

Molpro 2021.3.1 (HPE)

Webpage

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

Version

2021.3.1 (latest commit: Tue Nov 23 17:31:27 2021 +0100)

Build Environment

- GCC 10.3.1 (gcc-toolset-10)
- GCC 11.2.1 (gcc-toolset-11)
- HPC-X 2.11
- openblas 0.3.15 (of Rocky Linux 8 package)

Files Required

- Molpro_release.tar.gz (downloaded Molpro_release directory was tar-gzipped.)
- ga-5.8.2.tar.gz
- work.patch
- patch-argos-bininput.F
- patch-cic-ItfFortranInt.h
- patch-common_modules-common_cconf1
 - For details, please check those files in /apl/molpro/2021.3.1/patches.
- token

Build Procedure

```
#!/bin/sh

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

MOLPRO_VERSION=2021.3.1
MOLPRO_DIRNAME=Molpro_release
PARALLEL=12
BASEDIR=/home/users/${USER}/Software/Molpro/${MOLPRO_VERSION}
MOLPRO_TARBALL=${BASEDIR}/${MOLPRO_DIRNAME}.tar.gz

PATCH_SNPRINTF=${BASEDIR}/secure_snprintf.patch
PATCH0=${BASEDIR}/work.patch
PATCH1=${BASEDIR}/patch-argos-bininput.F
PATCH2=${BASEDIR}/patch-cic-ItfFortranInt.h
PATCH3=${BASEDIR}/patch-common_modules-common_cconf1

TOKEN=${BASEDIR}/token

WORKDIR=/gwork/users/${USER}
GA_INSTALLDIR=${WORKDIR}/ga-temporary
INSTALLDIR=/apl/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 gcc-toolset/10
module load openmpi/4.1.4-hpcx/gcc11

tar xzf `${GA_ARCHIVE}`
cd ga-`${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"

./autogen.sh
./configure --enable-i8 \
    --with-mpi-pr \
    --prefix=${GA_INSTALLDIR}

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

module switch gcc-toolset/11

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

patch -p0 < `${PATCH0}`
patch -p0 < `${PATCH1}`
patch -p0 < `${PATCH2}`
patch -p0 < `${PATCH3}`

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

CPPFLAGS="-I${GA_INSTALLDIR}/include -I/usr/include/openblas" \
LDLDFLAGS="-L${GA_INSTALLDIR}/lib" \
./configure --prefix=${INSTALLDIR} \
    --with-lapack="-L/usr/lib64 -lopenblas" \
    --enable-slater

```

```
sed -i -e "s/\.\/" CONFIG # ?
```

```
make -j ${PARALLEL}
```

```
cp $TOKEN lib/.token
```

```
make tuning
```

```
MOLPRO_OPTIONS="" make quicktest
```

```
MOLPRO_OPTIONS="-n2" make test
```

```
make install
```

Notes

- While --enable-slater is added, it does not seem to work correctly. (same as in the previous system)
 - Slater test was failed. All the other tests have passed.