

## CP2K 7.1.0 (intel)

### Webpage

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

### Version

7.1.0

### Build Environment

- Intel Parallel Studio 2018 Update 4
- GCC 7.3.1 (devtoolset-7)
- cmake 3.16.3

### Files Required

- cp2k-7.1.0.tar.gz
- dbcsr-2.0.1.tar.gz
- tc\_install\_cp2k\_toolchain.sh.diff

```
--- install_cp2k_toolchain.sh.org 2020-01-31 17:07:19.000000000 +0900
+++ install_cp2k_toolchain.sh 2020-01-31 17:07:30.000000000 +0900
@@ -942,8 +942,8 @@
  ./scripts/install_superlu.sh
  ./scripts/install_pexsi.sh
  ./scripts/install_quip.sh
- ./scripts/install_plumed.sh
  ./scripts/install_gsl.sh
+ ./scripts/install_plumed.sh
  ./scripts/install_spglib.sh
  ./scripts/install_hdf5.sh
  ./scripts/install_libvdx.sh
```

- tc\_install\_mkl.sh.intel.diff

```
--- install_mkl.sh.org 2020-01-31 15:58:56.000000000 +0900
+++ install_mkl.sh 2020-02-04 17:20:01.000000000 +0900
@@ -66,37 +66,38 @@
  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="-Wl,--start-group ${mkl_lib_dir}/libmkl_gf_lp64.a ${mkl_lib_dir}/libmkl_core.a ${mkl_lib_dir}/libmkl_sequential.a"
+ MKL_LIBS="-L${mkl_lib_dir} -Wl,--no-as-needed -lmkl_scalapack_lp64 -lmkl_blacs_intelmpi_lp64 -lmkl_intel_lp64 -lmkl_sequential -lmkl_core -
lpthread -lm -ldl"
  # check optional libraries
- if [ $MPI_MODE != no ]; then
+ #if [ $MPI_MODE != no ]; then
  enable_mkl_scalapack="__TRUE__"
- mkl_optional_libs="libmkl_scalapack_lp64.a"
- case $MPI_MODE in
-   mpich)
-     mkl_blacs_lib="libmkl_blacs_intelmpi_lp64.a"
-     ;;
-   openmpi)
-     mkl_blacs_lib="libmkl_blacs_openmpi_lp64.a"
-     ;;
-   *)
-     enable_mkl_scalapack="__FALSE__"
-     ;;
-   esac
- mkl_optional_libs="$mkl_optional_libs $mkl_blacs_lib"
```

```

-   for ii in $mkl_optional_libs ; do
-       if ! [ -f "${mkl_lib_dir}/${ii}" ] ; then
-           enable_mkl_scalapack="__FALSE_"
-       fi
-   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}"
-   fi
- else
-   echo "Not using MKL provided ScaLAPACK and BLACS"
-   enable_mkl_scalapack="__FALSE_"
- fi
- MKL_LIBS="${MKL_LIBS} -Wl,--end-group -lpthread -lm -ldl"
+ # mkl_optional_libs="libmkl_scalapack_lp64.a"
+ # case $MPI_MODE in
+ #   mpich)
+ #     mkl_blacs_lib="libmkl_blacs_intelmpi_lp64.a"
+ #     ;;
+ #   openmpi)
+ #     mkl_blacs_lib="libmkl_blacs_openmpi_lp64.a"
+ #     ;;
+ #   *)
+ #     enable_mkl_scalapack="__FALSE_"
+ #     ;;
+ # esac
+ mkl_optional_libs=""
+ # for ii in $mkl_optional_libs ; do
+ #   if ! [ -f "${mkl_lib_dir}/${ii}" ] ; then
+ #     enable_mkl_scalapack="__FALSE_"
+ #   fi
+ # 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}"
+ # fi
+ #else
+ # echo "Not using MKL provided ScaLAPACK and BLACS"
+ # enable_mkl_scalapack="__FALSE_"
+ #fi
+ #MKL_LIBS="${MKL_LIBS} -Wl,--end-group -lpthread -lm -ldl"
MKL_CFLAGS="${MKL_CFLAGS} -I${MKLROOT}/include -I${MKLROOT}/include/fftw"

# write setup files

```

- tc\_install\_mpich.sh.intel.diff

```

--- install_mpich.sh.org      2020-01-29 15:58:59.000000000 +0900
+++ install_mpich.sh        2020-01-29 16:03:53.000000000 +0900
@@ -50,14 +50,14 @@
    ;;
    _SYSTEM_)
        echo "===== Finding MPICH from system paths ====="
-       check_command mpirun "mpich"
-       check_command mpicc "mpich"
-       check_command mpif90 "mpich"
-       check_command mpic++ "mpich"
-       check_lib -lmpi "mpich"
-       check_lib -lmpicxx "mpich"
-       add_include_from_paths MPICH_CFLAGS "mpi.h" $INCLUDE_PATHS
-       add_lib_from_paths MPICH_LDFLAGS "libmpi.*" $LIB_PATHS
+       #check_command mpirun "mpich"
+       #check_command mpicc "mpich"
+       #check_command mpif90 "mpich"
+       #check_command mpic++ "mpich"

```

```

+ #check_lib -Impi "mpich"
+ #check_lib -Impicxx "mpich"
+ #add_include_from_paths MPICH_CFLAGS "mpi.h" $INCLUDE_PATHS
+ #add_lib_from_paths MPICH_LDFLAGS "libmpi.*" $LIB_PATHS
+ ;;
+ __DONTUSE__
+ ;;
@@ -87,15 +87,17 @@
+ mpi_bin=mpirun
+ fi
+ # check MPICH version, versions less than 3.0 will get -D_MPI_VERSION=2 flag
- raw_version=$(($mpi_bin --version | \
-     grep "Version:" | awk '{print $2}')
- major_version=$(echo $raw_version | cut -d '.' -f 1)
- minor_version=$(echo $raw_version | cut -d '.' -f 2)
- if [ $major_version -lt 3 ]; then
-     mpi2_dflags="-D_MPI_VERSION=2"
- else
+ #raw_version=$(($mpi_bin --version | \
+ #     grep "Version:" | awk '{print $2}')
+ #major_version=$(echo $raw_version | cut -d '.' -f 1)
+ #minor_version=$(echo $raw_version | cut -d '.' -f 2)
+ #if [ $major_version -lt 3 ]; then
+ #     mpi2_dflags="-D_MPI_VERSION=2"
+ #else
+     mpi2_dflags=""
- fi
+ #fi
+ MPICH_CFLAGS="-I${_MPI_ROOT}/include64"
+ MPICH_LDFLAGS="-L${_MPI_ROOT}/lib64 -Wl,-rpath=${_MPI_ROOT}/lib64"
+ cat <<EOF >> "${BUILDDIR}/setup_mpich"
export MPI_MODE="${MPI_MODE}"
export MPICH_CFLAGS="${MPICH_CFLAGS}"

```

- tc\_install\_libint.sh.intel.diff (avoiding fortran test build error which are completely unnecessary for cp2k)

```

--- install_libint.sh.org 2020-02-03 18:13:20.000000000 +0900
+++ install_libint.sh 2020-02-03 19:16:36.000000000 +0900
@@ -72,6 +72,8 @@
+ #cmake --build . > cmake.log 2>&1
+ #cmake --build . --target install > install.log 2>&1
+
+ # extremely ad hoc workaround
+ sed -i -e "s/fortran_example check_test/libint_f.o check_test/" fortran/Makefile.in
+ ./configure --prefix=${pkg_install_dir} \
+     --with-cxx="$CXX $LIBINT_CXXFLAGS" \
+     --with-cxx-opts="$LIBINT_CXXFLAGS" \

```

- tc\_install\_sirius.sh.diff

```

--- install_sirius.sh.org 2020-02-25 14:50:50.000000000 +0900
+++ install_sirius.sh 2020-02-25 14:48:01.000000000 +0900
@@ -131,8 +131,8 @@
+ -DspFFT_DIR="${SPFFT_ROOT}/lib/cmake/SpFFT" \
+ -DCMAKE_CXXFLAGS_RELEASE="${SIRIUS_OPT}" \
+ -DCMAKE_CXX_FLAGS_RELWITHDEBINFO="${SIRIUS_DBG}" \
- -DCMAKE_CXX_COMPILER=mpic++ \
- -DCMAKE_C_COMPILER=mpicc \
+ -DCMAKE_CXX_COMPILER=${MPICXX} \
+ -DCMAKE_C_COMPILER=${MPICC} \
+ ${COMPILE_OPTIONS} .. > compile.log 2>&1
+ make -j $NPROCS -C src >> compile.log 2>&1
@@ -155,8 +155,8 @@
+ -DCMAKE_CXX_FLAGS_RELWITHDEBINFO="${SIRIUS_DBG}" \
+ -DUSE_CUDA=ON \

```

```

-DGPU_MODEL=P100 \
-
-DCMAKE_CXX_COMPILER=mpic++ \
-DCMAKE_C_COMPILER=mpicc ${COMPILE_OPTIONS} .. >> compile.log 2>&1
+
-DCMAKE_CXX_COMPILER=${MPICXX} \
+
-DCMAKE_C_COMPILER=${MPICC} ${COMPILE_OPTIONS} .. >> compile.log 2>&1
make -j $NPROCS -C src >> compile.log 2>&1
install -d ${pkg_install_dir}/lib/cuda
install -d ${pkg_install_dir}/include/cuda

```

- tc\_install\_superlu.sh.intel.diff

```

--- install_superlu.sh.org 2020-02-04 11:46:01.000000000 +0900
+++ install_superlu.sh 2020-02-04 11:46:22.000000000 +0900
@@ -46,12 +46,12 @@
    cat <<EOF >> make.inc
PLAT=${OPENBLAS_ARCH}
DSUPERLULIB= ${PWD}/lib/libsuperlu_dist.a
-LIBS=$(DSUPERLULIB) ${PARMETIS_LDFLAGS} ${METIS_LDFLAGS} ${MATH_LDFLAGS} ${PARMETIS_LIBS} ${METIS_LIBS} $(resolve_string
"${MATH_LIBS}" OMP) -lgfortran
+LIBS=$(DSUPERLULIB) ${PARMETIS_LDFLAGS} ${METIS_LDFLAGS} ${MATH_LDFLAGS} ${PARMETIS_LIBS} ${METIS_LIBS} $(resolve_string
"${MATH_LIBS}" OMP)
ARCH=ar
ARCHFLAGS=cr
RANLIB=ranlib
CC=${MPICC}
-CFLAGS=${CFLAGS} ${PARMETIS_CFLAGS} ${METIS_CFLAGS} ${MATH_CFLAGS}
+CFLAGS=${CFLAGS} -std=c99 -fpic ${PARMETIS_CFLAGS} ${METIS_CFLAGS} ${MATH_CFLAGS}
NOOPTS=-O0
FORTRAN=${MPIFC}
F90FLAGS=${FFLAGS}

```

- tc\_install\_libvdxwxc.sh.intel.diff

```

--- install_libvdxwxc.sh.org 2020-02-04 16:23:50.000000000 +0900
+++ install_libvdxwxc.sh 2020-02-04 16:48:35.000000000 +0900
@@ -65,7 +65,7 @@
    unset MPICC MPICXX MPIF90 MPIFC MPIF77
    if [ "$MPI_MODE" = "no" ]; then
        # compile libvdxwxc without mpi support since fftw (or mkl) do not have mpi support activated
-
- ./configure \
+
+ CC=${CC} FC=${FC} ./configure \
    --prefix="${pkg_install_dir}" \
    --libdir="${pkg_install_dir}/lib" \
    --with-fftw3=${FFTW_ROOT} \
@@ -73,12 +73,11 @@
    --without-mpi \
    >> configure.log 2>&1
    else
-
- CC=mpicc FC=mpifort ./configure \
+
+ MPICC=mpiicc MPIFC=mpiifort ./configure \
    --prefix="${pkg_install_dir}" \
    --libdir="${pkg_install_dir}/lib" \
    --with-fftw3=${FFTW_ROOT} \
    --disable-shared \
-
- --with-mpi \
    >> configure.log 2>&1
    fi
    make -j $NPROCS > compile.log 2>&1

```

- tc\_install\_plumed.sh.diff

```

--- install_plumed.sh.org 2020-02-04 15:13:41.986747619 +0900
+++ install_plumed.sh 2020-02-04 16:00:15.980396838 +0900
@@ -40,7 +40,7 @@

```

```

echo "Installing from scratch into ${pkg_install_dir}"
cd plumed-${plumed_ver}
- ./configure CXX="${MPICXX}" --prefix=${pkg_install_dir} --libdir="${pkg_install_dir}/lib" > configure.log 2>&1
+ ./configure CXX="${MPICXX}" --prefix=${pkg_install_dir} --libdir="${pkg_install_dir}/lib" CXXFLAGS="-I${GSLROOT}/include" LIBS="-
L${GSLROOT}/lib -L${MKLROOT}/lib/intel64 -Wl,--no-as-needed -lmkl_intel_lp64 -lmkl_sequential -lmkl_core -lphread -lm -ldl" > configure.log 2>&1
make -j $NPROCS > make.log 2>&1
make install > install.log 2>&1
write_checksums "${install_lock_file}" "${SCRIPT_DIR}/${basename ${SCRIPT_NAME}}"
@@ -63,7 +63,7 @@
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"

```

## Build Procedure

```

#!/bin/sh

INSTDIR=/local/apl/lx/cp2k710

VERSION=7.1.0
DBCSR_VERSION=2.0.1

SOURCE_ROOT=/home/users/${USER}/Software/CP2K/${VERSION}

TARBALL=${SOURCE_ROOT}/cp2k-${VERSION}.tar.gz
TARBALL_DBCSR=${SOURCE_ROOT}/dbcsr-${DBCSR_VERSION}.tar.gz

TC_PATCH0=${SOURCE_ROOT}/tc_install_cp2k_toolchain.sh.diff
TC_PATCH1=${SOURCE_ROOT}/tc_install_mkl.sh.intel.diff
TC_PATCH2=${SOURCE_ROOT}/tc_install_mpich.sh.intel.diff
TC_PATCH3=${SOURCE_ROOT}/tc_install_libint.sh.intel.diff
#TC_PATCH4=${SOURCE_ROOT}/tc_install_quip.sh.intel.diff
TC_PATCH5=${SOURCE_ROOT}/tc_install_sirius.sh.diff
TC_PATCH6=${SOURCE_ROOT}/tc_install_superlu.sh.intel.diff
TC_PATCH7=${SOURCE_ROOT}/tc_install_libvdx.sh.intel.diff
TC_PATCH8=${SOURCE_ROOT}/tc_install_plumed.sh.diff

PARALLEL=12

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

module purge
module load scl/devtoolset-7
module load intel_parallelstudio/2018update4
module load cmake/3.16.3

cd $INSTDIR
if [ -d cp2k-${VERSION} ]; then
  mv cp2k-${VERSION} cp2k-erase
  rm -rf cp2k-erase &
fi
tar xzf ${TARBALL}
sleep 5
mv cp2k-${VERSION}/* .
sleep 5
rm -f cp2k-${VERSION}/.dockerignore
rmdir cp2k-${VERSION}

```

```

cd ${INSTDIR}/tools/toolchain
patch < ${TC_PATCH0}

cd scripts
patch < ${TC_PATCH1}
patch < ${TC_PATCH2}
patch < ${TC_PATCH3}
#patch < ${TC_PATCH4}
patch < ${TC_PATCH5}
patch < ${TC_PATCH6}
patch < ${TC_PATCH7}
patch < ${TC_PATCH8}
cd ../

export CC=icc
export CXX=icpc
export FC=ifort
export MPICC=mpiicc
export MPICXX=mpiicpc
export MPIFC=mpiifort

./install_cp2k_toolchain.sh --math-mode=mkl \
    --mpi-mode=mpich \
    --with-cmake=system \
    --with-mpich=system \
    --with-openmpi=no \
    --with-libxc=install \
    --with-libint=install \
    --with-fftw=install \
    --with-openblas=no \
    --with-scalapack=no \
    --with-reflapack=no \
    --with-libxsmm=install \
    --with-elpa=install \
    --with-ptscotch=install \
    --with-pexsi=install \
    --with-parmetis=install \
    --with-superlu=install \
    --with-quip=no \
    --with-plumed=install \
    --with-gsl=install \
    --with-libvdx=install \
    --with-spglib=install \
    --with-hdf5=install \
    --with-spfft=install \
    -j ${PARALLEL}

sed -e "/^LIBS /s/\$/ -nofor_main/" \
    install/arch/local.psm > ../arch/rccs.psm

cd ${INSTDIR}/exts
rmdir dbcsr
tar xzf ${TARBALL_DBCSR}
mv dbcsr-${DBC_SR_VERSION} dbcsr
cd ../
make -j ${PARALLEL} ARCH=rccs VERSION=psmp

```

## Tests

Test script below was executed on ccfep.

```

#!/bin/sh

export LC_ALL=C
export LANG=""

```

```
# intel
module purge
module load scl/devtoolset-7
module load intel_parallelstudio/2018update4
module load cmake/3.16.3
CP2K=/local/apl/lx/cp2k710

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}

```

### ■ Result: MPI1 - OMP1

```

----- Summary -----
Number of FAILED tests 1
Number of WRONG tests 2
Number of CORRECT tests 3214
Number of NEW tests 3
Total number of tests 3220

```

- QS/regtest-ri-mp2/opt\_basis\_O\_auto\_gen.inp: WRONG
- QS/regtest-also-2/ion-pair.inp: RUNTIME FAIL
- Fist/regtest-3/2d\_pot.inp: WRONG

### ■ Result: MPI1 - OMP2

```

----- Summary -----
Number of FAILED tests 2
Number of WRONG tests 2
Number of CORRECT tests 3213
Number of NEW tests 3
Total number of tests 3220

```

- SIRIUS/regtest-1/He-full-potential.inp: RUNTIME FAIL
- QS/regtest-ri-mp2/opt\_basis\_O\_auto\_gen.inp: WRONG
- QS/regtest-also-2/ion-pair.inp: RUNTIME FAIL
- Fist/regtest-3/2d\_pot.inp: WRONG

### ■ Result: MPI2 - OMP1

```

----- Summary -----
Number of FAILED tests 0
Number of WRONG tests 2
Number of CORRECT tests 3275
Number of NEW tests 8
Total number of tests 3285

```

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

- Fist/regtest-3/2d\_pot.inp: WRONG

## ■ Result: MPI2 - OMP2

```
----- Summary -----
Number of FAILED tests 1
Number of WRONG tests 2
Number of CORRECT tests 3274
Number of NEW tests 8
Total number of tests 3285
```

- SIRIUS/regtest-1/He-full-potential.inp: RUNTIME FAIL
- QS/regtest-ri-mp2/opt\_basis\_O\_auto\_gen.inp: WRONG
- Fist/regtest-3/2d\_pot.inp: WRONG

## ■ Result: MPI8 - OMP1

```
----- Summary -----
Number of FAILED tests 7
Number of WRONG tests 10
Number of CORRECT tests 3219
Number of NEW tests 6
Total number of tests 3242
```

- QS/regtest-mp2-lr/H2O-mp2-gpw-lr.inp: WRONG
- QS/regtest-mp2-grad/H2O\_grad\_mme.inp: WRONG
- QS/regtest-gpw-4/H2O-debug-5.inp: WRONG
- QS/regtest-gpw-4/H2O-debug-6.inp: WRONG
- QS/regtest-ri-mp2/opt\_basis\_O\_auto\_gen.inp: WRONG
- Fist/regtest-3/2d\_pot.inp: WRONG
- QS/regtest-mp2-4/H2O\_NO\_HFX.inp: WRONG
- QS/regtest-rma-3D/H2O-32-dftb-ls-2\_mult.inp: RUNTIME FAIL
- QS/regtest-rma-3D/H2O-32-dftb-ls-2.inp: RUNTIME FAIL
- QS/regtest-rma-3D/H2O-OT-ASPC-1.inp: RUNTIME FAIL
- QS/regtest-rma-3D/H2-big-nimages.inp: RUNTIME FAIL
- QS/regtest-rma-3D/H2O\_grad\_gpw.inp: RUNTIME FAIL
- QS/regtest-rma-3D/OH-H2O-bsse.inp: RUNTIME FAIL
- QS/regtest-rma-3D/H2O-6.inp: RUNTIME FAIL
- TMC/regtest\_ana\_on\_the\_fly/TMC\_ana\_start\_with\_exist\_traj.inp: WRONG
- TMC/regtest\_ana\_on\_the\_fly/TMC\_ana\_restart.inp: WRONG
- QS/regtest-mp2-2/H2O-02.inp: WRONG

## ■ Result: MPI8 - OMP2

```
----- Summary -----
Number of FAILED tests 8
Number of WRONG tests 10
Number of CORRECT tests 3218
Number of NEW tests 6
Total number of tests 3242
```

- QS/regtest-mp2-lr/H2O-mp2-gpw-lr.inp: WRONG
- SIRIUS/regtest-1/He-full-potential.inp: RUNTIME FAIL
- QS/regtest-mp2-grad/H2O\_grad\_mme.inp: WRONG
- QS/regtest-gpw-4/H2O-debug-5.inp: WRONG
- QS/regtest-gpw-4/H2O-debug-6.inp: WRONG
- QS/regtest-ri-mp2/opt\_basis\_O\_auto\_gen.inp: WRONG
- Fist/regtest-3/2d\_pot.inp: WRONG
- QS/regtest-mp2-4/H2O\_NO\_HFX.inp: WRONG
- QS/regtest-rma-3D/H2O-32-dftb-ls-2\_mult.inp: RUNTIME FAIL
- QS/regtest-rma-3D/H2O-32-dftb-ls-2.inp: RUNTIME FAIL
- QS/regtest-rma-3D/H2O-OT-ASPC-1.inp: RUNTIME FAIL
- QS/regtest-rma-3D/H2-big-nimages.inp: RUNTIME FAIL
- QS/regtest-rma-3D/H2O\_grad\_gpw.inp: RUNTIME FAIL
- QS/regtest-rma-3D/OH-H2O-bsse.inp: RUNTIME FAIL
- QS/regtest-rma-3D/H2O-6.inp: RUNTIME FAIL

- TMC/regtest\_ana\_on\_the\_fly/TMC\_ana\_start\_with\_exist\_traj.inp: WRONG
- TMC/regtest\_ana\_on\_the\_fly/TMC\_ana\_restart.inp: WRONG
- QS/regtest-mp2-2/H2O-02.inp: WRONG

## Benchmark

H2O-64.inp was employed for benchmark as in 6.1.0. (output of `grep "CP2K " *.log` is used)  
Ran 21 times, and average of last 20 runs is listed below.

jobtype	# of nodes	# of cores	MPI	OMP	GPU	elapse(sec)
core	18 (1)	18	1	-	-	68.154
small	40 (1)	40	1	-	-	45.426
small	80 (2)	80	1	-	-	31.327
small	160 (4)	32	5	-	-	23.398

## Notes

- GPU versions were skipped for this version; they are not so useful in RCCS for now.
  - SIRIUS GPU version might be efficient if correctly built with MAGMA etc. But skipped this time.
- We couldn't get performance improvement from libgrid (bit slower than the vanilla one).
  - pyratemp 0.3.2 was used when building libgrid.a. But this version of pyratemp cannot handle \*.template files in xyz\_to\_vab correctly.
  - Applying `sed -i -e "s/\$/!/g" -e "s/^\</!/g" -e "s/>\!/!/g"` to \*.template files can solve the issue, although the libgrid.a didn't bring any performance improvement...
    - (Use `sed -i -e "s/\$/!/g" -e "s/^\</!/g" -e "s/>\!/!/g"` in the script; above one is valid only when manual execution on terminal.)
- libsmm is simply ignored as in the case of 6.1.0.
- This version of cp2k was built with -O2 option. We also tried "-O2 -xHost" and "-O3 -xHost", but couldn't get performance improvement.
- Released version of dbcsr was used in this build. Using master branch of dbcsr is not a good way to build reliable binary.
- QUIP test couldn't be passed in this build. So we finally remove it from the build. QUIP works fine in GCC version.
  - Patch file used when building with QUIP support. (Not used in this build; just as reference information.)

```

--- install_quip.sh.org 2020-02-04 13:38:25.000000000 +0900
+++ install_quip.sh 2020-02-04 12:53:16.000000000 +0900
@@ -68,34 +68,24 @@
     -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_${quip_arch}_gfortran
- echo "F77FLAGS += -g" >> arch/Makefile.linux_${quip_arch}_gfortran
- echo "CFLAGS += -g" >> arch/Makefile.linux_${quip_arch}_gfortran
- echo "CPLUSPLUSFLAGS += -g" >> arch/Makefile.linux_${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

```

