OpenMolcas v23.06

Webpage

https://gitlab.com/Molcas/OpenMolcas

Version

v23.06

Build Environment

- GCC 9.2.1
- Intel MKL 2023.1.0
- HPC-X 2.11 (Open MPI 4.1.4)

Files Required

- OpenMolcas.tar.gz (git cloned directory was tar-gzipped)
- ga-5.8.2.tar.gz

Build Procedure

GlobalArrays

```
#!/bin/sh

GA_VERSION=5.8.2
GA_DIR=/home/users/${USER}/Software/GlobalArrays/${GA_VERSION}
GA_SOURCE=${GA_DIR}/ga-${GA_VERSION}.tar.gz

WORKDIR=/gwork/users/${USER}
INSTALLDIR=/apl/openmolcas/v23.06/ga-5.8.2

#------------------------------------------------------------------------
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 gcc-toolset/9
module load mkl/2023.1.0
module load openmpi/4.1.4-hpcx/gcc9

tar zxf ${GA_SOURCE}
cd ga-${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"
export GA_COPT="-O3"
export GA_CXXOPT="-O3"

sh autogen.sh

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

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

OpenMolcas

```
#!/bin/sh

VERSION=v23.06
SOURCEDIR=/home/users/${USER}/Software/OpenMolcas/${VERSION}
TARBALL=${SOURCEDIR}/OpenMolcas.tar.gz

INSTALL_DIR=/apl/openmolcas/${VERSION}
GAROOT=${INSTALL_DIR}/ga-5.8.2
PARALLEL=8

WORKDIR=/gwork/users/${USER}
VERIFYTMP=/gwork/users/${USER}/openmolcas-tmp-v23.06-gcc9-openib

# note: locally installed pyparsing was used in the installation

PATCH=${SOURCEDIR}/cmakelists.patch

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

export LANG=
export LC_ALL=C
export MOLCAS_TIMELIM=1800

module purge
module load gcc-toolset/9
module load mkl/2023.1.0
module load openmpi/4.1.4-hpcx/gcc9

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

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

sed -i -e "/environ/s/= 1/= '1'/" \
       -e "/environ/s/= opt\['parallel'\]/= str(opt['parallel'])/" \
```

```
    sbin/verify

mkdir build && cd build

export FC=mpif90
export CC=mpicc
export CXX=mpicxx

PYTHONEXE=/usr/bin/python3.6
PYTHONINC=/usr/include/python3.6
PYTHONLIB=/usr/lib64/python3.6

cmake .. -DCMAKE_INSTALL_PREFIX=${INSTALL_DIR} \
      -DMPI_Fortran_COMPILER=${FC} \
      -DMPI_C_COMPILER=${CC} \
      -DMPI_CXX_COMPILER=${CXX} \
      -DPython_EXECUTABLE=${PYTHONEXE} \
      -DPython_INCLUDE_DIR=${PYTHONINC} \
      -DPython_LIBRARY=${PYTHONLIB} \
      -DMPI=ON \
      -DGA=ON \
      -DOPENMP=ON \
      -DLINALG=MKL \
      -DHDF5=ON \
      -DTOOLS=ON \
      -DFDE=ON \
      -DEFPLIB=ON \
      -DMSYM=ON \
      -DNEVPT2=OFF \
      -DDMRG=OFF \
      -DWFA=ON

make -j${PARALLEL}

mkdir -p ${VERIFYTMP}

export OMP_NUM_THREADS=2
./pymolcas verify --parallel 4 --tmp ${VERIFYTMP}

make install
```

Tests

Serial version:

- grayzone:832 (only serial version tested): minor numerical error
- grayzone:898 (only serial version tested): numerical error

Parallel version (4 MPI, 2 OpenMP):

- additional:221: it took too much time and timed out eventually.
- additional:826: INTERNAL ERROR
- (OpenMP is applied only for external libraries such as MKL)

Notes

- Copy of testlog is available in /apl/openmolcas/v23.06/test_results.
- Error of additional:221 and 826 for parallel version is very hard to avoid.
    - GA compiled with -with-mpi-pr or --with-mpi-mt do not work well with openmolcas. --mpi-pt might result in the same error (not yet tried).
    - GA built with --with-mpi, --with-mpi-ts, --with-mpi-spawn, --with-mpi3, or --with-openib work fine with openmolcas. But the errors above do not disappear.
    - Changing gcc version (8,9,10,11) doesn't help.
    - Replacing MKL with OpenBLAS (ilp64 version) does not help, either.
    - Intel compiler version (with Intel MPI) met the same issue. Some of openmolcas tests were failed additionally.