CP2K 9.1

Webpage

https://www.cp2k.org/

Version

9.1 (9.1.0)

Build Environment

- GCC 11.2.1 (gcc-toolset-11)
- HPC-X 2.13.1 (Open MPI 4.1.5)

Files Required

- cp2k-9.1.0.tar.gz
- tc-install-libint.sh.diff

```
--- scripts/stage3/install_libint.sh.org        2022-01-26 09:34:28.922143775 +0900
+++ scripts/stage3/install_libint.sh    2022-01-26 09:41:44.440708192 +0900
@@ -90,6 +90,7 @@
         # Fix bug in makefile for Fortran module
         sed -i "s/\$(CXX) \$(CXXFLAGS)/\$(FC) \$(FCFLAGS)/g" fortran/Makefile
       fi
+      sed -i 's/FCLIBS)/FCLIBS) -lstdc++/' fortran/Makefile

       make -j $(get_nprocs) > make.log 2>&1
       make install > install.log 2>&1
```

- patch-openblas-makefile

```
--- scripts/stage2/install_openblas.sh.org      2023-01-17 10:19:31.000000000 +0900
+++ scripts/stage2/install_openblas.sh  2023-01-17 10:20:21.000000000 +0900
@@ -47,6 +47,7 @@
       [ -d OpenBLAS-${openblas_ver} ] && rm -rf OpenBLAS-${openblas_ver}
       tar -zxf ${openblas_pkg}
       cd OpenBLAS-${openblas_ver}
+      sed -i -e "/NOTPARALLEL/s/$/ shared/" Makefile

       # First attempt to make openblas using auto detected
       # TARGET, if this fails, then make with forced
```

Build Procedure

```
#!/bin/sh

INSTDIR=/apl/cp2k/9.1

GITHUB_VERSION=9.1.0
VERSION=9.1.0
DBCSR_VERSION=v2.2.0

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

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

TC_PATCH_3_1=${SOURCE_ROOT}/tc-install-libint.sh.diff
TC_PATCH_2_OB=${SOURCE_ROOT}/patch-openblas-makefile

PARALLEL=12

#------------------------------------------------------------------------------
```

```
umask 0022
export LANG=C
export LC_ALL=C
ulimit -s unlimited

module purge
module load gcc-toolset/11
module load openmpi/4.1.5-hpcx/gcc11

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

cd ${INSTDIR}/tools/toolchain

# apply patches
patch -p0 < ${TC_PATCH_3_1}
patch -p0 < ${TC_PATCH_2_OB}

# ad hoc...
sed -i -e "s/https:.*/https:\/\/github.com\/spglib\/spglib\/archive\/refs\/tags\/v1.16.2.tar.gz \\\/" scripts/stage7/install_spglib.sh

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

./install_cp2k_toolchain.sh --mpi-mode=openmpi \
                            --math-mode=openblas \
                            --with-gcc=system \
                            --with-cmake=system \
                            --with-openmpi=system \
                            --with-mpich=no \
                            --with-intelmpi=no \
                            --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=no \
                            --with-superlu=no \
                            --with-pexsi=no \
                            --with-quip=install \
                            --with-plumed=install \
                            --with-sirius=install \
                            --with-gsl=install \
                            --with-libvdwxc=install \
                            --with-spglib=install \
                            --with-hdf5=install \
                            --with-spfft=install \
```

```
                    --with-spla=install \
                    --with-cosma=no \
                    --with-libvori=install \
                    -j ${PARALLEL}

cp install/arch/local.psmp ../../arch/rccs.psmp

cd ${INSTDIR}
cd ${INSTDIR}/exts
rmdir dbcsr
git clone https://github.com/cp2k/dbcsr.git
cd dbcsr
git checkout refs/tags/${DBCSR_VERSION}
git submodule update --init --recursive
cd ${INSTDIR}

make -j ${PARALLEL} ARCH=rccs VERSION=psmp
make -j ${PARALLEL} ARCH=rccs VERSION=psmp libcp2k
```

Tests

Following scripts was used for testing.

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

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

module purge
module load gcc-toolset/11
module load openmpi/4.1.5-hpcx/gcc11

CP2K=/apl/cp2k/9.1

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

# 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}
```

results

```
$ grep GREPME regtest_mpi*
regtest_mpi1_omp1.log:GREPME 0 0 3586 0 3586 X
regtest_mpi1_omp2.log:GREPME 0 0 3586 0 3586 X
regtest_mpi2_omp1.log:GREPME 0 0 3642 0 3642 X
regtest_mpi2_omp2.log:GREPME 0 0 3642 0 3642 X
regtest_mpi8_omp1.log:GREPME 11 16 3629 0 3656 X
regtest_mpi8_omp2.log:GREPME 11 17 3628 0 3656 X
```

Test results are available at /apl/cp2k/9.1/regtesting/rccs/psmp.

Notes

- elpa doesn't work well. Simply disabled.
- If openmpi is employed, superlu can't be enabled. pexsi and ptscotch (depends on superlu) are also disabled.
- (intel mpi version is not intensively tested. At this time, there was no workaround available for the Intel MPI issue solved on Feb 3.)
- (Jul 26, 2024) Runtime library of HPC-X 2.11 or 2.13.1 cause significant performance loss for calculation of H20-256 system with 128 MPI processes. This problem can be removed by switching to Open MPI 4.1.5, 4.1.6 or HPC-X 2.16 runtime libraries.