

Molpro 2020.1.2

Webpage

<https://www.molpro.net/>

Version

2020.1.2

Build Environment

- ▶ GCC 9.3.1 (devtoolset-9)
- ▶ Intel Parallel Studio 2018 update4 (mkl and mpi)
- ▶ Global Arrays Toolkit 5.7.2

Files Required

- ▶ Molpro_release.tar.gz (compressed Molpro_release 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}

# -----
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-9
module load intel_parallelstudio/2018update4

#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="-mpc80"
export FFLAGS="-mpc80"
export FCFLAGS="-mpc80"
export CXXFLAGS="-mpc80"

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"

# --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 xzf ${MOLPRO_TARBALL}
cd ${MOLPRO_DIRNAME}

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

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

CPPFLAGS="-I${GA_INSTALLDIR}/include" \
LDFLAGS="-L${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

```

The last two lines, "make install" of molpro and installation of token, were done manually.

Tests

Global Arrays Toolkit

- ▶ Error on global/testing/elempatch.x (gcc 8 also failed on this test)

Molpro

- ▶ MPI parallel runs failed in the following tests. OpenMP parallel runs finished successfully.
 - ▶ h2odim_pnorccsd.test
 - ▶ h2odim_pno_singdom.test
 - ▶ gly2_pnorccsd.test
 - ▶ form_pnoccsd.test

Notes

- ▶ According to the official manual, current versions of molpro are well tested with GCC.
 - ▶ The performance of GCC version binary seems to be better than that of Intel version.
 - ▶ PNO-LCCSD runs are available in this GCC version. (Intel version cannot run them.)
- ▶ Some types of run do not work correctly with MPI parallel. On the other hand, OpenMP parallel works well for those kinds of inputs.