

Molpro 2024.2.0

Webpage

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

Version

2024.2.0

Build Environment

- GCC 13.1.1 (gcc-toolset-13)
- Intel MPI 2021.13
- Eigen 3.4.0
- MKL 2024.2

Files Required

- molpro-2024.2.0.tar.gz
- ga-5.8.2.tar.gz
- work.patch
- patch-argos-bininput.F
- patch-cic-ltfFortranInt.h
- patch-common_modules-common_cconf
 - Parameter values for large CI calculations and default path of temporary directory were changed.
 - Patch files are available in /apl/molpro/2024.2.0/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=2024.2.0
MOLPRO_DIRNAME=molpro-${MOLPRO_VERSION}
PARALLEL=12
BASEDIR=/home/users/${USER}/Software/Molpro/${MOLPRO_VERSION}
MOLPRO_TARBALL=${BASEDIR}/${MOLPRO_DIRNAME}.tar.gz

PATCH0=${BASEDIR}/work.patch
PATCH1=${BASEDIR}/patch-argos-bininput.F
PATCH2=${BASEDIR}/patch-cic-ltfFortranInt.h
PATCH3=${BASEDIR}/patch-common_modules-common_cconf

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 -s purge
module -s load gcc-toolset/13
module -s load intelmpi/2021.13
module -s load eigen/3.4.0

tar zxf ${GA_ARCHIVE}
cd ga-${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

# mkl for molpro
module -s load mkl/2024.2

cd ${WORKDIR}
tar zxf ${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${GA_INSTALLDIR}/include" \
LDLFLAGS="-L${GA_INSTALLDIR}/lib64" \
  ./configure --prefix=${INSTALLDIR} \
  --enable-slater

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

```

```
make tuning
```

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

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

```
make install
```

```
cp -a testjobs ${INSTALLDIR}/molpro*
```

```
cp -a bench ${INSTALLDIR}/molpro*
```

Tests

All the tests have passed successfully.

Notes

- Built only with Intel MPI. Open MPI was not verified this time.