

## CP2K 6.1.0 for LX

### Webpage

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

### Version

6.1.0

### Build Environment

- Intel Parallel Studio 2017 Update 8
- CUDA Toolkit 9.1.85 (only for GPU version)
- spglib/1.11.1

### Files Required

- cp2k-6.1.0.tar.gz
- plumed-2.4.3.tgz
- (some files are obtained during the installation process)
- install\_openmpi.patch

```
-- scripts/install_openmpi.sh.org 2018-11-20 10:08:10.000000000 +0900
+++ scripts/install_openmpi.sh 2018-11-20 10:07:47.000000000 +0900
@@ -56,13 +56,13 @@
;;
__SYSTEM__)
echo "===== Finding OpenMPI from system paths ====="
=====
- check_command mpirun "openmpi"
- check_command mpicc "openmpi"
- check_command mpif90 "openmpi"
- check_command mpic++ "openmpi"
- check_lib -lmpi "openmpi"
- add_include_from_paths OPENMPI_CFLAGS "mpi.h" $INCLUDE_PATHS
- add_lib_from_paths OPENMPI_LDFLAGS "libmpi.*" $LIB_PATHS
+ #check_command mpirun "openmpi"
+ #check_command mpicc "openmpi"
+ #check_command mpif90 "openmpi"
+ #check_command mpic++ "openmpi"
+ #check_lib -lmpi "openmpi"
+ #add_include_from_paths OPENMPI_CFLAGS "mpi.h" $INCLUDE_PATHS
+ #add_lib_from_paths OPENMPI_LDFLAGS "libmpi.*" $LIB_PATHS
;;
__DONTUSE__)
;;
@@ -90,24 +90,26 @@
else
  mpi_bin=mpirun
fi
- # check openmpi version as reported by mpirun
- raw_version=$(($mpi_bin --version 2>&1 | \
-             grep "(Open MPI)" | awk '{print $4}')
- major_version=$(echo $raw_version | cut -d '.' -f 1)
- minor_version=$(echo $raw_version | cut -d '.' -f 2)
- # old versions required -lmpi_cxx to link cxx code, new version don't
- if [ $major_version -gt 1 ] ; then
+ ## check openmpi version as reported by mpirun
+ #raw_version=$(($mpi_bin --version 2>&1 | \
+ #             grep "(Open MPI)" | awk '{print $4}')
+ #major_version=$(echo $raw_version | cut -d '.' -f 1)
+ #minor_version=$(echo $raw_version | cut -d '.' -f 2)
+ ## old versions required -lmpi_cxx to link cxx code, new version don't
+ #if [ $major_version -gt 1 ] ; then
```

```

OPENMPI_LIBS="-lmpi"
-
- else
-   OPENMPI_LIBS="-lmpi -lmpi_cxx"
- fi
+
# else
+ # OPENMPI_LIBS="-lmpi -lmpi_cxx"
+ #fi
#
# old versions didn't support MPI 3, so adjust __MPI_VERSION accordingly (needed e.g. for pexsi)
- if [ $major_version -lt 1 ] || \
-   [ $major_version -eq 1 -a $minor_version -lt 7 ] ; then
-   mpi2_dflags="-D__MPI_VERSION=2"
- else
+ #if [ $major_version -lt 1 ] || \
+ # [ $major_version -eq 1 -a $minor_version -lt 7 ] ; then
+ #   mpi2_dflags="-D__MPI_VERSION=2"
+ #else
+   mpi2_dflags=""
- fi
+ #fi
+
OPENMPI_CFLAGS="-I${I_MPI_ROOT}/include64"
+
OPENMPI_LDFLAGS="-L${I_MPI_ROOT}/lib64 -WI,-rpath=${I_MPI_ROOT}/lib64"
cat <<EOF >> "${BUILDDIR}/setup_openmpi"
export OPENMPI_CFLAGS="${OPENMPI_CFLAGS}"
export OPENMPI_LDFLAGS="${OPENMPI_LDFLAGS}"

```

- `install_mkl_intel_intelmpi.patch`

```

--- scripts/install_mkl.sh.org 2018-11-12 14:44:45.000000000 +0900
+++ scripts/install_mkl.sh    2018-11-12 14:50:40.000000000 +0900
@@@ -66,7 +66,7 @@
          fi
done
# set the correct lib flags from MLK link adviser
-MKL_LIBS="-WI,--start-group ${mkl_lib_dir}/libmkl_gf_lp64.a ${mkl_lib_dir}/
libmkl_core.a ${mkl_lib_dir}/libmkl_sequential.a"
+MKL_LIBS="-lmkl_intel_lp64 -lmkl_sequential -lmkl_core"
# check optional libraries
if [ $MPI_MODE != no ] ; then
  enable_mkl_scalapack="__TRUE__"
@@@ -74,11 +74,11 @@
      case $MPI_MODE in
        mpich)
          mkl_optional_libs="$mkl_optional_libs libmkl_blacs_lp64.a"
-         mkl_blacs_lib="libmkl_blacs_lp64.a"
+         mkl_blacs_lib="-lmkl_blacs_lp64"
          ;;
        openmpi)
          mkl_optional_libs="$mkl_optional_libs libmkl_blacs_openmpi_lp64
.a"
-         mkl_blacs_lib="libmkl_blacs_openmpi_lp64.a"
+         mkl_blacs_lib="-lmkl_blacs_intelmpi_lp64"
          ;;
        *)
          enable_mkl_scalapack="__FALSE__"
@@@ -91,13 +91,13 @@
      done
      if [ $enable_mkl_scalapack = "__TRUE__" ] ; then
        echo "Using MKL provided ScALAPACK and BLACS"
-       MKL_LIBS="${mkl_lib_dir}/libmkl_scalapack_lp64.a ${MKL_LIBS} ${mkl_lib_dir}/${mkl_blacs_lib}"
+       MKL_LIBS="-lmkl_scalapack_lp64 ${MKL_LIBS} ${mkl_blacs_lib}"
      fi
    else
      enable_mkl_scalapack="__FALSE__"
    fi
-     MKL_LIBS="${MKL_LIBS} -WI,--end-group -lpthread -lm -ldl"

```

```
- MKL_CFLAGS="${MKL_CFLAGS} -I${MKLROOT}/include"
+ MKL_LIBS="-L${mkl_lib_dir}/lib/intel64 ${MKL_LIBS} -lpthread -lm"
+ MKL_CFLAGS="${MKL_CFLAGS} -I${MKLROOT}/include"
```

```
# write setup files
cat <<EOF > "${BUILDDIR}/setup_mkl"
```

- [install\\_elpa.patch](#)

```
-- scripts/install_elpa.sh.org 2018-11-16 16:22:07.000000000 +0900
+++ scripts/install_elpa.sh 2018-11-16 16:29:20.000000000 +0900
@@@ -92,6 +92,8 @@
        LDFLAGS="-WI,--enable-new-dtags ${MATH_LDFLAGS} ${SCALAPACK_LDFLAGS} ${cray_ldflags}" \
        LIBS="$${SCALAPACK_LIBS} ${MATH_LIBS}" \
        > configure.log 2>&1
+     sed -i -e "s/^wl=\\\"/wl=-WI,/\\\" \
+ -e "s/^pic_flag=\\\"/pic_flag=-fPIC\\\" libtool
make -j $NPROCS > make.log 2>&1
make install > install.log 2>&1
cd ..
@@@ -114,6 +116,8 @@
        LDFLAGS="-WI,--enable-new-dtags ${MATH_LDFLAGS} ${SCALAPACK_LDFLAGS} ${cray_ldflags}" \
        LIBS="$${SCALAPACK_LIBS} ${MATH_LIBS}" \
        > configure.log 2>&1
+     sed -i -e "s/^wl=\\\"/wl=-WI,/\\\" \
+ -e "s/^pic_flag=\\\"/pic_flag=-fPIC\\\" libtool
make -j $NPROCS > make.log 2>&1
make install > install.log 2>&1
cd ..
```

- [install\\_quip.patch](#)

```
-- scripts/install_quip.sh.org 2018-11-16 16:39:15.000000000 +0900
+++ scripts/install_quip.sh 2018-11-16 16:50:31.000000000 +0900
@@@ -66,34 +66,24 @@
-e "s|\\(cd build.*\\)|\\1 >&- 2>&-|g" \
bin/find_sizeof_fortran_t
fi
sed -i \
-e "s|\\(F77 *=\\).*|\\1 ${FC}|g" \
-e "s|\\(F90 *=\\).*|\\1 ${FC}|g" \
-e "s|\\(F95 *=\\).*|\\1 ${FC}|g" \
-e "s|\\(CC *=\\).*|\\1 ${CC}|g" \
-e "s|\\(CPLUSPLUS *=\\).*|\\1 ${CXX}|g" \
-e "s|\\(LINKER *=\\).*|\\1 ${FC}|g" \
-e "s|\\(FPP *=\\).*|\\1 ${FC} -E -x f95-cpp-input|g" \
-e "s|\\(QUIPPY_FCOMPILER *=\\).*|\\1 ${FC}|g" \
-e "s|\\(QUIPPY_CPP *=\\).*|\\1 ${FC} -E -x f95-cpp-input|g" \
arch/Makefile.linux_${quip_arch}_gfortran
# enable debug symbols
echo "F95FLAGS += -g" >> arch/Makefile.linux_${quip_arch}_gfo
rtran
echo "F77FLAGS += -g" >> arch/Makefile.linux_${quip_arch}_gfo
rtran
echo "CFLAGS += -g" >> arch/Makefile.linux_${quip_arch}_gfo
rtran
echo "CPLUSPLUSFLAGS += -g" >> arch/Makefile.linux_${quip_arch}_gfortran
export QUIP_ARCH=linux_${quip_arch}_gfortran
echo "F95FLAGS += -g" >> arch/Makefile.linux_${quip_arch}_ifort_icc
echo "F77FLAGS += -g" >> arch/Makefile.linux_${quip_arch}_ifort_icc
echo "CFLAGS += -g" >> arch/Makefile.linux_${quip_arch}_ifort_icc
echo "CPLUSPLUSFLAGS += -g" >> arch/Makefile.linux_${quip_arch}_ifort_icc
export QUIP_ARCH=linux_${quip_arch}_ifort_icc
# hit enter a few times to accept defaults
echo -e "${MATH_LDFLAGS} ${MATH_LIBS} \\n\\n\\n\\n\\n\\n\\n\\n\\n\\n\\n\\n\\n\\n\\n\\n\\n\\n\\n" | make config > configure.log
QUIP_MATH_LIBS="-lmkl_intel_lp64 -lmkl_sequential -lmkl_core -lpthread -lm -ldl"
```

```

+ echo -e "${MATH_LDFLAGS} ${QUIP_MATH_LIBS} \n\n\n\n\n\n\n\n\n\n\n\n\n\n\n\n\n\n" | make config > configure.log
# make -j does not work :-(

make > make.log 2>&1
! [ -d "${pkg_install_dir}/include" ] && mkdir -p "${pkg_install_dir}/include"
! [ -d "${pkg_install_dir}/lib" ] && mkdir -p "${pkg_install_dir}/lib"
- cp build/linux_x86_64_gfortran/quip_unified_wrapper_module.mod \
+ cp build/linux_x86_64_ifort_icc/quip_unified_wrapper_module.mod \
    "${pkg_install_dir}/include/"
- cp build/linux_x86_64_gfortran/*.a \
+ cp build/linux_x86_64_ifort_icc/*.a \
    "${pkg_install_dir}/lib/"
- cp src/FoX-4.0.3/objs.linux_${quip_arch}_gfortran/lib/*.a \
+ cp src/FoX-4.0.3/objs.linux_${quip_arch}_ifort_icc/lib/*.a \
    "${pkg_install_dir}/lib/"
cd ..
touch "${install_lock_file}"

```

## Build Procedure

```

#!/bin/sh

INSTDIR=/local/apl/lx/cp2k610
WORKDIR=/work/users/${USER}

VERSION=6.1.0

TARBALL=/home/users/${USER}/Software/CP2K/${VERSION}/cp2k-${VERSION}.tar.gz
#LIBGRID=/home/users/${USER}/Software/CP2K/${VERSION}/libgrid/cp2k-${VERSION}-i1708/tools/autotune_grid
PATCH_INST_OPENMPI=/home/users/${USER}/Software/CP2K/${VERSION}/install_openmpi.patch
PATCH_INST_MKL=/home/users/${USER}/Software/CP2K/${VERSION}/install_mkl_intel_intelmpi.patch
PATCH_INST_ELPA=/home/users/${USER}/Software/CP2K/${VERSION}/install_elpa.patch
PATCH_INST QUIP=/home/users/${USER}/Software/CP2K/${VERSION}/install_quip.patch

PLUMED_VERSION=2.4.3
PLUMED_TARBALL=/home/users/${USER}/Software/PLUMED/${PLUMED_VERSION}/plumed-${PLUMED_VERSION}.tgz

PARALLEL=12

# NOTE: Some of header and library paths are defined in CPATH and
#       LIBRARY_PATH environment variables from modulefiles.

#-----
umask 0022
export LANG=""
export LC_ALL=C

module purge
module load intel_parallelstudio/2017update8
module load spglib/1.11.1

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

tar zxf ${TARBALL}
mv cp2k-${VERSION}/* .
rm -rf cp2k-${VERSION}/{.dockerignore,.gitignore}
rmdir cp2k-${VERSION}
#rm -rf tools/autotune_grid
#cp ${LIBGRID} tools/autotune_grid
#cp ${LIBGRID}/libgrid.a tools/autotune_grid

# plumed

```

```

mkdir ${INSTDIR}/plumed
cd $WORKDIR
if [ -d plumed-${PLUMED_VERSION} ]; then
  mv plumed-${PLUMED_VERSION} plumed-erase
  rm -rf plumed-erase &
fi

tar zxf ${PLUMED_TARBALL}
cd plumed-${PLUMED_VERSION}
CC=mpiicc FC=mpifort CXX=mpiicpc \
./configure --prefix=${INSTDIR}/plumed
make -j ${PARALLEL}
make check
make install

# cp2k toolchain
cd ${INSTDIR}/tools/toolchain
sed -e "s/blacs_openmpi/blacs_intelmpi/" scripts/install_mkl.sh > scripts/install_mkl.sh.impi
chmod 755 scripts/install_mkl.sh.impi

patch -p0 < $PATCH_INST_OPENMPI
patch -p0 < $PATCH_INST_MKL
patch -p0 < $PATCH_INST_ELPA
patch -p0 < $PATCH_INST_QUIP

CC=icc FC=ifort F77=ifort F90=ifort CXX=icpc \
MPICC=mpiicc MPICXX=mpiicpc MPIFC=mpifort MPIF77=mpifort MPIF90=mpifort \
./install_cp2k_toolchain.sh --math-mode=mkl \
--mpi-mode=openmpi \
--with-elpa=install \
--with-cmake=system \
--with-mpich=no \
--with-openmpi=system \
--with-reflapack=no \
-j ${PARALLEL}

# cheat the script
mv -f scripts/install_mkl.sh.impi scripts/install_mkl.sh

CC=icc FC=ifort F77=ifort F90=ifort CXX=icpc \
MPICC=mpiicc MPICXX=mpiicpc MPIFC=mpifort MPIF77=mpifort MPIF90=mpifort \
./install_cp2k_toolchain.sh --math-mode=mkl \
--mpi-mode=openmpi \
--with-elpa=install \
--with-ptscotch=install \
--with-parmetis=install \
--with-superlu=install \
--with-pexsi=install \
--with-quip=install \
--with-cmake=system \
--with-mpich=no \
--with-openmpi=system \
--with-reflapack=no \
-j ${PARALLEL}

#LIBGRID_ESC=`echo ${INSTDIR}/tools/autotune_grid | sed -e 's//\\\\\\\\\\//g'`
```

# finish building toolchain, copy arch file to the proper place

## modify arch for cpu-only version

```

sed -e "/^CFLAGS    =/s/CFLAGS    =/CFLAGS    = -O2 /" \
-e "/^FCFLAGS   =/s/FCFLAGS   =/FCFLAGS   = -O2 /" \
-e "/^DFLAGS   /s/$/-D_SPGLIB -D_PLUMED2/" \
-e "/^LIBS     /s/$/-lsympg -lz -lgsl -nofor_main/" \
install/arch/local.psmp > ${INSTDIR}/arch/rccs.psmp
echo "include ${INSTDIR}/plumed/lib/plumed/src/lib/Plumed.inc" >> ${INSTDIR}/arch/rccs.psmp
```

```

echo "EXTERNAL_OBJECTS=\$(PLUMED_STATIC_DEPENDENCIES)" >> ${INSTDIR}/arch/rccs.psmp

## modify arch for cpu-gpu version
sed -e "/^CFLAGS    =/s/CFLAGS    =/CFLAGS    = -O2 /" \
-e "/^FCFLAGS   =/s/FCFLAGS   =/FCFLAGS   = -O2 /" \
-e "/^DFLAGS /s/$/-D_SPGLIB -D_PLUMED2 -D_ACC -D_DBCSR_ACC -D_PW_CUDA/" \
-e "/^LIBS /s/$/-lsympg -lz -lgsl -lcudart -lcublas -nofor_main/" \
install/arch/local.psmp > ${INSTDIR}/arch/rccs_cuda.psmp
echo "include ${INSTDIR}/plumed/lib/plumed/src/lib/Plumed.inc" >> ${INSTDIR}/arch/rccs_cuda.psmp
echo "EXTERNAL_OBJECTS=\$(PLUMED_STATIC_DEPENDENCIES)" >> ${INSTDIR}/arch/rccs_cuda.psmp
echo "NVCC      = nvcc -D_GNUC_=5 -D_GNUC_MINOR_=3 -Xcompiler=--std=gnu++98" >> ${INSTDIR}/arch/rccs_cuda.psmp
echo "NVFLAGS   = -gencode=arch=compute_60,code=sm_60 -gencode=arch=compute_70,code=sm_70 \$(DFLAGS)" >>
${INSTDIR}/arch/rccs_cuda.psmp

#--

cd ${INSTDIR}/makefiles
make -j ${PARALLEL} ARCH=rccs VERSION=psmp

module load cuda/9.1
make -j ${PARALLEL} ARCH=rccs_cuda VERSION=psmp

```

## Test

### plumed

All of these three errors are minor numerical errors.

```

+ check file ves/rt-td-vonmises/report.txt for more information
+ ERROR in test isdb/rt-emmi/
+ check file isdb/rt-emmi/report.txt for more information
+ ERROR in test isdb/rt-jcouplings-mi/
+ check file isdb/rt-jcouplings-mi/report.txt for more information
+ ERROR in test isdb/rt-jcouplings/
+ check file isdb/rt-jcouplings/report.txt for more information
+++++
+ Final report:
+ 248 tests performed, 161 tests not applicable
+ 3 errors found
+ Find the bug!
+ To replace references, go to the test directory and
+ type 'make reset'
+++++

```

### cp2k

Test results are available at /local/apl/lx/cp2k610/regtesting/rccs/psmp and  
 /local/apl/lx/cp2k610/regtesting/rccs\_cuda/psmp.

All the tests except GPU version were performed on ccfep.

```

#!/bin/sh

export LC_ALL=C
export LANG=""

module purge
module load intel_parallelstudio/2017update8
module load spglib/1.11.1

CP2K=/local/apl/lx/cp2k610/
CP2K_ARCH=rccs
CP2K_VER=psmp
TIMEOUT=120
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 \
-nosvn \
-arch ${CP2K_ARCH} \
-version ${CP2K_VER} \
-mpiranks 1 \
-ompthreads 1 \
-jobmaxtime ${TIMEOUT} \
-cp2kdir ../../ \
-maxtasks ${PARALLEL} >& regtest_mpi1_omp1.log
rm -rf LAST-${CP2K_ARCH}-${CP2K_VER}

# omp test
../../tools/regtesting/do_regtest \
-nobuild \
-nosvn \
-arch ${CP2K_ARCH} \
-version ${CP2K_VER} \
-mpiranks 1 \
-ompthreads 2 \
-jobmaxtime ${TIMEOUT} \
-cp2kdir ../../ \
-maxtasks ${PARALLEL} >& regtest_mpi1_omp2.log
rm -rf LAST-${CP2K_ARCH}-${CP2K_VER}

# mpi test
../../tools/regtesting/do_regtest \
-nobuild \
-nosvn \
-arch ${CP2K_ARCH} \
-version ${CP2K_VER} \
-mpiranks 2 \
-ompthreads 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 \
-nosvn \
-arch ${CP2K_ARCH} \
-version ${CP2K_VER} \
-mpiranks 2 \
-ompthreads 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 \
-nosvn \
-arch ${CP2K_ARCH} \
-version ${CP2K_VER} \
-mpiranks 8 \
-ompthreads 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 \
-nosvn \
-arch ${CP2K_ARCH} \
-version ${CP2K_VER} \
-mpiranks 8 \
-ompthreads 2 \
-jobmaxtime ${TIMEOUT} \
-cp2kdir ..../../
-maxtasks ${PARALLEL} >& regtest_mpi8_omp2.log
rm -rf LAST-${CP2K_ARCH}-${CP2K_VER}

```

## ■ Test Result: MPI1 - OMP1

```

----- Summary -----
Number of FAILED tests 1
Number of WRONG tests 0
Number of CORRECT tests 3008
Number of NEW tests 14
Total number of tests 3023
GREPME 1 0 3008 14 3023 X
-----
```

- QS/regtest-ri-mp2/opt\_basis\_O\_auto\_gen.inp : RUNTIME FAIL

## ■ Test Result: MPI1 - OMP2

```

----- Summary -----
Number of FAILED tests 1
Number of WRONG tests 0
Number of CORRECT tests 3008
Number of NEW tests 14
Total number of tests 3023
GREPME 1 0 3008 14 3023 X
-----
```

- QS/regtest-ri-mp2/opt\_basis\_O\_auto\_gen.inp : RUNTIME FAIL

## ■ Test Result: MPI2 - OMP1

```

----- Summary -----
Number of FAILED tests 1
Number of WRONG tests 0
Number of CORRECT tests 3053
Number of NEW tests 19
Total number of tests 3073
GREPME 1 0 3053 19 3073 X
-----
```

- QS/regtest-ri-mp2/opt\_basis\_O\_auto\_gen.inp : RUNTIME FAIL

## ■ Test Result: MPI2 - OMP2

```

----- Summary -----
Number of FAILED tests 1
Number of WRONG tests 0
Number of CORRECT tests 3053
Number of NEW tests 19
Total number of tests 3073
GREPME 1 0 3053 19 3073 X
-----
```

- QS/regtest-ri-mp2/opt\_basis\_O\_auto\_gen.inp : RUNTIME FAIL

## ■ Test Result: MPI8 - OMP1

```
----- Summary -----  
Number of FAILED tests 8  
Number of WRONG tests 2  
Number of CORRECT tests 3012  
Number of NEW tests 16  
Total number of tests 3038  
GREPME 8 2 3012 16 3038 X  
-----
```

- QS/regtest-ri-mp2/opt\_basis\_O\_auto\_gen.inp : RUNTIME FAIL
- QS/regtest-rma-3D/\* : RUNTIME FAIL

## ■ Test Result: MPI8 - OMP2

```
----- Summary -----  
Number of FAILED tests 8  
Number of WRONG tests 2  
Number of CORRECT tests 3012  
Number of NEW tests 16  
Total number of tests 3038  
GREPME 8 2 3012 16 3038 X  
-----
```

- QS/regtest-ri-mp2/opt\_basis\_O\_auto\_gen.inp : RUNTIME FAIL
- QS/regtest-rma-3D/\* : RUNTIME FAIL

## ■ Test Result: GPU version, MPI2 - OMP2 (@ccca)

```
----- Summary -----  
Number of FAILED tests 3  
Number of WRONG tests 0  
Number of CORRECT tests 3052  
Number of NEW tests 19  
Total number of tests 3074  
GREPME 3 0 3052 19 3074 X  
-----
```

- QS/regtest-pao-2/H2O\_pao\_rotinv.inp : RUNTIME FAIL
- QS/regtest-rel/Hg\_rel.inp : RUNTIME FAIL
- QS/regtest-ri-mp2/opt\_basis\_O\_auto\_gen.inp : RUNTIME FAIL

## Benchmark

Input file is tests/QS/benchmark/H2O-64.inp. (The elapse times below are from output of 'grep "CP2K" \*.log').

jobtype	Total # of cores (# of nodes)	MPI	OMP	GPU	elapse(sec)
core	18 (1)	18	1	-	77.148
small	40 (1)	40	1	-	45.537
small	80 (2)	80	1	-	36.421
small	160 (4)	160	1	-	27.490
small	160 (4)	80	2	-	33.158
small	160 (4)	32	5	-	27.090
gpu	12 (1)	12	1	1	130.869

## Misc

- Compiler support information on the official website. [https://www.cp2k.org/dev/compiler\\_support](https://www.cp2k.org/dev/compiler_support)
- libsmm is not verified. (libxsmm is expected to be enough for x86\_64 system.)
- Intel17-OpenMPI3.1.0 version yields more errors than Intel17-Intelmpi (even on serial (mpi1\*omp1) run).

- Intelmpi seems to be better than openmpi.
- Strangely, intel17-openmpi3.1.0-mkl2017.x version is terribly slow when MPI paralleled.
  - But intel17-openmpi3.1.0-mkl2018.x version is free from the slow MPI issue. Terribly curious.
- libgrid.a didn't work when multiple OpenMP threads employed.
  - libgrid.a (built with -fopenmp option) works fine for intel17-openmpi3.1.0-mkl version.
  - If libgrid.a works fine, ~5 % speedup is available.
- Intel18 version met more errors than intel17 one.
- Other versions of Intel MPI are not tested.
- In H2O-64 benchmark, -O3 -xHost -ip version binary is slower than -O2 one.
- GPU version maybe advantageous for large (>1000 atoms) system.