

Molpro 2022.3.0 (mvapich)

Webpage

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

Version

2022.3.0

Build Environment

- GCC 10.3.1 (gcc-toolset-10)
- GCC 11.2.1 (gcc-toolset-11)
- MVAPICH 2.3.7
- openblas 0.3.15 (of Rocky Linux 8)

Files Required

- molpro-2022.3.0.tar.gz
- 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/2022.3.0/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=2022.3.0
MOLPRO_DIRNAME=molpro-${MOLPRO_VERSION}
PARALLEL=12
BASEDIR=/home/users/${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}-mva

#-----
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 mvapich/2.3.7/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" \
        --enable-slater

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

```

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

make tuning

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

make install
```

Notes

- Unlike [hpc-x \(openmpi\) version](#), this version works fine when disk option is active.
 - HPC-X 2.13.1, HPC-X 2.11, or Intel MPI 2021.7.1 version hangs when disk option is enabled. (In case of IMPI 2021.7.1, job freezes immediately after start running. In case of HPC-X, job freezes randomly(?).)
 - In case of HPC-X, job often freezes in the libhcoll routine. However, disabling libhcoll (add "-mca coll_hcoll_enable 0" to mpirun) did not help.
 - In case of Open MPI 3.1.6, disk options works without problem. However, another error message is constantly shown. (This probably does not affect results, though.)
 - Intel MPI 2021.5.1, 2021.8.0, and 2021.9.0 are free from this issue. The problem occurs only when runtime library of Intel MPI 2021.7.1 is used.
 - If you don't use disk option (add "--ga-impl ga" option to molpro), those freezes do not happen even when those problematic versions are employed.