

Molpro 2022.2.2 (HPE)

Webpage

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

Version

2022.2.2 (latest commit: 2022/6/8 11:34:24 +0200)

Build Environment

- GCC 10.3.1 (gcc-toolset-10)
- GCC 11.2.1 (gcc-toolset-11)
- HPC-X 2.13.1
- openblas 0.3.15 (of Rocky Linux 8)

Files Required

- Molpro_release.tar.gz (downloaded "Molpro_release" was tar-gzipped)
- ga-5.8.2.tar.gz
- work.patch
- patch-argos-bininput.F
- patch-cic-ItfFortranInt.h
- patch-common_modules-common_cconf1
 - Patch files are copied to /apl/molpro/2022.2.2/patches. Please check them by yourself.
- 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=2022.2.2
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/4.1.5-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${GA_INSTALLDIR}/include -I/usr/include/openblas" \
LDLFLAGS="-L${GA_INSTALLDIR}/lib" \
./configure --prefix=${INSTALLDIR} \
    --with-lapack="-L/usr/lib64 -lopenblas"

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

```

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

make tuning

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

make install
```

Notes

- (forgot to add --enable-slater...)
- Gcc11 versions of GA-5.8.2 failed in some tests. There are no problems for gcc10 version.
- Disk option has problem? Sometimes hang up during the job.
 - Intel MPI version didn't work well. So far disk option does not work stably.
- If MKL is employed, the build failed with Eigen error. OpenBlas is used to avoid this error.
 - Loading Eigen module may fix this problem. (not yet tried.)