

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 xzf ${TARBALL}
sleep 5
mv cp2k-${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-libvdx=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.psmpl ../../arch/rccs.psmpl

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

```

Tests

Following scripts was used for testing.

```

#!/bin/sh
#PBS -l select=1:ncpus=16:mpiprocs=16:omphreads=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=psmpl
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 \
  -omphreads 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 \

```

```

-omphthreads 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 \
-omphthreads 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 \
-omphthreads 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 \
-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 \
-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}

```

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

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- 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.