

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:mpiexecs=16:omphreads=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 \
    --omphreads 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.