

Molpro 2021.3.1

Webpage

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

Version

2021.3.1 (latest commit: 2021/11/23 17:31:27 +0100)

Build Environment

- GCC 9.3.1 (devtoolset-9)
- Intel Parallel Studio 2018 update4 (mkl and mpi)
- Global Arrays Toolkit 5.8

Files Required

- Molpro_release.tar.gz (downloaded Molpro_release directory was tar-gzipped.)
- ga-5.8.tar.gz
- work.patch
 - to change default work directory setting
- patch-argos-bininput.F
- patch-cic-ltfFortranInt.h
- patch-common_modules-common_cconf1
 - change parameters for huge CI calculations
- patch-mpp-ga_impl_select
 - change default scratch file setting for single node runs from "disk" to "ga"
- patch-common_modules-common_cftypes
- patch-util-iom
- patch-util-iow
 - work-around for character type "findloc" Fortran 2008 function
 - (On CentOS 7 + devtoolset-9 environment, shared link of molpro executable failed.)
- secure_snprintf.patch
 - to avoid ga build error
- token

Build Procedure

```
#!/bin/sh

GA_VERSION=5.8
GA_ARCHIVE=/home/users/${USER}/Software/GlobalArrays/${GA_VERSION}/ga-${GA_VERSION}.zip

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-ltfFortranInt.h
PATCH3=${BASEDIR}/patch-common_modules-common_cconf1
PATCHX=${BASEDIR}/patch-mpp-ga_impl_select

PATCH10=${BASEDIR}/patch-common_modules-common_cftypes
PATCH11=${BASEDIR}/patch-util-iom
PATCH12=${BASEDIR}/patch-util-iow

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 mk/2018.0.4
module load mpi/intelmpi/2018.4.274
```

```
unzip -q ${GA_ARCHIVE}
#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"
```

```
# --with-ofi failed...
```

```
./autogen.sh
cp -f $PATCH_SNPRINTF autotools/m4-1.4.17/
cd $WORKDIR/ga-${GA_VERSION}
./autogen.sh
./configure --enable-i8 \
  --with-mpi3 \
  --prefix=${GA_INSTALLDIR}
```

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

```

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

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

patch -p0 < ${PATCH10}
patch -p0 < ${PATCH11}
patch -p0 < ${PATCH12}

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

CPPFLAGS="-I${GA_INSTALLDIR}/include" \
LDLFLAGS="-L${GA_INSTALLDIR}/lib" \
./configure --prefix=${INSTALLDIR}

sed -i -e "s/^VERBOSE.*$/VERBOSE=/" CONFIG

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

make tuning

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

```

Notes

- (patch files are available at /local/apl/lx/molpro2021.3.1/patches)
- one of ga tests failed [as in the previous version](#).
- all the molpro tests have passed successfully.
 - slater is disabled, since its test can't be passed.
- Molpro 2021.2 or later employs "disk option" for scratch files of single node runs. However, local disk is not available in RCCS system; /wor/users is on network (lustre) filesystem. We thus change the default setting to the conventional memory one.
 - default "disk option" can be utilised by adding "--ga-impl disk" option.
- some parameters (such as permissions) were modified after the installation (not mentioned in the procedure above)
- On CentOS 7 + devtoolset-9 env, link of molpro.exe failed due to findloc for character type function (not very sure about this error, though).
 - we avoided this error by manually adding equivalent function to findloc of character type.
 - (instead of adding findloc equivalent, static linking of molpro.exe might be another solution (not tried))