

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
```

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

[illegible]

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.