Molpro 2024.1.0

Webpage

https://www.molpro.net/

Version

2024.1.0

Build Environment

- GCC 12.1.1 (gcc-toolset-12)
- Intel MPI 2021.11 / Open MPI 4.1.6
- Eigen 3.4.0
- MKL 2024.0

Files Required

- molpro-2024.1.0.tar.gz
- ga-5.8.2.tar.gz
- work.patch
- patch-argos-binput.F
- patch-cic-ItfFortranInt.h
- patch-common_modules-common_cconf1
    - Change some parameters for huge CI calculations and modify default path for temporary files.
    - Patch files are placed at /apl/molpro/2024.1.0/patches directory.
- 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=2024.1.0
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-binput.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 -s purge
module -s load gcc-toolset/12
module -s load intelmpi/2021.11
#module -s load openmpi/4.1.6/gcc12
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/2024.0

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${GA_INSTALLDIR}/include" \
LDFLAGS="-L${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*
```

Test Results

Failed on h2o_rvci_dip test. The value of RVCI_DIP(4:6) may be the problem.

```
SETTING RVCI_TEST(1)  =     140.24404946  CM-1
SETTING RVCI_TEST(2)  =    2040.72148410  CM-1
SETTING RVCI_TEST(3)  =    4309.43539874  CM-1
SETTING RVCI_DIP(1)   =    6.6023777D-20
SETTING RVCI_DIP(2)   =    6.9439373D-20
SETTING RVCI_DIP(3)   =    5.6819299D-19
SETTING RVCI_DIP(4)   =    9.6702224D-20
SETTING RVCI_DIP(5)   =    1.2687290D-18
SETTING RVCI_DIP(6)   =    4.3975422D-19
SETTING RVCI_DIP(7)   =    4.5351150D-20
SETTING RVCI_DIP(8)   =    3.5013711D-19
SETTING RVCI_DIP(9)   =    1.3565481D-20
RVCI_TEST(1:3)  = [    140.24404946  2040.72148410  4309.43539874] CM-1
SETTING RVCIFREQ_REF(1)=      140.24000000
SETTING RVCIFREQ_REF(2)=     2040.72000000
SETTING RVCIFREQ_REF(3)=     4309.44000000
SETTING RVCIDIP_REF(1) =     6.6023777D-20
SETTING RVCIDIP_REF(2) =     6.9439373D-20
SETTING RVCIDIP_REF(3) =     5.6819299D-19
SETTING RVCIDIP_REF(4) =     3.2234075D-20
SETTING RVCIDIP_REF(5) =     4.2290966D-19
SETTING RVCIDIP_REF(6) =     1.3192627D-18
SETTING RVCIDIP_REF(7) =     4.5351150D-20
SETTING RVCIDIP_REF(8) =     3.5013711D-19
SETTING RVCIDIP_REF(9) =     1.3565481D-20
SETTING DRVCI       =       0.00460126  CM-1
SETTING DRVCI_DIP   =       2.00000008
```

This error occurs both on Open MPI and Intel MPI. GCC11, Non-parallel (without -n2 option), and OpenBLAS versions also failed with this test.

Notes

- (openmpi version was built using "module -s load openmpi/4.1.6/gcc12" instead of intelmpi line.)
- Intel MPI version is so far free from the disk option problem.
    - Open MPI version occasionally hung during the calcualtion if disk option is enabled.
    - (Regarding performance, Disk option can be faster or slower than GA option. It depends on the input.)
- On average, Open MPI version is slightly faster than Intel MPI version. But Open MPI version has an issue regarding disk option. We thus chose Intel MPI version as a standard version.
- Eigen 3.4 is necessary? We failed to build with Eigen 3.3 (Rocky Linux rpm).
    - MKL+Eigen 3.3 failed on configure. OpenBLAS+Eigen 3.3 failed during the compilation.