CP2K 8.2

Webpage

https://www.cp2k.org/

Version

8.2 (8.2.0)

Build Environment

- Intel Parallel Studio 2020 Update 2 (MPI only)
- GCC 9.3.1 (devtoolset-9)
- cmake 3.16.3

Files Required

- cp2k-8.2.tar.bz2
- tc_install_fftw3.sh.diff (to avoid build error of libvdwxc)

```
--- install_fftw.sh.org 2021-06-09 09:56:30.000000000 +0900
+++ install_fftw.sh     2021-06-09 09:56:56.000000000 +0900
@@ -96,10 +96,10 @@
   # we may also want to cover FFT_SG
   cat << EOF >> "${BUILDDIR}/setup_fftw"
 export FFTW3_INCLUDES="${FFTW_CFLAGS}"
-export FFTW3_LIBS="${FFTW_LIBS}"
+export FFTW3_LIBS="-L${pkg_install_dir}/lib ${FFTW_LIBS}"
 export FFTW_CFLAGS="${FFTW_CFLAGS}"
 export FFTW_LDFLAGS="${FFTW_LDFLAGS}"
-export FFTW_LIBS="${FFTW_LIBS}"
+export FFTW_LIBS="-L${pkg_install_dir}/lib ${FFTW_LIBS}"
 export CP_DFLAGS="\${CP_DFLAGS} -D__FFTW3 IF_COVERAGE(IF_MPI(|-U__FFTW3)|)"
 export CP_CFLAGS="\${CP_CFLAGS} ${FFTW_CFLAGS}"
 export CP_LDFLAGS="\${CP_LDFLAGS} ${FFTW_LDFLAGS}"
```

- tc_install_plumed.sh.gcc.diff (to simplify path specification)

```
--- install_plumed.sh.org       2021-06-09 11:57:44.000000000 +0900
+++ install_plumed.sh   2021-06-09 11:58:39.000000000 +0900
@@ -83,7 +84,7 @@
 esac

 if [ "$with_plumed" != "__DONTUSE__" ]; then
-  PLUMED_LIBS='-lplumed -ldl -lstdc++ -lz -ldl'
+  PLUMED_LIBS='-lplumedKernel -lplumed -ldl -lstdc++ -lz -ldl'
   if [ "$with_plumed" != "__SYSTEM__" ]; then
     cat << EOF > "${BUILDDIR}/setup_plumed"
 prepend_path LD_LIBRARY_PATH "$pkg_install_dir/lib"
```

Build Procedure

```
#!/bin/sh

INSTDIR=/local/apl/lx/cp2k820

GITHUB_VERSION=8.2.0
VERSION=8.2

SOURCE_ROOT=/home/users/${USER}/Software/CP2K/${GITHUB_VERSION}

TARBALL=${SOURCE_ROOT}/cp2k-${VERSION}.tar.bz2
#export RCCS_COSMA_TARBALL=${SOURCE_ROOT}/COSMA-vrccs.tar.gz
```

```
TC_PATCH_3_1=${SOURCE_ROOT}/tc_install_fftw3.sh.diff
#TC_PATCH_4_1=${SOURCE_ROOT}/tc_install_cosma.sh.diff
TC_PATCH_6_1=${SOURCE_ROOT}/tc_install_plumed.sh.gcc.diff

PARALLEL=12

#-------------------------------------------------------------------------
umask 0022
export LANG=C
export LC_ALL=C

module purge
module load mpi/intelmpi/2019.8.254
module load scl/devtoolset-9
module load cmake/3.16.3

cd $INSTDIR
if [ -d cp2k-${VERSION} ]; then
  mv cp2k-${VERSION} cp2k-erase
  rm -rf cp2k-erase &
fi
tar jxf ${TARBALL}
sleep 5
mv cp2k-${VERSION}/* .
sleep 5
rm -f cp2k-${VERSION}/.dockerignore
rmdir cp2k-${VERSION}

cd ${INSTDIR}/tools/toolchain

# apply patches
cd scripts
cd stage3 && patch < ${TC_PATCH_3_1} && cd -
#cd stage4 && patch < ${TC_PATCH_4_1} && cd -
cd stage6 && patch < ${TC_PATCH_6_1} && cd -
cd ../

export CC=gcc
export CXX=g++
export FC=gfortran
export MPICC=mpicc
export MPICXX=mpicxx
export MPIFC=mpif90

./install_cp2k_toolchain.sh --mpi-mode=intelmpi \
                            --math-mode=openblas \
                            --with-cmake=system \
                            --with-openmpi=no \
                            --with-mpich=no \
                            --with-intelmpi=system \
                            --with-libxc=install \
                            --with-libint=install \
                            --with-fftw=install \
                            --with-acml=no \
                            --with-mkl=no \
                            --with-openblas=install \
                            --with-scalapack=install \
                            --with-libsmm=no \
                            --with-libxsmm=install \
                            --with-elpa=no \
                            --with-ptscotch=install \
                            --with-superlu=install \
                            --with-pexsi=install \
                            --with-quip=install \
```

```
                    --with-plumed=install \
                    --with-sirius=no \
                    --with-gsl=install \
                    --with-libvdwxc=install \
                    --with-spglib=install \
                    --with-hdf5=install \
                    --with-spfft=install \
                    --with-cosma=no \
                    --with-libvori=install \
                    -j ${PARALLEL}

sed -e "s/-Werror / /g" install/arch/local.psmp > ../../arch/rccs.psmp

cd ${INSTDIR}
make -j ${PARALLEL} ARCH=rccs VERSION=psmp
```

Tests

```
#!/bin/sh
#PBS -l select=1:ncpus=16:mpiprocs=16:ompthreads=1:jobtype=core
#PBS -l walltime=12:00:00

export LC_ALL=C
export LANG=""
export OMP_STACKSIZE=64M

# gcc9
module purge
module load mpi/intelmpi/2019.8.254
module load scl/devtoolset-9
module load cmake/3.16.3
CP2K=/local/apl/lx/cp2k820

CP2K_ARCH=rccs
CP2K_VER=psmp
TIMEOUT=600
PARALLEL=16

ulimit -s unlimited
cd ${CP2K}/regtesting/${CP2K_ARCH}/${CP2K_VER}
rm -rf LAST-${CP2K_ARCH}-${CP2K_VER}

# serial test
../../../tools/regtesting/do_regtest \
      -nobuild \
      -arch ${CP2K_ARCH} \
      -version ${CP2K_VER} \
      -mpiranks 1 \
      -ompthreads 1 \
      -jobmaxtime ${TIMEOUT} \
      -cp2kdir ../../../ \
      -maxtasks ${PARALLEL} >& regtest_mpi1_omp1.log
rm -rf LAST-${CP2K_ARCH}-${CP2K_VER}

# omp test
../../../tools/regtesting/do_regtest \
      -nobuild \
      -arch ${CP2K_ARCH} \
      -version ${CP2K_VER} \
      -mpiranks 1 \
      -ompthreads 2 \
      -jobmaxtime ${TIMEOUT} \
      -cp2kdir ../../../ \
      -maxtasks ${PARALLEL} >& regtest_mpi1_omp2.log
rm -rf LAST-${CP2K_ARCH}-${CP2K_VER}
```

```
# mpi test
../../../tools/regtesting/do_regtest \
      -nobuild \
      -arch ${CP2K_ARCH} \
      -version ${CP2K_VER} \
      -mpiranks 2 \
      -ompthreads 1 \
      -jobmaxtime ${TIMEOUT} \
      -cp2kdir ../../../ \
      -maxtasks ${PARALLEL} >& regtest_mpi2_omp1.log
rm -rf LAST-${CP2K_ARCH}-${CP2K_VER}

# mpi/openmp test
../../../tools/regtesting/do_regtest \
      -nobuild \
      -arch ${CP2K_ARCH} \
      -version ${CP2K_VER} \
      -mpiranks 2 \
      -ompthreads 2 \
      -jobmaxtime ${TIMEOUT} \
      -cp2kdir ../../../ \
      -maxtasks ${PARALLEL} >& regtest_mpi2_omp2.log
rm -rf LAST-${CP2K_ARCH}-${CP2K_VER}

# yet another mpi test
../../../tools/regtesting/do_regtest \
      -nobuild \
      -arch ${CP2K_ARCH} \
      -version ${CP2K_VER} \
      -mpiranks 8 \
      -ompthreads 1 \
      -jobmaxtime ${TIMEOUT} \
      -cp2kdir ../../../ \
      -maxtasks ${PARALLEL} >& regtest_mpi8_omp1.log
rm -rf LAST-${CP2K_ARCH}-${CP2K_VER}

# yet another mpi/openmp test
../../../tools/regtesting/do_regtest \
      -nobuild \
      -arch ${CP2K_ARCH} \
      -version ${CP2K_VER} \
      -mpiranks 8 \
      -ompthreads 2 \
      -jobmaxtime ${TIMEOUT} \
      -cp2kdir ../../../ \
      -maxtasks ${PARALLEL} >& regtest_mpi8_omp2.log
rm -rf LAST-${CP2K_ARCH}-${CP2K_VER}
```

Test Results

```
[root@ccfep4 psmp]# grep "GREPME" regtest_mpi*
regtest_mpi1_omp1.log:GREPME 0 0 3396 0 3396 X
regtest_mpi1_omp2.log:GREPME 0 0 3396 0 3396 X
regtest_mpi2_omp1.log:GREPME 0 0 3447 0 3447 X
regtest_mpi2_omp2.log:GREPME 0 0 3447 0 3447 X
regtest_mpi8_omp1.log:GREPME 0 10 3407 0 3417 X
regtest_mpi8_omp2.log:GREPME 0 10 3407 0 3417 X
```

- Errors occurred only on 8 MPI cases.
  - MPI*8, OMP*1
    - QS/regtest-mp2-lr/H2O-mp2-gpw-lr.inp: ENERGY| Total FORCE_EVAL : ref = -16.964068900743456 new = -16.964157811107025
    - QS/regtest-mp2-grad/H2O_grad_mme.inp: ENERGY| Total FORCE_EVAL : ref = -16.766973106034889 new = -16.766973179928165
    - QS/regtest-gpw-4/H2O-debug-5.inp: DIPOLE : CheckSum = : ref = -0.535129866059 new = -

0.535129747930E+00
        - QS/regtest-gpw-4/H2O-debug-6.inp: DIPOLE : CheckSum = : ref = -0.535125994114 new = -0.535125875984E+00
        - QS/regtest-mp2-4/H2O_NO_HFX.inp: ENERGY| Total FORCE_EVAL : ref = -17.253519557463612 new = -17.291360866609697
        - QS/regtest-rma-3D/H2O-32-dftb-ls-2_mult.inp: ENERGY| Total FORCE_EVAL : ref = -32.574187310759356 new = -32.563908850166179
        - QS/regtest-rma-3D/H2O-32-dftb-ls-2.inp: ENERGY| Total FORCE_EVAL : ref = -32.574187310759356 new = -32.563908850166179
        - QS/regtest-rma-3D/H2O-OT-ASPC-1.inp: Total energy: : ref = -17.13993294716182 new = -17.13993294752104
        - QS/regtest-rma-3D/H2O-6.inp: Total energy: : ref = -17.14603641576940 new = -17.14603641519600
        - QS/regtest-mp2-2/H2O-02.inp: ENERGY| Total FORCE_EVAL : ref = -17.157097357548857 new = -17.181101307832947
    - MPI*8, OMP*2
        - QS/regtest-mp2-lr/H2O-mp2-gpw-lr.inp: ENERGY| Total FORCE_EVAL : ref = -16.964068900743456 new = -16.964157811107032
        - QS/regtest-mp2-grad/H2O_grad_mme.inp: ENERGY| Total FORCE_EVAL : ref = -16.766973106034889 new = -16.766973179928165
        - QS/regtest-gpw-4/H2O-debug-5.inp.out: DIPOLE : CheckSum = : ref = -0.535129866059 new = -0.535129747930E+00
        - QS/regtest-gpw-4/H2O-debug-6.inp: DIPOLE : CheckSum = : ref = -0.535125994114 new = -0.535125875984E+00
        - QS/regtest-mp2-4/H2O_NO_HFX.inp: ENERGY| Total FORCE_EVAL : ref = -17.253519557463612 new = -17.291360866609637
        - QS/regtest-rma-3D/H2O-32-dftb-ls-2_mult.inp: ENERGY| Total FORCE_EVAL : ref = -32.574187310759356 new = -32.563908850166179
        - QS/regtest-rma-3D/H2O-32-dftb-ls-2.inp: ENERGY| Total FORCE_EVAL : ref = -32.574187310759356 new = -32.563908850166179
        - QS/regtest-rma-3D/H2O-OT-ASPC-1.inp: Total energy: : ref = -17.13993294716182 new = -17.13993294752103
        - QS/regtest-rma-3D/H2O-6.inp: Total energy: : ref = -17.14603641576940 new = -17.14603641519601
        - QS/regtest-mp2-2/H2O-02.inp: ENERGY| Total FORCE_EVAL : ref = -17.157097357548857 new = -17.181101307832943

Benchmark

We employed H2O-64.inp as in the case of cp2k-7.1. (Output of grep "CP2K " *.log was used.) Run 20 times and average of last 19 runs were shown below. The 1st run was excluded since that result is bit unstable (often slow).

jobtype	# of cores (# of nodes)	MPI	OMP	GPU	elapse(sec)
core	18 (1)	18	1	-	59.96
small	40 (1)	40	1	-	46.00
small	80 (2)	80	1	-	29.05
small	160 (4)	160	1	-	21.61

- OpenMP parallelization is not so effective than the pervious version (7.1.0).
- (7.1.0 intel version might be faster for single node jobtype=small jobs.)
- In jobtype=core benchmark, we reserved whole node and use only 18 cores to exclude other jobs' influence.

Notes

- For this version, GCC build shows clearly better performance than Intel one. This is quite different result from version 7.1 case.
- OpenMP parallelization is not so good in this version unlike the version 7.1.0.
- GPU version not tested.
- We avoid ELPA for this version since BFGS stuck in some cases.
    - In case of regtest, tests with 8-MPI failed on (all?) the BFGS tests, while tests with 1-2 MPI are free from this issue.
    - reference: https://groups.google.com/g/cp2k/c/BAvvW_qGG2I
- We also avoid COSMA for this version.
    - CP2K binary built with COSMA-v2.5.0 does not work regardless of the compiler type (Intel/GCC); all the tests

failed. Unittests of COSMA also failed.
- Changing COSMA version to 2.5.1 did't help.
- The latest snapshot on GitHub (latest commit on Jun 18, 2021) works perfectly. But unfortunately, we couldn't see significant performance improvements and to use this unnamed snapshot (not yet released version) may not be a welcome option. We thus decided not to use COSMA for now.
- tc_install_cosma.sh.diff: a patch to use the latest COSMA, which were archvied (COSMA-vrccs.tar.gz) beforehand. (See installation script above.)

```
--- install_cosma.sh.org        2021-06-21 13:52:52.000000000 +0900
+++ install_cosma.sh    2021-06-21 13:58:10.000000000 +0900
@@ -9,7 +9,7 @@
 [ "${BASH_SOURCE[0]}" ] && SCRIPT_NAME="${BASH_SOURCE[0]}" || SCRIPT_NAME=$0
 SCRIPT_DIR="$(cd "$(dirname "$SCRIPT_NAME")/.." && pwd -P)"

-cosma_ver="2.5.0"
+cosma_ver="rccs"
 cosma_sha256="7f68bb0ee5c80f9b8df858afcbd017ad4ed87ac09439d13d7d890844dbdd3d54"
 source "${SCRIPT_DIR}"/common_vars.sh
 source "${SCRIPT_DIR}"/tool_kit.sh
@@ -37,9 +37,7 @@
       if [ -f COSMA-v${cosma_ver}.tar.gz ]; then
         echo "COSMA-v${cosma_ver}.tar.gz is found"
       else
-        download_pkg ${DOWNLOADER_FLAGS} ${cosma_sha256} \
-          "https://github.com/eth-cscs/COSMA/releases/download/v${cosma_ver}/COSMA-v${cosma_ver}.tar.gz" \
-          -o COSMA-v${cosma_ver}.tar.gz
+        cp ${RCCS_COSMA_TARBALL} .
       fi
       echo "Installing from scratch into ${pkg_install_dir}"
       [ -d COSMA-${cosma_ver} ] && rm -rf COSMA-${cosma_ver}
```