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_libvdwxc.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 -lmpi "mpich"
+       #check_lib -lmpicxx "mpich"
+       #add_include_from_paths MPICH_CFLAGS "mpi.h" $INCLUDE_PATHS
+       #add_lib_from_paths MPICH_LDFLAGS "libmpi.*" $LIB_PATHS
        ;;
    __DONTUSE__)
        ;;
@@ -87,15 +87,17 @@
        mpi_bin=mpirun
    fi
    # check MPICH version, versions less than 3.0 will get -D__MPI_VERSION=2 flag
-   raw_version=$($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 [ $major_version -lt 3 ] ; then
+   #   mpi2_dflags="-D__MPI_VERSION=2"
+   #else
       mpi2_dflags=''
-   fi
+   #fi
+   MPICH_CFLAGS="-I${I_MPI_ROOT}/include64"
+   MPICH_LDFLAGS="-L${I_MPI_ROOT}/lib64 -Wl,-rpath=${I_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 $LIBINT_CXXFLAGS" \
                      --with-cxx-optflags="$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} \
               ${COMPILATION_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 ${COMPILATION_OPTIONS} .. >> compile.log 2>&1
+                  -DCMAKE_CXX_COMPILER=${MPICXX} \
+                  -DCMAKE_C_COMPILER=${MPICC} ${COMPILATION_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_libvdwxc.sh.intel.diff

```
--- install_libvdwxc.sh.org     2020-02-04 16:23:50.000000000 +0900
+++ install_libvdwxc.sh 2020-02-04 16:48:35.000000000 +0900
@@ -65,7 +65,7 @@
          unset MPICC MPICXX MPIF90 MPIFC MPIF77
          if [ "$MPI_MODE" = "no" ]; then
              # compile libvdwxc without mpi support since fftw (or mkl) do not have mpi support activated
-             ./configure \
+              CC=${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 -lpthread -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_libvdwxc.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 zxf ${TARBALL}
sleep 5
mv cp2k-${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-libvdwxc=install \
                            --with-spglib=install \
                            --with-hdf5=install \
                            --with-spfft=install \
                            -j ${PARALLEL}

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

cd ${INSTDIR}/exts
rmdir dbcsr
tar zxf ${TARBALL_DBCSR}
mv dbcsr-${DBCSR_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-almo-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-almo-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 cores (# of nodes)	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
```

```
          # hit enter a few times to accept defaults
-         echo -e "${MATH_LDFLAGS} $(resolve_string "${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
+          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 ..
          write_checksums "${install_lock_file}" "${SCRIPT_DIR}/$(basename ${SCRIPT_NAME})"
```

- Intel 2019 build shows lesser performance than Intel 2018 one. Also, behaviour of MPI version was bit strange and the number of failed tests was larger.
- Intel 2018 is the fastest among Intel 207, 2018, and 2019 build. In terms of test result, 2018 version is also the best. (Numbers of errors in 2017 and 2018 versions were comparable, though.)
- Modification of source code was required for Intel 2017. Some values in iso_fortran_env are not available in 2017.
    - Patch file for src/start/cp2k.F for intel 2017.

```
--- src/start/cp2k.F.org        2020-02-17 15:26:54.474087502 +0900
+++ src/start/cp2k.F    2020-02-17 15:40:07.489475278 +0900
@@ -55,8 +55,6 @@
   USE input_cp2k,                      ONLY: create_cp2k_root_section
   USE input_section_types,             ONLY: section_release,&
                                              section_type
-  USE iso_fortran_env,                 ONLY: compiler_options,&
-                                             compiler_version
   USE kinds,                           ONLY: default_path_length,&
                                              default_string_length
   USE machine,                         ONLY: default_output_unit
@@ -245,14 +243,6 @@
              cp2k_version//TRIM(dev_flag), &
              "Source code revision "//TRIM(compile_revision), &
              TRIM(cp2k_flags())
-            compiler_options_string = compiler_options()
-            WRITE (output_unit, "(T2,A,A)") "compiler: ", compiler_version()
-            WRITE (output_unit, "(T2,A)") "compiler options:"
-            DO i = 0, (LEN(compiler_options_string) - 1)/68
-              WRITE (output_unit, "(T4,A)") &
-                compiler_options_string(i*68 + 1:MIN(LEN(compiler_options_string), (i + 1)*68))
-            END DO
-            DEALLOCATE (compiler_options_string)
           END IF
         END IF
```