.78 min	17.89 s	273.98 h	6.91 h	41.98 s	1.12 s	97.13 min	3.91 min
excited state (right)	44.25 min	4.98 min	647.19 h	16.31 h	35.43 s	0.96 s	3.03 h	8.57 min
excited state (left)	10.31 min	32.93 s	623.25 h	15.76 h	29.15 s	0.77 s	56.40 min	118.47 s
Time to calculate EOM properties	80.84 s	2.59 s	83.89 h	2.25 h	0.23 s	0.01 s	24.80 s	1.16 s

Table 12: tryptophane aug-cc-pVDZ

Task	cc2		ccs		ccsd	
	cpu	wall	cpu	wall	cpu	wall
SCF solver	3.34 h	5.02 min	3.32 h	5.00 min	3.31 h	4.98 min
Cholesky decomposition of ERIs	14.28 min	25.06 s	14.35 min	25.24 s	14.72 min	25.66 s
CC GS solver time	32.23 min	50.13 s	2.27 min	3.47 s	16.82 h	28.66 min
multipliers	106.14 min	2.72 min	4.37 min	6.58 s	34.84 h	64.71 min
excited state (right)	3.64 h	17.09 min	3.47 min	5.37 s	36.89 h	70.33 min
excited state (left)	74.14 min	3.66 min	3.15 min	4.77 s	20.62 h	35.99 min
Time to calculate EOM properties	11.28 min	23.43 s	0.38 s	0.01 s	4.27 min	12.25 s