OpenMolcas v21.10

Webpage

https://gitlab.com/Molcas/OpenMolcas

Version

v21.10

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.tar.gz
    - "git submodule" didn't work in source tree of release tarball. We built a tarball of v21.10 as described below.

```
[user@ccfep v21.10]$ git clone https://gitlab.com/Molcas/OpenMolcas.git
[user@ccfep v21.10]$ cd OpenMolcas
[user@ccfep OpenMolcas]$ git tag
molcas-8.4
molcas-8.4-sp1
v18.09
v19.11
v20.10
v21.02
v21.06
v21.10
[user@ccfep OpenMolcas]$ git checkout refs/tags/v21.10
[user@ccfep OpenMolcas]$ cd ../
[user@ccfep v21.10]$ tar zcvf OpenMolcas.tar.gz OpenMolcas/
```

- ga-5.8.zip (Global Arrays)
    - Symbolic link /local/apl/lx/openmolcas21.10/ga-5.8 pointing to ga ofv20.10 installation.

Build Procedure

(We reused GlobalArrays of v20.10 installation via symbolic link /local/apl/lx/openmolcas21.10/ga-5.8.)

```
#!/bin/sh

VERSION=v21.10
SOURCEDIR=/home/users/${USER}/Software/OpenMolcas/${VERSION}
TARBALL=${SOURCEDIR}/OpenMolcas.tar.gz

INSTALL_DIR=/local/apl/lx/openmolcas21.10
GAROOT=${INSTALL_DIR}/ga-5.8 # reuse prev version's one
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 ]; 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

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 \
        -DMSYM=ON \
        -DNEVPT2=OFF \
        -DDMRG=OFF \
        -DWFA=ON

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

OpenMolcas test results are copied to /local/apl/lx/openmolcas21.10/test_results directory.

serial

- grayzone: 834 Skipped (not enabled gromacs function)
- there were no errors on manually tested extra/835.input (for WFA).

parallel

- standard: all the tests passed
- additional: following tests were skipped (not available). Other tests have passed without problems.

    - 310, 330, 339, 340, 341, 343, 344, 411, 806, 809, 810, 811, 812, 822, 855
- grayzone: 834 Skipped.

Notes

- Almost the same installation procedure as v20.10.
    - libwfa was enabled additionally in this build.