

## CP2K 2025.2

## Web Page

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

## Version

2025.2

## Build Environment

- GCC 13.1.1 (gcc-toolset-13)
- Open MPI 4.1.8

## Files Required for Build

- cp2k-2025.2.tar.bz2

## Build Procedure

```
#!/bin/sh
set -e # Exit immediately on error

VERSION=2025.2
DBCSR_VERSION=v2.5.0
INSTDIR=/apl/cp2k/${VERSION}
SOURCE_ROOT=/home/users/${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/4.1.8/gcc13
module -s load cmake/3.31.6

rm -rf $INSTDIR/*
cd $INSTDIR
if [ -d cp2k-${VERSION} ]; then
  mv cp2k-${VERSION} cp2k-erase
  rm -rf cp2k-erase &
```

fi

```
tar jxf ${TARBALL}
sleep 5
rsync -aq cp2k-${VERSION}/ ./
sleep 5
rm -rf cp2k-${VERSION} # Use rm -rf instead of rmdir

cd ${INSTDIR}/tools/toolchain
```

```
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-libgrpp=install \
    --with-acml=no \
    --with-mkl=no \
    --with-openblas=install \
    --with-scalapack=install \
    --with-libxsmm=install \
    --with-elpa=install \
    --with-deepmd=no \
    --with-plumed=install \
    --with-sirius=install \
    --with-gsl=install \
    --with-libvdxwc=install \
    --with-spglib=install \
    --with-hdf5=install \
    --with-spfft=install \
    --with-spla=install \
    --with-cosma=install \
    --with-libvori=install \
    --with-libtorch=no \
    --with-libsmeagol=install \
```

```
--with-dftd4=install \
--with-tblite=install \
--with-trexio=install \
--with-greenx=install \
--with-gmp=install \
--with-ace=install \
-j ${PARALLEL}
```

source install/setup

cd \${INSTDIR}

**# Delete build directory if it exists**

if [ -d "build" ]; then

echo "Deleting existing build directory..."

rm -rf build

fi

mkdir build

cd build

**# CMake configuration**

cmake -S .. -B . \

```
-DCMAKE_BUILD_TYPE=Release \
-DCMAKE_INSTALL_PREFIX=${INSTDIR} \
-DCP2K_USE_ACCEL=OFF \
-DCP2K_WITH_CUDA_PROFILING=OFF \
-DCP2K_USE_MPI=ON \
-DCP2K_USE_MPI_F08=ON \
-DCP2K_ENABLE_DBM_GPU=OFF \
-DCP2K_ENABLE_GRID_GPU=OFF \
-DCP2K_ENABLE_PW_GPU=OFF \
-DCP2K_USE_COSMA=ON \
-DCP2K_USE_ELPA=ON \
-DCP2K_ENABLE_ELPA_OPENMP_SUPPORT=ON \
-DCP2K_USE_SPLA=ON \
-DCP2K_USE_SPLA_GEMM_OFFLOADING=OFF \
-DCP2K_USE_LIBXSMM=ON \
-DCP2K_USE_FFTW3=ON \
-DCP2K_ENABLE_FFTW3_OPENMP_SUPPORT=ON \
-DCP2K_USE_LIBXC=ON \
-DCP2K_USE_LIBINT2=ON \
-DCP2K_USE_SIRIUS=ON \
-DCP2K_USE_LIBVDWXC=ON \
-DCP2K_USE_SIRIUS_DFTD4=ON \
-DCP2K_USE_SIRIUS_VCSQNM=ON \
-DCP2K_USE_SIRIUS_NLCG=ON \
-DCP2K_USE_DFTD4=ON \
-DCP2K_USE_TBLITE=ON \
```

```
-DCP2K_USE_ACE=OFF \
-DCP2K_USE_GRPP=ON \
-DCP2K_USE_DEEPMD=OFF \
-DCP2K_USE_PLUMED=ON \
-DCP2K_USE_PEXSI=OFF \
-DCP2K_USE_LIBSMEAGOL=ON \
-DCP2K_USE_GREENX=ON \
-DCP2K_USE_HDF5=ON \
-DCP2K_USE_SPGLIB=ON \
-DCP2K_USE_VORI=ON \
-DCP2K_USE_TREXIO=ON \
-DBUILD_SHARED_LIBS=OFF \
-DCMAKE_POSITION_INDEPENDENT_CODE=ON
```

# **Execute build**

```
cmake --build . -j ${PARALLEL}
```

```
cmake --build . --target install -j ${PARALLEL}
```

## Testing

Execute with the following job script:

```
#!/bin/sh
#PBS -l select=1:ncpus=2:mpiprocs=2:omphreads=1
#PBS -l walltime=72:00:00

set -e

VERSION=2025.2
INSTDIR=/apl/cp2k/${VERSION}
WORKDIR=$(pwd)

module -s purge
module -s load openmpi/4.1.8/gcc13

cd ${INSTDIR}

source tools/toolchain/install/setup

export CP2K_DATA_DIR=${INSTDIR}/data/
python3.11 ./tests/do_regtest.py ${INSTDIR}/bin psmp --mpiranks=1 --omphreads=1 --timeout=4000 >
${WORKDIR}/mpi1_omp1.log

python3.11 ./tests/do_regtest.py ${INSTDIR}/bin psmp --mpiranks=2 --omphreads=1 --timeout=4000 >
${WORKDIR}/mpi2_omp1.log

python3.11 ./tests/do_regtest.py ${INSTDIR}/bin psmp --mpiranks=1 --omphreads=2 --timeout=4000 >
${WORKDIR}/mpi1_omp2.log
```

The following error occurs in the test with MPI=1, OMP=2:

----- Errors -----

XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX

SE/regtest-2-2/ZrF2-PM6.inp.out

Spec: {'matcher': 'M003', 'tol': 4e-12, 'ref': -985.9930664264728}

Difference too large: 4.64e-12 > 4e-12, value: -985.9930664218987.

Regarding Library Selection

- gcc14 produces numerical errors in several tests.
- Open MPI 5 series may have slower computation speed.