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${I_MPI_ROOT}/lib64 -Wl,-rpath=${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="-Wl,--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} -Wl,--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="-Wl,--enable-new-dtags ${MATH_LDFLAGS} ${SCALAPACK_LDFLAGS} ${cray_ldflags}" \
                        LIBS="${SCALAPACK_LIBS} ${MATH_LIBS}" \
                        > configure.log 2>&1
+           sed -i -e "s/^wl=\"\"/wl=\"-Wl,\"/" \
+                -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="-Wl,--enable-new-dtags ${MATH_LDFLAGS} ${SCALAPACK_LDFLAGS} ${cray_ldflags}" \
                          LIBS="${SCALAPACK_LIBS} ${MATH_LIBS}" \
                          > configure.log 2>&1
+              sed -i -e "s/^wl=\"\"/wl=\"-Wl,\"/" \
+                   -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\n\n\n" | make config > configure.log
+            QUIP_MATH_LIBS="-lmkl_intel_lp64 -lmkl_sequential -lmkl_core -lpthread -lm -ldl"
```

```
+           echo -e "${MATH_LDFLAGS} ${QUIP_MATH_LIBS} \n\n\n\n\n\n\n\n\n\n\n\n\n\n\n\n\n\n\n\n\n\n\n\n" | make config > configure.log
            # make -j does not work :-(
            make > make.log 2>&1
            ! [ -d "${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 -rf ${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=mpiifort 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=mpiifort MPIF77=mpiifort MPIF90=mpiifort \
    ./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=mpiifort MPIF77=mpiifort MPIF90=mpiifort \
    ./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/\$/ -lsymspg -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/\$/ -lsymspg -lz -lgsl -lcudart -lcufft -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
- 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 if free from the slow MPI issue. Terribly curious.
- libgrid.a didn't work when multiple OpenMP threads employed.
    - libgrid.a (built with -qopenmp 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.