

## 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 xzf /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=mplifort
export FC=mplifort
export CC=mplifort
export CXX=mplifort
export MPIF77=mplifort
export MPICC=mplifort
export MPICXX=mplifort
export GA_FOFT="-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-blas \
    --enable-i8 \
    --prefix=${GA_INSTALLDIR}

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

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

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

export PATH="${GA_INSTALLDIR}/bin:$PATH" # where ga-config exists
CPPFLAGS="-I${GA_INSTALLDIR}/include" \
LDLDFLAGS="-L${GA_INSTALLDIR}/lib" \
./configure --prefix=${INSTALLDIR} \
    --enable-integer8 \
    --enable-slater

LD_LIBRARY_PATH_ESC="echo $LD_LIBRARY_PATH | sed -e 's/v/\\\\v/g'"
sed -i -e "s/^VERBOSE.*$/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\_pnolccsdf12.test, h2o\_pnormp2f12.test, auh\_cabs.test, c2h4\_pnoccd.test, ch3oh\_srm2.test, embed\_pno-lccsd-in-dft.test, form\_pnoccd.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\_lif.test, h2o\_pnolccsdf12.test, h2o\_pnormp2f12.test, h2o\_pnotriples.test, h2o\_rhfpr.test, h2odim\_mlt2p.test, h2odim\_pno\_singdom.test, h2odim\_pnolccsd.test, h2odim\_pnolccsd\_f12.test, h2odim\_pnolccsd\_proj.test, h2odim\_pnolccsdf12.test, h2odim\_pnolccsdf12.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.