Molpro 2020.1.2 (intel)

Webpage

https://www.molpro.net/

Version

2020.1.2

Build Environment

- GCC 6.3.1 (devtoolset-6)
- Intel Compiler 19.1.2 (parallel studio 2020 update 2)
- Intel MPI 2018.0.4 (parallel studio 2018 update 4)
- Intel MKL 2020.0.2 (parallel studio 2020 update 2)
- Global Arrays Toolkit 5.7.2

Files Required

- Molpro_release.tar.gz (downloaded source code was archived with tar and gzip)
- ga-5.7.2.tar.gz
- work.patch (/local/apl/lx/molpro2020.1.2/patches/work.patch; to change default working directory)
- binput.patch (/local/apl/lx/molpro2020.1.2/patches/binput.patch; for huge CI calculations)
- token

Build Procedure

```
#!/bin/sh

GA_VERSION=5.7.2
MOLPRO_VERSION=2020.1.2
MOLPRO_DIRNAME=Molpro_release
PARALLEL=12
BASEDIR=/home/users/${USER}/Software/Molpro/2020.1.2
MOLPRO_TARBALL=${BASEDIR}/${MOLPRO_DIRNAME}.tar.gz
PATCH0=${BASEDIR}/work.patch
PATCH1=${BASEDIR}/binput.patch
TOKEN=${BASEDIR}/token

WORKDIR=/work/users/${USER}
GA_INSTALLDIR=${WORKDIR}/ga-temporary
INSTALLDIR=/local/apl/lx/molpro${MOLPRO_VERSION}-intel

#-----------------------------------------
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
if [ -d ga-temporary ]; then
  mv ga-temporary ga_tmp_tmp
  rm -rf ga_tmp_tmp &
fi
if [ -d ${MOLPRO_DIRNAME} ]; then
  mv ${MOLPRO_DIRNAME} molpro_tmp
  rm -rf molpro_tmp &
```

```
fi

module purge
module load scl/devtoolset-6
module load intel/19.1.2
module load mpi/intelmpi/2018.4.274
module load mkl/2020.0.2

#tar zxf /home/users/${USER}/Software/GlobalArrays/${GA_VERSION}/ga-${GA_VERSION}.tar.gz
unzip /home/users/${USER}/Software/GlobalArrays/${GA_VERSION}/ga-${GA_VERSION}.zip
cd ga-${GA_VERSION}

export CFLAGS="-pc80"
export FFLAGS="-pc80"
export FCFLAGS="-pc80"
export CXXFLAGS="-pc80"

export F77=mpiifort
export F90=mpiifort
export FC=mpiifort
export CC=mpiicc
export CXX=mpiicpc
export MPIF77=mpiifort
export MPICC=mpiicc
export MPICXX=mpiicpc
export GA_FOPT="-O3 -ip -w -xHost"
export GA_COPT="-O3 -ip -w -xHost"
export GA_CXXOPT="-O3 -ip -w -xHost"

# --with-ofi failed...
./autogen.sh
./configure --with-blas8 \
            --enable-i8 \
            --prefix=${GA_INSTALLDIR}

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

cd ../
tar zxf ${MOLPRO_TARBALL}
cd ${MOLPRO_DIRNAME}

patch -p0 < ${PATCH0}
patch -p0 < ${PATCH1}

export PATH="${GA_INSTALLDIR}/bin:$PATH" # where ga-config exists

CPPFLAGS="-I${GA_INSTALLDIR}/include" \
LDFLAGS="-L${GA_INSTALLDIR}/lib" \
   ./configure --prefix=${INSTALLDIR} \
               --enable-integer8 \
               --enable-slater

LD_LIBRARY_PATH_ESC=`echo $LD_LIBRARY_PATH | sed -e 's/\//\\\\\//g'`
sed -i -e "s/^VERBOSE.*$/VERBOSE=/" \
      -e "s/^LD_ENV=.*$/LD_ENV=$LD_LIBRARY_PATH_ESC/" CONFIG
unset LD_LIBRARY_PATH_ESC

make -j ${PARALLEL}
cp $TOKEN lib/.token

make tuning
```

```
## manually modify tuning parameters!
#sed -i -e "s/tuning-mindgm.*/tuning-mindgm 0001/" \
#       -e "s/tuning-mindgc.*/tuning-mindgc 0001/" \
#       -e "s/tuning-mindgr.*/tuning-mindgr 0001/" \
#       -e "s/tuning-mindgl.*/tuning-mindgl 0001/" \
#       -e "s/tuning-mindgv.*/tuning-mindgv 0001/" lib/tuning.rc

MOLPRO_OPTIONS=-n2 make quicktest
MOLPRO_OPTIONS=-n2 make test

# failed tests
# loc_eom3.test and PNO-[RU]CCSD tests

#make install
#install -m 644 lib/.token ${INSTALLDIR}/molpro*/lib
```

Installation of the binary and token were done manually.

Tests

- All the GA tests were passed.
- All of PNO-LCCSD tests failed.
    - (h2odim_pnolmp2.test, h2o_rhfpr.test, h2odim_pnolccsdtf12.test, h2o_pnormp2f12.test, auh_cabs.test, c2h4_pnoccd.test, ch3oh_srmp2.test, embed_pno-lccsd-in-dft.test, form_pnoccsd.test, gly1_pnolmp2f12_xyz.test, gly1_pnolmp2f12_zmat.test, gly2_pnof12.test, gly2_pnolccd.test, gly2_pnolccsd.test, gly2_pnolmp2.test, gly2_pnolmp2_2.test, gly2_pnolmp2f12.test, gly2_pnorccsd.test, gly2_pnotriples.test, gly2_pnotriples_disk.test, h2o_pno_litf.test, h2o_pnolccsdf12.test, h2o_pnormp2f12.test, h2o_pnotriples.test, h2o_rhfpr.test, h2odim_mltp.test, h2odim_pno_singdom.test, h2odim_pnolccsd.test, h2odim_pnolccsd_f12.test, h2odim_pnolccsd_proj.test, h2odim_pnolccsdf12.test, h2odim_pnolccsdtf12.test, h2odim_pnolmp2.test, h2odim_pnolmp2_2.test, h2odim_pnolmp2_3.test, h2odim_pnolmp2f12.test, h2odim_pnorccsd.test, h2odim_pnormp2.test, ldfhf.test, ldfhf2.test)

Notes

- PNO-LCCSD would not work in Intel version.
- GCC version showed a better performance than Intel version on DFT and MRCI benchmark tests.
- Intel MPI from parallel studio 2020 update 2 did not work well.