New implementation of high-level correlated methods using a general block-tensor library for high-performance electronic structure calculations: Supplemetary Materals

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1 Q-Chem inputs used for benchmark calculations

1.1 Test 1

```
$comment
Test1: mU_H2O_t1_6311+Gdp
Nuclear repulsion energy: 634.4898796969 hartrees
SCF energy                 = -566.71127749
CCSD total energy          = -568.56092723
$end

$molecule
0 1
C       1.196324    -1.576666     0.000000
N       0.259910    -0.449875     0.000000
C       0.742908     0.865744     0.000000
C      -0.279791     1.892522     0.000000
C      -1.582150     1.551615     0.000000
N      -1.997135     0.248535     0.000000
C      -1.083721    -0.799793     0.000000
```

```
O      -1.457784    -1.959681     0.000000
C      -3.409405    -0.117777     0.000000
H      -3.644189    -0.710833     0.885731
H      -4.001716     0.797650     0.000000
H      -3.644189    -0.710833    -0.885731
H      -2.371808     2.294716     0.000000
H       0.045628     2.922569     0.000000
O       1.944130     1.111909     0.000000
H       1.027445    -2.191281     0.885562
H       1.027445    -2.191281    -0.885562
H       2.210065    -1.189296     0.000000
O       4.406416    -0.287521     0.000000
H       3.660618     0.332238     0.000000
H       5.204191     0.244198     0.000000
$end

$rem
JOBTYPE SP
CORRELATION CCSD
BASIS 6-311+G**
cc_memory 90000
mem_static 1000
MAX_SUB_FILE_NUM 50
n_frozen_core fc
CC_T_CONV 4
CC_E_CONV 6
$end
```

1.2 Test 2

```
$comment
Test2: mU_H2O_t1_6311+Gdp
First job is HF calculation for the neutral; second job uses RHF orbitals
as a guess for ROHF.
Nuclear Repulsion Energy: 634.489880 hartrees
SCF energy (1st job): -566.711278 hartrees
SCF energy (2nd job): -566.395034 hartrees
$end

$molecule
0 1
C       1.196324    -1.576666     0.000000
N       0.259910    -0.449875     0.000000
C       0.742908     0.865744     0.000000
C      -0.279791     1.892522     0.000000
C      -1.582150     1.551615     0.000000
```

```
N      -1.997135     0.248535     0.000000
C      -1.083721    -0.799793     0.000000
O      -1.457784    -1.959681     0.000000
C      -3.409405    -0.117777     0.000000
H      -3.644189    -0.710833     0.885731
H      -4.001716     0.797650     0.000000
H      -3.644189    -0.710833    -0.885731
H      -2.371808     2.294716     0.000000
H       0.045628     2.922569     0.000000
O       1.944130     1.111909     0.000000
H       1.027445    -2.191281     0.885562
H       1.027445    -2.191281    -0.885562
H       2.210065    -1.189296     0.000000
O       4.406416    -0.287521     0.000000
H       3.660618     0.332238     0.000000
H       5.204191     0.244198     0.000000
$end

$rem
JOBTYPE SP
EXCHANGE HF
CORRELATION NONE
UNRESTRICTED FALSE
BASIS 6-311+G**
mem_static 1000
MAX_SUB_FILE_NUM 50
$end

@@@
$molecule
1 2
C       1.196324    -1.576666     0.000000
N       0.259910    -0.449875     0.000000
C       0.742908     0.865744     0.000000
C      -0.279791     1.892522     0.000000
C      -1.582150     1.551615     0.000000
N      -1.997135     0.248535     0.000000
C      -1.083721    -0.799793     0.000000
O      -1.457784    -1.959681     0.000000
C      -3.409405    -0.117777     0.000000
H      -3.644189    -0.710833     0.885731
H      -4.001716     0.797650     0.000000
H      -3.644189    -0.710833    -0.885731
H      -2.371808     2.294716     0.000000
H       0.045628     2.922569     0.000000
O       1.944130     1.111909     0.000000
```

```
H       1.027445    -2.191281     0.885562
H       1.027445    -2.191281    -0.885562
H       2.210065    -1.189296     0.000000
O       4.406416    -0.287521     0.000000
H       3.660618     0.332238     0.000000
H       5.204191     0.244198     0.000000
$end

$rem
JOBTYPE SP
CORRELATION CCSD
UNRESTRICTED FALSE
BASIS 6-311+G**
SCF_GUESS  =  Read
cc_memory 48000
mem_static 1000
MAX_SUB_FILE_NUM 50
n_frozen_core fc
CC_T_CONV 4
CC_E_CONV 6
$end
```

1.3 Test 3

```
$comment
Nuclear Repulsion Energy =  1945.8695484535 hartrees
SCF energy                = -1057.14315983
CCSD total energy         = -1060.47718627
$end

$molecule
0 1
C       1.545064    -1.804675     1.545512
N       0.285229    -1.677479     0.814467
C       0.166397    -2.272594    -0.454951
C      -1.158084    -2.205915    -1.027086
C      -2.123943    -1.485110    -0.421915
N      -1.915212    -0.838218     0.765459
C      -0.711456    -0.945786     1.443811
O      -0.534470    -0.411004     2.527996
C      -2.963688    -0.035285     1.390765
H      -2.554141     0.934756     1.673037
H      -3.754361     0.115182     0.656665
H      -3.348163    -0.532963     2.284131
H      -3.103137    -1.340172    -0.861695
H      -1.323978    -2.684906    -1.981367
```

```
O       1.140501    -2.781078    -1.001905
H       1.993313    -0.823547     1.711752
H       1.361558    -2.269153     2.515745
H       2.202198    -2.425695     0.941117
N       2.116658     0.486447    -0.992980
C       1.138568     0.344926    -1.934601
H       1.385874    -0.312748    -2.759747
C      -0.064934     0.942510    -1.826581
H      -0.842390     0.791306    -2.561735
C      -0.368309     1.729061    -0.655415
O      -1.466447     2.252072    -0.438769
N       0.670508     1.858510     0.264464
C       0.451963     2.605626     1.505261
H       1.218312     3.374252     1.608281
H      -0.538173     3.050400     1.453806
H       0.510460     1.916115     2.349498
C       1.929937     1.284546     0.127945
O       2.806299     1.456191     0.958016
C       3.395448    -0.205179    -1.147009
H       4.063549     0.371938    -1.791451
H       3.849480    -0.298544    -0.163000
H       3.207981    -1.196199    -1.563228
O      -3.551228     0.952796    -1.702837
H      -4.133353     1.534797    -2.195201
H      -2.874319     1.525783    -1.290891
$end

$rem
JOBTYPE SP
EXCHANGE HF
CORRELATION CCSD
BASIS 6-31+G**
cc_memory 48000
mem_static 1500
MAX_SUB_FILE_NUM 100
n_frozen_core fc
CC_T_CONV 4
CC_E_CONV 6
$end
```

1.4 AATT tetramer

```
$molecule
0 1
N 4.933372 -0.652401 1.567963
C 4.782400 0.482761 2.335118
```

```
N 3.531384 0.774553 2.612804
C 2.808187 -0.230005 1.978375
C 1.430371 -0.498997 1.888625
N 0.484454 0.242012 2.472008
N 1.050473 -1.577325 1.168217
C 1.996652 -2.327480 0.583704
N 3.315014 -2.181833 0.600479
C 3.660963 -1.105872 1.324195
N 4.648954 0.062237 -2.370046
C 5.222661 1.044161 -1.595124
N 4.354894 1.743856 -0.892815
C 3.124382 1.191641 -1.234691
C 1.796538 1.473710 -0.820053
N 1.477058 2.412334 0.063341
N 0.802690 0.730580 -1.347517
C 1.118897 -0.233683 -2.222372
N 2.315056 -0.597666 -2.682467
C 3.287489 0.159535 -2.145551
N -4.119880 1.175240 -1.668947
C -2.788993 0.852210 -1.845154
O -2.385787 0.134394 -2.748531
N -1.937862 1.401121 -0.916872
C -2.275607 2.205332 0.157303
O -1.389232 2.644961 0.899530
C -3.691851 2.470201 0.309209
C -4.156175 3.291113 1.475440
C -4.531960 1.955432 -0.607897
N -3.093123 -2.936903 -1.004080
C -1.789262 -2.710900 -0.630457
O -0.840457 -3.167912 -1.243704
N -1.636359 -1.922963 0.479694
C -2.636971 -1.336214 1.225506
O -2.346142 -0.645842 2.195441
C -3.987755 -1.598884 0.766076
C -5.137909 -0.995328 1.511021
C -4.143924 -2.378097 -0.316323
H 5.634063 1.064617 2.657101
H 0.746500 1.082317 2.959601
H -0.501938 -0.002634 2.391471
H 1.608242 -3.155126 -0.004534
H 6.291440 1.207255 -1.586397
H 2.216641 2.881413 0.561742
H 0.519215 2.485870 0.406134
H 0.269720 -0.796087 -2.601331
H -0.930607 1.148159 -1.047409
H -5.240856 3.424662 1.455065
```

```
H -3.680063 4.275568 1.470584
H -3.878536 2.804296 2.415249
H -5.602410 2.125849 -0.555843
H -0.639080 -1.781127 0.770889
H -6.090057 -1.247239 1.035981
H -5.040838 0.094030 1.551165
H -5.161876 -1.348358 2.546381
H -5.126930 -2.611972 -0.712652
H 5.785419 -1.049962 1.208988
H 5.101053 -0.601273 -2.978111
H -4.769876 0.803247 -2.342853
H -3.229023 -3.459136 -1.855586
$end

$rem
jobtype = sp
basis = 6-311+G(d,p)
aux_basis = rimp2-cc-pvtz
n_frozen_core = fc
correlation = ccsd
cc_t_conv = 4
cc_e_conv = 6
cc_fno_thresh = 9950
cc_direct_ri = false

mem_static = 2000
mem_total = 8000
cc_memory = 100000
max_sub_file_num = 256
$end
```

1.5 Oligoporphyrin

```
$molecule
0 1
H        -12.82461990    -1.34441500     0.00000000
H        -12.82461990     1.34441500     0.00000000
C        -11.97841099    -0.67594620     0.00000000
C        -11.97841099     0.67594620     0.00000000
H        -10.94514224    -3.16984607     0.00000000
H        -10.94514224     3.16984607     0.00000000
C        -10.58266488    -1.08330946     0.00000000
C        -10.58266488     1.08330946     0.00000000
C        -10.16826656    -2.41701954     0.00000000
C        -10.16826656     2.41701954     0.00000000
N         -9.76211904     0.00000000     0.00000000
```

H	-9.07947451	-5.10429627	0.00000000
H	-9.07947451	5.10429627	0.00000000
C	-8.86504393	-2.89173199	0.00000000
C	-8.86504393	2.89173199	0.00000000
C	-8.42239241	-4.25076494	0.00000000
C	-8.42239241	4.25076494	0.00000000
H	-7.74886175	-1.10580132	0.00000000
H	-7.74886175	1.10580132	0.00000000
N	-7.73584565	-2.11519955	0.00000000
N	-7.73584565	2.11519955	0.00000000
C	-7.05528398	-4.25103467	0.00000000
C	-7.05528398	4.25103467	0.00000000
C	-6.61124147	-2.89159923	0.00000000
C	-6.61124147	2.89159923	0.00000000
H	-6.39726669	-5.10356325	0.00000000
H	-6.39726669	5.10356325	0.00000000
N	-5.65561541	0.00000000	0.00000000
C	-5.29948753	-2.42966649	0.00000000
C	-5.29948753	2.42966649	0.00000000
C	-4.87131225	-1.11006337	0.00000000
C	-4.87131225	1.11006337	0.00000000
H	-4.52044475	-3.17947259	0.00000000
H	-4.52044475	3.17947259	0.00000000
C	-3.46110145	-0.71787974	0.00000000
C	-3.46110145	0.71787974	0.00000000
N	-2.38191028	-1.44279686	0.00000000
N	-2.38191028	1.44279686	0.00000000
C	-1.21241473	-0.72467625	0.00000000
C	-1.21241473	0.72467625	0.00000000
H	0.00000000	-2.48972260	0.00000000
C	0.00000000	-1.40938137	0.00000000
C	0.00000000	1.40938137	0.00000000
H	0.00000000	2.48972260	0.00000000
C	1.21241473	-0.72467625	0.00000000
C	1.21241473	0.72467625	0.00000000
N	2.38191028	-1.44279686	0.00000000
N	2.38191028	1.44279686	0.00000000
C	3.46110145	-0.71787974	0.00000000
C	3.46110145	0.71787974	0.00000000
H	4.52044475	-3.17947259	0.00000000
H	4.52044475	3.17947259	0.00000000
C	4.87131225	-1.11006337	0.00000000
C	4.87131225	1.11006337	0.00000000
C	5.29948753	-2.42966649	0.00000000
C	5.29948753	2.42966649	0.00000000
N	5.65561541	0.00000000	0.00000000

```
H          6.39726669    -5.10356325     0.00000000
H          6.39726669     5.10356325     0.00000000
C          6.61124147    -2.89159923     0.00000000
C          6.61124147     2.89159923     0.00000000
C          7.05528398    -4.25103467     0.00000000
C          7.05528398     4.25103467     0.00000000
N          7.73584565    -2.11519955     0.00000000
N          7.73584565     2.11519955     0.00000000
H          7.74886175    -1.10580132     0.00000000
H          7.74886175     1.10580132     0.00000000
C          8.42239241    -4.25076494     0.00000000
C          8.42239241     4.25076494     0.00000000
C          8.86504393    -2.89173199     0.00000000
C          8.86504393     2.89173199     0.00000000
H          9.07947451    -5.10429627     0.00000000
H          9.07947451     5.10429627     0.00000000
N          9.76211904     0.00000000     0.00000000
C         10.16826656    -2.41701954     0.00000000
C         10.16826656     2.41701954     0.00000000
C         10.58266488    -1.08330946     0.00000000
C         10.58266488     1.08330946     0.00000000
H         10.94514224    -3.16984607     0.00000000
H         10.94514224     3.16984607     0.00000000
C         11.97841099    -0.67594620     0.00000000
C         11.97841099     0.67594620     0.00000000
H         12.82461990    -1.34441500     0.00000000
H         12.82461990     1.34441500     0.00000000
$end

$rem
jobtype = sp
exchange = hf
basis = cc-pvdz
aux_basis = rimp2-cc-pvdz
correlation = ccsd
n_frozen_core = fc
cc_t_conv = 4
cc_e_conv = 6
cc_direct_ri = false
mem_static = 1000
mem_total = 8000
cc_memory = 100000
max_sub_file_num = 256
$end
```

2 Molpro inputs used for benchmark calculations

2.1 Test 1

```
memory,15000,m
basis,6-311+g**
angstrom
geometry={
  21
C1 0.00000000 0.00000000 0.00000000
N2 -0.93641400 1.12679100 0.00000000
C3 -0.45341600 2.44241000 0.00000000
C4 -1.47611500 3.46918800 0.00000000
C5 -2.77847400 3.12828100 0.00000000
N6 -3.19345900 1.82520100 0.00000000
C7 -2.28004500 0.77687300 0.00000000
O8 -2.65410800 -0.38301500 0.00000000
C9 -4.60572900 1.45888900 0.00000000
H10 -4.84051300 0.86583300 0.88573100
H11 -5.19804000 2.37431600 0.00000000
H12 -4.84051300 0.86583300 -0.88573100
H13 -3.56813200 3.87138200 0.00000000
H14 -1.15069600 4.49923500 0.00000000
O15 0.74780600 2.68857500 0.00000000
H16 -0.16887900 -0.61461500 0.88556200
H17 -0.16887900 -0.61461500 -0.88556200
H18 1.01374100 0.38737000 0.00000000
O19 3.21009200 1.28914500 0.00000000
H20 2.46429400 1.90890400 0.00000000
H21 4.00786700 1.82086400 0.00000000
}
rhf
ccsd(t)
```

2.2 Test 2

```
memory,16812,m
angstrom
geometry={
C
N, 1 ,B1
C, 2 ,B2 , 1, A1
C, 3 ,B3 , 2, A2 , 1, D1
C, 4 ,B4 , 3, A3 , 2, D2
N, 5 ,B5 , 4, A4 , 3, D3
C, 2 ,B6 , 1, A5 , 3, D4
```

```
O, 7 ,B7 , 2, A6 , 1, D5
C, 6 ,B8 , 5, A7 , 4, D6
H, 9 ,B9 , 6, A8 , 5, D7
H, 9 ,B10, 6, A9 , 5, D8
H, 9 ,B11, 6, A10, 5, D9
H, 5 ,B12, 4, A11, 3, D10
H, 4 ,B13, 3, A12, 2, D11
O, 3 ,B14, 2, A13, 1, D12
H, 1 ,B15, 2, A14, 3, D13
H, 1 ,B16, 2, A15, 3, D14
H, 1 ,B17, 2, A16, 3, D15
O, 1 ,B18, 2, A17, 3, D16
H, 19,B19, 1, A18, 2, D17
H, 19,B20,20, A19, 1, D18
}

 B1= 1.4651044
 B2= 1.4014777
 B3= 1.4492020
 B4= 1.3462383
 B5= 1.3675631
 B6= 1.3884474
 B7= 1.2187133
 B8= 1.4590038
 B9= 1.0914936
B10= 1.0903384
B11= 1.0914936
B12= 1.0843242
B13= 1.0802284
B14= 1.2261854
B15= 1.0910969
B16= 1.0910969
B17= 1.0852307
B18= 3.4592753
B19= 0.9696993
B20= 0.9587335
A1 =120.11237
A2 =114.95453
A3 =120.21724
A4 =122.33356
A5 =115.13094
A6 =122.47166
A7 =122.20569
A8 =110.15925
A9 =108.36333
A10= 110.15925
```

```
A11= 122.07109
A12= 117.58138
A13= 121.74075
A14= 109.52998
A15= 109.52998
A16= 108.81526
A17= 107.84814
A18= 61.606574
A19= 106.58984
D1 =180.00000
D2 =0.0000000
D3 =0.0000000
D4 =180.00000
D5 =0.0000000
D6 =180.00000
D7 =-120.18090
D8 =0.0000000
D9 =120.18090
D10= 180.00000
D11= 180.00000
D12= 0.0000000
D13= 120.55162
D14= -120.55162
D15= 0.0000000
D16= 0.0000000
D17= 0.0000000
D18= 180.00000

cartesian
basis=6-311+g**
{rhf;wf,charge=1,spin=1}
gprint,cpu,micro,io,threshol,mpperr,disk,domains,extensions
{uccsd
wf,charge=1,spin=1}
```

2.3 Test 3

```
memory,16830,m
angstrom
geometry={
39
C1 0.00000000 0.00000000 0.00000000
N2 -1.25983500 0.12719600 -0.73104500
C3 -1.37866700 -0.46791900 -2.00046300
C4 -2.70314800 -0.40124000 -2.57259800
C5 -3.66900700 0.31956500 -1.96742700
```

```
N6 -3.46027600 0.96645700 -0.78005300
C7 -2.25652000 0.85888900 -0.10170100
O8 -2.07953400 1.39367100 0.98248400
C9 -4.50875200 1.76939000 -0.15474700
H10 -4.09920500 2.73943100 0.12752500
H11 -5.29942500 1.91985700 -0.88884700
H12 -4.89322700 1.27171200 0.73861900
H13 -4.64820100 0.46450300 -2.40720700
H14 -2.86904200 -0.88023100 -3.52687900
O15 -0.40456300 -0.97640300 -2.54741700
H16 0.44824900 0.98112800 0.16624000
H17 -0.18350600 -0.46447800 0.97023300
H18 0.65713400 -0.62102000 -0.60439500
N19 0.57159400 2.29112200 -2.53849200
C20 -0.40649600 2.14960100 -3.48011300
H21 -0.15919000 1.49192700 -4.30525900
C22 -1.60999800 2.74718500 -3.37209300
H23 -2.38745400 2.59598100 -4.10724700
C24 -1.91337300 3.53373600 -2.20092700
O25 -3.01151100 4.05674700 -1.98428100
N26 -0.87455600 3.66318500 -1.28104800
C27 -1.09310100 4.41030100 -0.04025100
H28 -0.32675200 5.17892700 0.06276900
H29 -2.08323700 4.85507500 -0.09170600
H30 -1.03460400 3.72079000 0.80398600
C31 0.38487300 3.08922100 -1.41756700
O32 1.26123500 3.26086600 -0.58749600
C33 1.85038400 1.59949600 -2.69252100
H34 2.51848500 2.17661300 -3.33696300
H35 2.30441600 1.50613100 -1.70851200
H36 1.66291700 0.60847600 -3.10874000
O37 -5.09629200 2.75747100 -3.24834900
H38 -5.67841700 3.33947200 -3.74071300
H39 -4.41938300 3.33045800 -2.83640300
}

cartesian
basis,6-31+g**
rhf
gprint,cpu,micro,io,threshol,mpperr,disk,domains,extensions                    !,tasks
{ccsd
}
```