# Bastion 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 | – | – | – | – |
| 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 2: 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 3: 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 4: 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 5: 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 6: 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 7: 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 8: 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 9: 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 10: 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 | – | – | – | – | – | – |

Table 11: 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 12: 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 | – | – | – | – | – | – |