

CP2K 7.1.0 (gnu)

Webpage

<https://www.cp2k.org/>

Version

7.1.0

Build Environment

- OpenMPI 4.0.2 (GCC 7.3 version)
- GCC 7.3.1 (devtoolset-7)
- cmake 3.16.3

Files Required

- cp2k-7.1.0.tar.gz
- dbcsr-2.0.1.tar.gz
- tc_install_cp2k_toolchain.sh.diff

```
--- install_cp2k_toolchain.sh.org 2020-01-31 17:07:19.000000000 +0900
+++ install_cp2k_toolchain.sh 2020-01-31 17:07:30.000000000 +0900
@@ -942,8 +942,8 @@
  ./scripts/install_superlu.sh
  ./scripts/install_pexsi.sh
  ./scripts/install_quip.sh
- ./scripts/install_plumed.sh
  ./scripts/install_gsl.sh
+ ./scripts/install_plumed.sh
  ./scripts/install_spglib.sh
  ./scripts/install_hdf5.sh
  ./scripts/install_libvdwxc.sh
```

- tc_install_sirius.sh.diff

```
--- install_sirius.sh.org 2020-02-25 14:50:50.000000000 +0900
+++ install_sirius.sh 2020-02-25 14:48:01.000000000 +0900
@@ -131,8 +131,8 @@
  -DSpFFT_DIR="${SPFFT_ROOT}/lib/cmake/SpFFT" \
  -DCMAKE_CXXFLAGS_RELEASE="${SIRIUS_OPT}" \
  -DCMAKE_CXX_FLAGS_RELWITHDEBINFO="${SIRIUS_DBG}" \
- -DCMAKE_CXX_COMPILER=mpic++ \
- -DCMAKE_C_COMPILER=mpicc \
+ -DCMAKE_CXX_COMPILER=${MPICXX} \
+ -DCMAKE_C_COMPILER=${MPICC} \
  ${COMPILE_OPTIONS} .. > compile.log 2>&1
  make -j $NPROCS -C src >> compile.log 2>&1

@@ -155,8 +155,8 @@
  -DCMAKE_CXX_FLAGS_RELWITHDEBINFO="${SIRIUS_DBG}" \
  -DUSE_CUDA=ON \
  -DGPU_MODEL=P100 \
- -DCMAKE_CXX_COMPILER=mpic++ \
- -DCMAKE_C_COMPILER=mpicc ${COMPILE_OPTIONS} .. >> compile.log 2>&1
+ -DCMAKE_CXX_COMPILER=${MPICXX} \
+ -DCMAKE_C_COMPILER=${MPICC} ${COMPILE_OPTIONS} .. >> compile.log 2>&1
  make -j $NPROCS -C src >> compile.log 2>&1
  install -d ${pkg_install_dir}/lib/cuda
  install -d ${pkg_install_dir}/include/cuda
```

- tc_install_plumed_noext.sh.diff

```

--- install_plumed.sh.org    2020-02-19 13:43:07.000000000 +0900
+++ install_plumed.sh    2020-02-19 13:42:49.000000000 +0900
@@ -40,7 +40,7 @@

    echo "Installing from scratch into ${pkg_install_dir}"
    cd plumed-${plumed_ver}
-   ./configure CXX="${MPICXX}" --prefix=${pkg_install_dir} --libdir="${pkg_install_dir}/lib" > configure.log 2>&1
+   ./configure CXX="${MPICXX}" --prefix=${pkg_install_dir} --libdir="${pkg_install_dir}/lib" CXXFLAGS="-I${GSLROOT}/include" LIBS="-L${GSLROOT}/lib" --enable-external-lapack=no --enable-external-blas=no > configure.log 2>&1
    make -j $NPROCS > make.log 2>&1
    make install > install.log 2>&1
    write_checksums "${install_lock_file}" "${SCRIPT_DIR}/${basename ${SCRIPT_NAME}}"
@@ -63,7 +63,7 @@
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/cp2k710-gnu

VERSION=7.1.0
DBCSR_VERSION=2.0.1

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

TARBALL=${SOURCE_ROOT}/cp2k-${VERSION}.tar.gz
TARBALL_DBCSR=${SOURCE_ROOT}/dbscr-${DBCSR_VERSION}.tar.gz

TC_PATCH0=${SOURCE_ROOT}/tc_install_cp2k_toolchain.sh.diff
TC_PATCH5=${SOURCE_ROOT}/tc_install_sirius.sh.diff
TC_PATCH9=${SOURCE_ROOT}/tc_install_plumed_noext.sh.diff

PARALLEL=12

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

module purge
module load scl/devtoolset-7
module load mpi/openmpi/4.0.2/gnu7.3
module load cmake/3.16.3

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

cd ${INSTDIR}/tools/toolchain

```

```

patch < ${TC_PATCH0}

cd scripts
patch < ${TC_PATCH5}
patch < ${TC_PATCH9}
cd ../

export MPICC=mpicc
export MPICXX=mpicxx
export MPIFC=mpif90

./install_cp2k_toolchain.sh --math-mode=openblas \
    --mpi-mode=openmpi \
    --with-cmake=system \
    --with-mpich=no \
    --with-libxc=install \
    --with-libint=install \
    --with-fftw=install \
    --with-openblas=install \
    --with-scalapack=install \
    --with-reflapack=no \
    --with-mkl=no \
    --with-libxsmm=install \
    --with-elpa=install \
    --with-ptscotch=install \
    --with-pexsi=install \
    --with-parmetis=install \
    --with-superlu=install \
    --with-quip=install \
    --with-plumed=install \
    --with-gsl=install \
    --with-libvdwxc=install \
    --with-spglib=install \
    --with-hdf5=install \
    --with-sfft=install \
    -j ${PARALLEL}

cp install/arch/local.psmf ../arch/rccs.psmf

cd ${INSTDIR}/exts
rmdir dbcscr
tar xzf ${TARBALL_DBCSR}
mv dbcscr-${DBCSCR_VERSION} dbcscr
cd ../
make -j ${PARALLEL} ARCH=rccs VERSION=psmf

```

Tests

Test script below was executed on ccfep.

```

#!/bin/sh

export LC_ALL=C
export LANG=""

# gcc8
module purge
module load scl/devtoolset-7
module load mpi/openmpi/4.0.2/gnu7.3
module load cmake/3.16.3
#CP2K=/home/users/qf7/Software/CP2K/7.1.0/cp2k-7.1.0-gcc7-openmpi4-openblas
CP2K=/local/apl/ix/cp2k710-gnu

CP2K_ARCH=rccs
CP2K_VER=psmf

```

TIMEOUT=120

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 \

-nosvn \

-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 \

-nosvn \

-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 \

-nosvn \

-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 \

-nosvn \

-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 \

-nosvn \

-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 \  
-nosvn \  
-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}
```

■ Result: MPI1 - OMP1

```
----- Summary -----  
Number of FAILED tests 1  
Number of WRONG tests 0  
Number of CORRECT tests 3217  
Number of NEW tests 3  
Total number of tests 3221
```

- QS/regtest-also-2/ion-pair.inp: RUNTIME FAIL

■ Result: MPI1 - OMP2

```
----- Summary -----  
Number of FAILED tests 1  
Number of WRONG tests 1  
Number of CORRECT tests 3216  
Number of NEW tests 3  
Total number of tests 3221
```

- QS/regtest-also-2/ion-pair.inp: RUNTIME FAIL
- SE/regtest/h2o_gks_e.inp: WRONG

■ Result: MPI2 - OMP1

```
----- Summary -----  
Number of FAILED tests 0  
Number of WRONG tests 0  
Number of CORRECT tests 3278  
Number of NEW tests 8  
Total number of tests 3286
```

■ Result: MPI2 - OMP2

```
----- Summary -----  
Number of FAILED tests 0  
Number of WRONG tests 0  
Number of CORRECT tests 3278  
Number of NEW tests 8  
Total number of tests 3286
```

■ Result: MPI8 - OMP1

```
----- Summary -----  
Number of FAILED tests 0  
Number of WRONG tests 9  
Number of CORRECT tests 3228
```


- Explicit legacy MPI1 support is required when built with OpenMPI 4.x. (Requested by scalapack (or mkl).)
- gcc8 build is not good as gcc7 one in terms of performance and reliability.