OpenMolcas v20.10

Webpage

https://gitlab.com/Molcas/OpenMolcas

Version

v20.10

Build Environment

- Intel Compiler 19.1.2 (intel parallel studio 2020 update 2)
- Intel MKL 2020.0.2 (intel parallel studio 2020 update 2)
- OpenMPI 3.1.0
- cmake 3.16.3

Files Required

- openmolcas-v20.10.tar.gz (git clone and then git checkout)
- ga-5.8.zip (Global Arrays)

Build Procedure

Global Arrays-5.8

```
#!/bin/sh

GA_VERSION=5.8
GA_DIR=/home/users/${USER}/Software/GlobalArrays/${GA_VERSION}
GA_SOURCE=${GA_DIR}/ga-${GA_VERSION}.zip

WORKDIR=/work/users/${USER}
INSTALLDIR=/local/apl/lx/openmolcas20.10/ga-5.8

#------------------------------------------------------------------------
umask 0022
ulimit -s unlimited

export LANG=
export LC_ALL=C
export OMP_NUM_THREADS=1

cd $WORKDIR
if [ -d ga-${GA_VERSION} ]; then
  mv ga-${GA_VERSION} ga_tmp
  rm -rf ga_tmp &
fi

module purge
module load intel/19.1.2
module load mkl/2020.0.2
module load mpi/openmpi/3.1.0/intel20

#tar zxf ${GA_SOURCE}
unzip ${GA_SOURCE}
cd ga-${GA_VERSION}

export F77=mpif90
export F90=mpif90
export FC=mpif90
export CC=mpicc
export CXX=mpicxx
export MPIF77=mpif90
export MPICC=mpicc
```

```
export MPICXX=mpicxx

export GA_FOPT="-O3 -ip -w -xHost"
export GA_COPT="-O3 -ip -w -xHost"
export GA_CXXOPT="-O3 -ip -w -xHost"

sh autogen.sh
./configure --with-blas8=-mkl \
            --with-scalapack8=-mkl \
            --enable-i8 \
            --prefix=${INSTALLDIR}

make -j ${PARALLEL}
make check
make install
cp config.log ${INSTALLDIR}
```

OpenMolcas-20.10

```
#!/bin/sh

VERSION=v20.10
SOURCEDIR=/home/users/${USER}/Software/OpenMolcas/${VERSION}
TARBALL=${SOURCEDIR}/OpenMolcas-${VERSION}.tar.gz

INSTALL_DIR=/local/apl/lx/openmolcas20.10
GAROOT=${INSTALL_DIR}/ga-5.8
PARALLEL=8

WORKDIR=/work/users/${USER}

export GAROOT
#-----------------------------------------------------------
umask 0022
ulimit -s unlimited

export LANG=
export LC_ALL=C

module purge
module load intel/19.1.2
module load mkl/2020.0.2
module load mpi/openmpi/3.1.0/intel20
module load cmake/3.16.3

cd $WORKDIR
if [ -d OpenMolcas-${VERSION} ]; then
  mv OpenMolcas-${VERSION} OpenMolcas_tmp
  rm -rf OpenMolcas_tmp
fi

tar zxf ${TARBALL}
cd OpenMolcas-${VERSION}
#git submodule update --init External/NECI
git submodule update --init External/libmsym
git submodule update --init External/efp

# simply ridiculous.
uniq src/integral_util/drvefp.f src/integral_util/drvefp.f.tmp
mv -f src/integral_util/drvefp.f.tmp src/integral_util/drvefp.f

mkdir build && cd build

export FC=mpif90
export CC=mpicc
```

```
export CXX=mpicxx

cmake .. -DCMAKE_INSTALL_PREFIX=${INSTALL_DIR} \
      -DMPI_Fortran_COMPILER=${FC} \
      -DMPI_C_COMPILER=${CC} \
      -DMPI_CXX_COMPILER=${CXX} \
      -DMPI=ON \
      -DGA=ON \
      -DOPENMP=ON \
      -DLINALG=MKL \
      -DHDF5=ON \
      -DTOOLS=ON \
      -DFDE=ON \
      -DEFPLIB=ON \
      -DNECI=OFF \
      -DMSYM=ON \
      -DNEVPT2=OFF \
      -DDDMRG=OFF

make -j${PARALLEL}
export MOLCAS_NPROCS=1
export OMP_NUM_THREADS=1
pymolcas verify
export MOLCAS_NPROCS=2
export OMP_NUM_THREADS=2
pymolcas verify

make install
```

Test Result

Tests of Global Arrays are passed without problems. OpenMolcas test results are available under /local/apl/lx/openmolcas20.10/test_results directory.

Serial version

- Only additional:409 failed.
    - # of iteration differs from the reference; may not be a serious problem.

Parallel version

- standard:076 (scf) = numerical error (minor?)
- additional
    - 139 (scf) = input error
    - 221 (alaska) = numerical error (minor?)
    - 259 (scf) = memory error
    - 308 (cht3) = memory error
    - 309 (cht3) = memory error
    - 310 (alaska) = parallel not supported
    - 330 (alaska) = parallel not supported
    - 339 (alaska) = parallel not supported
    - 358 (alaska) = numerical error (minor?)
    - 405 (rasscf) = input error
    - 409 (alaska) = numerical error (NOT minor one)
    - 801 (cht3) = memory error
    - 804 (scf) = input error
    - 806 (mbpt2) = numerical error (minor?)
    - 809 (alaska) = parallel not supported
    - 810 (alaska) = parallel not supported
    - 811 (mbpt2) = numerical error (minor?)
    - 812 (mbpt2) = numerical error (minor?)
    - 814 (alaska) = numerical error (minor?)
    - 820 (scf) = large numerical error only on "E_CNO". Others were OK.
    - 821 (scf) = internal error
    - 822 (alaska) = parallel not supported
    - 852 (rasscf) = input error
    - 863 (alaska) = numerical error (minor?)

- 864 (alaska) = numerical error (minor?)
- 898 (rasscf) = internal error

Notes

- If EFPLIB enabled, duplicated variables declaration in "drvefp.f" shall be dealt with.
- Do not add chemps2 support this time; it does not seem to be maintained.
  - https://gitlab.com/Molcas/OpenMolcas/-/issues/213
- QCMaquis didn't work with Intel compiler. Exactly the same reason as the following issue.
  - https://gitlab.com/Molcas/OpenMolcas/-/issues/125
  - gcc-8, gcc-9 failed to build QCMaquis.
  - We thus avoided QCMaquis in this build.
  - (NOTE: the license of QCMaquis may not be problem; the non-GPL binary executable was called as an external program.)
- Intelmpi 19-20 failed on GA.
- Intel 17-20 + intel mpi 2017/2018 failed on test000 (caspt2). (001, 002 were passed)
- gcc6 + intelmpi 2018 build can pass test000.
  - (patch to chovec_io and other files are required in intelmpi cases. (integer*4 => integer*8))
- Openmpi + intel18 or former needs special setting of "PSM2_MQ_RECVREQS_MAX" environment variable (maybe Omni-Path related; we employ 2097152 this time). Otherwise, perf_strided test of GA failed.
  - (Intel20 can pass the test without additional setting; libpsm2 version problem?)
- The performance of this build might be slightly worse than the previous build (2019/6/4 ver)?
  - (We only did some short (< 10 minutes) benchmark tests, though.)
  - No significant slowdown is observed for core computations (such as scf, rasscf).