

CP2K 2024.2

Webpage

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

Version

2024.2

Build Environment

- GCC 13.1.1 (gcc-toolset-13)
- HPC-X 2.16 (Open MPI 4.1.5)

Files Required

- cp2k-2024.2.tar.bz2

Build Procedure

```
#!/bin/sh
VERSION=2024.2
INSTDIR=/apl/cp2k/2024.2
SOURCE_ROOT=/home/users/${USER}/Software/CP2K/${VERSION}
TARBALL=${SOURCE_ROOT}/cp2k-${VERSION}.tar.bz2
PARALLEL=32
# -----
umask 0022
export LANG=C
export LC_ALL=C
ulimit -s unlimited
module -s purge
module -s load gcc-toolset/13
module -s load openmpi/4.1.5-hpcx2.16/gcc13

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 -rf cp2k-${VERSION}/.dockerignore
rmdir cp2k-${VERSION}
cd ${INSTDIR}/tools/toolchain

sed -i -e "/PARMETISLIB=FALSE/"a'-DCMAKE_C_COMPILER=${MPICC} -DCMAKE_CXX_COMPILER=${MPICXX} \' scripts/stage5/install_superlu.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-libxsmm=install \  
--with-elpa=install \  
--with-ptscotch=install \  
--with-superlu=install \  
--with-pexsi=install \  
--with-quip=install \  
--with-plumed=install \  
--with-sirius=install \  
--with-gsl=install \  
--with-libvdx=install \  
--with-spglib=install \  
--with-hdf5=install \  
--with-sfft=install \  
--with-spla=install \  
--with-cosma=install \  
--with-libvori=install \  
--with-libtorch=install
```

```
cp install/arch/local.psmpl ../arch/rccs.psmpl  
cd ${INSTDIR}  
# dcsr source code is already available  
make -j ${PARALLEL} ARCH=rccs VERSION=psmpl  
make -j ${PARALLEL} ARCH=rccs VERSION=psmpl libcp2k
```

Tests

Following job script was employed.

```
#!/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 -s purge  
module -s load gcc-toolset/13  
module -s load openmpi/4.1.5-hpcx2.16/gcc13  
  
CP2K=/apl/cp2k/2024.2  
  
CP2K_ARCH=rccs  
CP2K_VER=psmpl  
TIMEOUT=600  
PARALLEL=16  
  
ulimit -s unlimited  
  
cd ${CP2K}/regtesting/${CP2K_ARCH}/${CP2K_VER} || { echo "Failed to change directory"; exit 1; }  
rm -rf LAST-${CP2K_ARCH}-${CP2K_VER}  
  
#serial test  
echo "Starting serial test at $(date)"  
../..../tests/do_regtest.py \  
    --mpiranks 1 \  
    --ompthreads 1 \  
    --timeout ${TIMEOUT} \  
--workbasedir ../..../ \  
--maxtasks ${PARALLEL} \  
{CP2K_ARCH} {CP2K_VER} >& regtest_mpi1_omp1.log
```

```

rm -rf LAST-${CP2K_ARCH}-${CP2K_VER}

# # omp test
../../tests/do_regtest.py \
    --mpiranks 1 \
    --ompthreads 2 \
    --timeout ${TIMEOUT} \
--workbasedir ../../ \
--maxtasks ${PARALLEL} \
${CP2K_ARCH} ${CP2K_VER} >& regtest_mpi1_omp2.log
rm -rf LAST-${CP2K_ARCH}-${CP2K_VER}

# # mpi test
../../tests/do_regtest.py \
    --mpiranks 2 \
    --ompthreads 1 \
    --timeout ${TIMEOUT} \
--workbasedir ../../ \
--maxtasks ${PARALLEL} \
${CP2K_ARCH} ${CP2K_VER} >& regtest_mpi2_omp1.log
rm -rf LAST-${CP2K_ARCH}-${CP2K_VER}

# # mpi/openmp test
../../tests/do_regtest.py \
    --mpiranks 2 \
    --ompthreads 2 \
    --timeout ${TIMEOUT} \
--workbasedir ../../ \
--maxtasks ${PARALLEL} \
${CP2K_ARCH} ${CP2K_VER} >& regtest_mpi2_omp2.log
rm -rf LAST-${CP2K_ARCH}-${CP2K_VER}

# # yet another mpi test
../../tests/do_regtest.py \
    --mpiranks 8 \
    --ompthreads 1 \
    --timeout ${TIMEOUT} \
--workbasedir ../../ \
--maxtasks ${PARALLEL} \
${CP2K_ARCH} ${CP2K_VER} >& regtest_mpi8_omp1.log
rm -rf LAST-${CP2K_ARCH}-${CP2K_VER}

# # yet another mpi/openmp test
../../tests/do_regtest.py \
    --mpiranks 8 \
    --ompthreads 2 \
    --timeout ${TIMEOUT} \
--workbasedir ../../ \
--maxtasks ${PARALLEL} \
${CP2K_ARCH} ${CP2K_VER} >& regtest_mpi8_omp2.log
rm -rf LAST-${CP2K_ARCH}-${CP2K_VER}

```

Notes

- Please check [/apl/cp2k/2023.1/regtesting/rccs/psmp](#) and its sub-directory for details about tests.
 - `summary.txt`, `error_summary`, `timings.txt` may be informative.
- (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.