

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
- ▶ dbcsrc-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_libvdx.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=${SOURCE_ROOT}/dbcsr-${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-libvdx=install \
```

```
  --with-spglib=install \
```

```

--with-hdf5=install \
--with-spfft=install \
-j ${PARALLEL}

cp install/arch/local.psmpp ../arch/rccs.psmpp

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

```

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/lx/cp2k710-gnu

CP2K_ARCH=rccs
CP2K_VER=psmpp
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 \
-omphthreads 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 \
-omphthreads 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 \
-omphthreads 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
Number of NEW tests 6

```

Total number of tests 3243

- ▶ QS/regtest-mp2-lr/H2O-mp2-gpw-lr.inp: WRONG
- ▶ xTB/regtest-2/HF-field-gopt.inp: WRONG
- ▶ QS/regtest-mp2-grad/H2O_grad_mme.inp: WRONG
- ▶ QS/regtest-gpw-4/H2O-debug-5.inp: WRONG
- ▶ QS/regtest-gpw-4/H2O-debug-6.inp: WRONG
- ▶ QS/regtest-mp2-4/H2O_NO_HFX.inp: WRONG
- ▶ QS/regtest-rma-3D/H2O-32-dftb-ls-2_mult.inp: WRONG
- ▶ QS/regtest-rma-3D/H2O-32-dftb-ls-2.inp: WRONG
- ▶ QS/regtest-mp2-2/H2O-02.inp: WRONG

Result: MPI8 - OMP2

```
----- Summary -----  
Number of FAILED tests 0  
Number of WRONG tests 9  
Number of CORRECT tests 3228  
Number of NEW tests 6  
Total number of tests 3243
```

- ▶ QS/regtest-mp2-lr/H2O-mp2-gpw-lr.inp: WRONG
- ▶ xTB/regtest-2/HF-field-gopt.inp: WRONG
- ▶ QS/regtest-mp2-grad/H2O_grad_mme.inp: WRONG
- ▶ QS/regtest-gpw-4/H2O-debug-5.inp: WRONG
- ▶ QS/regtest-gpw-4/H2O-debug-6.inp: WRONG
- ▶ QS/regtest-mp2-4/H2O_NO_HFX.inp: WRONG
- ▶ QS/regtest-rma-3D/H2O-32-dftb-ls-2_mult.inp: WRONG
- ▶ QS/regtest-rma-3D/H2O-32-dftb-ls-2.inp: WRONG
- ▶ QS/regtest-mp2-2/H2O-02.inp: WRONG

Benchmark

H2O-64.inp was employed for benchmark as in 6.1.0. (output of `grep "CP2K" *.log` is used)
Ran 21 times, and average of last 20 runs is listed below.

jobtype	# of cores (# of nodes)	MPI	OMP	GPU	elapse(sec)
core	18 (1)	18	1	-	72.685
small	40 (1)	40	1	-	51.424
small	80 (2)	80	1	-	36.697
small	160 (4)	32	5	-	27.455

Notes

- ▶ GPU versions were skipped for this version; they are not so useful in RCCS for now.
 - ▶ SIRIUS GPU version might be efficient if correctly built with MAGMA etc. But skipped this time.
- ▶ We couldn't get performance improvement from libgrid (slower than the vanilla one).
 - ▶ pyratemp 0.3.2 was used when building libgrid.a. But this version of pyratemp cannot handle *.template files in xyz_to_vab correctly.
 - ▶ Applying `sed -i -e "s\\$\\!/g" -e "s^@<^\\!/g" -e "s/>^@\\!/g"` to *.template files can solve the issue, although the libgrid.a didn't bring any performance improvement...
 - ▶ (Use `sed -i -e "s\\$\\!/g" -e "s^@<^\\!/g" -e "s/>^@\\!/g"` in the script; above one is valid only when manual execution on terminal.)
- ▶ libsmm is simply ignored as in the case of 6.1.0.
- ▶ Released version of dcsr was used in this build. Using master branch of dcsr is not a good way to build reliable binary.
- ▶ At least for GCC build, OpenBlas is better than MKL in terms of performance.
- ▶ GCC + Intel MPI failed on building cp2k. MPI module is concerned with this error, but we cannot identify the cause of this error. It might come from the wrong include path setting.
- ▶ Couldn't build correctly with OpenMPI 3.1.0. It turned out to be a known issue.
 - ▶ <https://github.com/cp2k/dcsr/issues/141>
- ▶ 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.