

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

2023.1

- GCC 11.2.1 (gcc-toolset-11)
- HPC-X 2.11 (Open MPI 4.1.4)

- cp2k-2023.1.tar.gz
- patch-openblas.diff

```

--- 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

```

- patch-plumed.diff

```

--- scripts/stage6/install_plumed.sh.org 2023-04-04 15:56:54.000000000 +0900
+++ scripts/stage6/install_plumed.sh 2023-04-04 15:57:28.000000000 +0900
@@ -90,7 +90,7 @@
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"

```

- patch-spla-nogpu.diff

```

--- scripts/stage8/install_spla.sh.org 2023-04-04 15:31:42.000000000 +0900
+++ scripts/stage8/install_spla.sh 2023-04-04 15:37:09.000000000 +0900
@@ -204,6 +204,11 @@
export CP_LDFLAGS="\${CP_LDFLAGS}; IF_CUDA(\${SPLA_CUDA_LDFLAGS})\${SPLA_LDFLAGS}"
EOF
fi
+ if [ "$ENABLE_CUDA" != "__TRUE__" -a "$ENABLE_HIP" != "__TRUE__" ]; then
+ cat << EOF >> "${BUILDDIR}/setup_spla"
+export CP_LDFLAGS="\${CP_LDFLAGS} \${SPLA_LDFLAGS}"
+EOF
+ fi
  cat "${BUILDDIR}/setup_spla" >> $SETUPFILE
fi

```

#!/bin/sh

```

VERSION=2023.1
DBCSR_VERSION=v2.5.0

INSTDIR=/apl/cp2k/${VERSION}

SOURCE_ROOT=/home/users/${USER}/Software/CP2K/${VERSION}
TARBALL=${SOURCE_ROOT}/cp2k-${VERSION}.tar.bz2

TC_PATCH_2_1=${SOURCE_ROOT}/patch-openblas.diff
TC_PATCH_6_1=${SOURCE_ROOT}/patch-plumed.diff
TC_PATCH_8_1=${SOURCE_ROOT}/patch-spla-nogpu.diff

PARALLEL=32

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

module -s purge
module -s load gcc-toolset/11
module -s load openmpi/4.1.4-hpcx/gcc11

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

# apply patches
patch -p0 < ${TC_PATCH_2_1}
patch -p0 < ${TC_PATCH_6_1}
patch -p0 < ${TC_PATCH_8_1}
sed -i -e "/PARAMETISLIB=FALSE/"a'-DCMAKE_C_COMPILER=${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-spfft=install \  
--with-spla=install \  
--with-cosma=install \  
--with-libvori=install \  
--with-libtorch=install
```

```
cp install/arch/local.psmpl ../arch/rccs.psmpl  
cd ${INSTDIR}
```

```
# dbscr 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: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/11  
module -s load openmpi/4.1.4-hpcx/gcc11  
  
CP2K=/apl/cp2k/2023.1  
  
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
rm -rf LAST-#{CP2K_ARCH}-#{CP2K_VER}

# 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:

```
regtest_mpi1_omp1.log:GREPME 0 0 3868 0 3868 X
```

```
regtest_mpi1_omp2.log:GREPME 0 0 3868 0 3868 X
regtest_mpi2_omp1.log:GREPME 0 0 3926 0 3926 X
regtest_mpi2_omp2.log:GREPME 0 0 3926 0 3926 X
regtest_mpi8_omp1.log:GREPME 10 15 3908 0 3933 X
regtest_mpi8_omp2.log:GREPME 10 15 3908 0 3933 X
```

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.
- Superlu is successfully activated by passing compilers explicitly. (This was failed in [the previous build](#).)
- Cosma is enabled this time. There are no noticeable problems in the build/performance.
- GPU version is not released this time. Although performance is improved by GPUs in some cases, GPU version seems bit unstable.
 - Some investigations may be required to get good performance. (More difficult than CPU version.)
 - Memory usage level seems to be very high. Mpirun command often needs `"-mca coll_hcoll_enable 0"` to run correctly.
 - If GPUs are available only to toolchain part, the overall calculations and performances become stable. However, performance improvement is limited (performance is often worse than cpu only version).
- Following message may be harmless since the cp2k is built with `"-mtune=native"` option.
 - Most probably, this message is related to `-march` option in the build time. (`-march` is not specified)

```
*** HINT in environment.F:884 :: The compiler target flags (generic) used ***
*** to build this binary cannot exploit all extensions of this CPU model ***
*** (x86_avx2). Consider compiler target flags as part of FCFLAGS and ***
```

- (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.