Disco timing benchmark on (small) bigmem nodes on Saga

September 12, 2021

Table 1: acetamide aug-cc-pVDZ

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

Table 2: acetamide aug-cc-pVTZ

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

Table 3: thymine aug-cc-pVDZ

Task	ccsd		cc2		cc3		ccs	
	cpu	wall	cpu	wall	cpu	wall	cpu	wall
SCF solver	29.61 min	44.70 s	29.56 min	44.55 s	29.60 min	44.65 s	29.70 min	44.80 s
Cholesky decomposition of ERIs	3.44 min	6.94 s	3.74 min	7.38 s	3.89 min	10.09 s	3.45 min	6.91 s
CC GS solver time	83.15 min	8.49 min	4.25 min	6.92 s	128.39 h	3.33 h	33.01 s	0.85 s
multipliers	97.45 min	38.24 min	12.08 min	19.20 s	281.42 h	7.19 h	43.12 s	1.23 s
excited state (right)	3.20 h	9.44 min	44.61 min	4.96 min	657.90 h	16.61 h	33.30 s	0.89 s
excited state (left)	57.78 min	2.20 min	10.11 min	32.50 s	628.01 h	15.92 h	32.18 s	0.86 s
Time to calculate EOM properties	24.99 s	1.15 s	86.65 s	2.74 s	83.31 h	2.24 h	0.22 s	0.01 s

Table 4: betaine aug-cc-pVDZ

Task	lowmem-cc2		ccs	
	cpu	wall	cpu	wall
SCF solver	91.63 h	2.30 h	90.33 h	2.26 h
Cholesky decomposition of ERIs	6.45 h	10.82 min	6.47 h	10.59 min
CC GS solver time	199.30 h	6.07 h	119.21 min	10.36 min
multipliers	–	–	–	–
excited state (right)	1489.15 h	43.05 h	2.94 h	8.29 min
excited state (left)	–	–	–	–
Time to calculate EOM properties	–	–	–	–

Table 5: cytosine aug-cc-pVDZ

Task	ccs		ccsd		cc3		cc2	
	cpu	wall	cpu	wall	cpu	wall	cpu	wall
SCF solver	18.27 min	27.66 s	18.28 min	27.61 s	25.89 min	39.13 s	18.36 min	27.73 s
Cholesky decomposition of ERIs	2.44 min	4.99 s	2.40 min	4.90 s	2.35 min	5.88 s	2.26 min	4.70 s
CC GS solver time	21.32 s	0.55 s	51.31 min	100.98 s	47.80 h	76.21 min	2.66 min	4.18 s
multipliers	22.19 s	0.58 s	53.21 min	2.12 min	98.02 h	2.71 h	6.86 min	10.42 s
excited state (right)	20.99 s	0.56 s	62.96 min	2.62 min	307.38 h	7.86 h	37.12 min	4.68 min
excited state (left)	18.90 s	0.49 s	31.54 min	66.11 s	341.28 h	9.23 h	6.27 min	19.09 s
Time to calculate EOM properties	0.20 s	0.01 s	17.82 s	0.76 s	29.15 h	48.05 min	46.79 s	1.49 s

Table 6: formaldehyde aug-cc-pVDZ

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

Table 7: formaldehyde aug-cc-pVTZ

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

Table 8: ATP aug-cc-pVDZ

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

Table 9: tryptophane aug-cc-pVDZ

Task	ccs		ccsd		cc2	
	cpu	wall	cpu	wall	cpu	wall
SCF solver	3.33 h	5.01 min	3.33 h	5.01 min	3.35 h	5.05 min
Cholesky decomposition of ERIs	14.00 min	25.07 s	14.41 min	25.25 s	14.37 min	25.38 s
CC GS solver time	2.37 min	3.63 s	17.03 h	29.23 min	31.17 min	48.46 s
multipliers	4.55 min	6.86 s	34.53 h	63.77 min	106.27 min	2.73 min
excited state (right)	4.14 min	6.63 s	36.69 h	69.76 min	3.63 h	18.70 min
excited state (left)	3.24 min	4.91 s	20.34 h	35.26 min	74.05 min	3.67 min
Time to calculate EOM properties	0.76 s	0.02 s	4.12 min	12.20 s	11.28 min	23.67 s

Table 10: lsd aug-cc-pVDZ

Task	ccs		ccsd		cc2	
	cpu	wall	cpu	wall	cpu	wall
SCF solver	18.96 h	28.52 min	18.94 h	28.48 min	18.98 h	28.54 min
Cholesky decomposition of ERIs	82.07 min	2.22 min	75.72 min	2.02 min	76.15 min	2.03 min
CC GS solver time	16.43 min	25.27 s	296.53 h	8.24 h	4.38 h	6.97 min
multipliers	59.66 min	90.32 s	586.13 h	18.41 h	20.83 h	32.79 min
excited state (right)	25.67 min	40.20 s	1667.03 h	67.73 h	96.19 h	15.43 h
excited state (left)	31.29 min	47.46 s	442.52 h	12.88 h	19.58 h	59.44 min
Time to calculate EOM properties	1.92 s	0.05 s	37.31 min	105.06 s	118.06 min	3.96 min

Table 11: furan aug-cc-pVTZ

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

Table 12: furan aug-cc-pVDZ

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