

## Molpro 2020.1.2 (intel)

### ウェブページ

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

### バージョン

2020.1.2

### ビルド環境

- GCC 6.3.1 (devtoolset-6)
- Intel Compiler 19.1.2 (parallel studio 2020 update 2)
- Intel MPI 2018.0.4 (parallel studio 2018 update 4)
- Intel MKL 2020.0.2 (parallel studio 2020 update 2)
- Global Arrays Toolkit 5.7.2

### ビルドに必要なファイル

- Molpro\_release.tar.gz (ダウンロードした Molpro\_release を tar.gz で固めたもの)
- ga-5.7.2.tar.gz
- work.patch (/local/apl/lx/molpro2020.1.2/patches/work.patch; work directory のデフォルトを変更)
- binput.patch (/local/apl/lx/molpro2020.1.2/patches/binput.patch; 巨大な CI 計算のためのパラメータ変更)
- token

### ビルド手順

```
#!/bin/sh

GA_VERSION=5.7.2
MOLPRO_VERSION=2020.1.2
MOLPRO_DIRNAME=Molpro_release
PARALLEL=12
BASEDIR=/home/users/${USER}/Software/Molpro/2020.1.2
MOLPRO_TARBALL=${BASEDIR}/${MOLPRO_DIRNAME}.tar.gz
PATCH0=${BASEDIR}/work.patch
PATCH1=${BASEDIR}/binput.patch
TOKEN=${BASEDIR}/token

WORKDIR=/work/users/${USER}
GA_INSTALLDIR=${WORKDIR}/ga-temporary
INSTALLDIR=/local/apl/lx/molpro${MOLPRO_VERSION}-intel

#-----
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-6
module load intel/19.1.2
module load mpi/intelmpi/2018.4.274
module load mkl/2020.0.2

#tar zxf /home/users/${USER}/Software/GlobalArrays/${GA_VERSION}/ga-${GA_VERSION}.tar.gz
unzip /home/users/${USER}/Software/GlobalArrays/${GA_VERSION}/ga-${GA_VERSION}.zip
cd ga-${GA_VERSION}

export CFLAGS="-pc80"
export FFLAGS="-pc80"
export FCFLAGS="-pc80"
export CXXFLAGS="-pc80"

export F77=mpiifort
export F90=mpiifort
export FC=mpiifort
export CC=mpiicc
export CXX=mpiicpc
export MPIF77=mpiifort
export MPICC=mpiicc
export MPICXX=mpiicpc
export GA_FOPT="-O3 -ip -w -xHost"
export GA_COPT="-O3 -ip -w -xHost"
export GA_CXXOPT="-O3 -ip -w -xHost"

# --with-ofi failed...
./autogen.sh
./configure --with-blas8 \
    --enable-i8 \
    --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}

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

CPPFLAGS="-I${GA_INSTALLDIR}/include" \
LDLDFLAGS="-L${GA_INSTALLDIR}/lib" \
./configure --prefix=${INSTALLDIR} \
    --enable-integer8 \
    --enable-slater

LD_LIBRARY_PATH_ESC=`echo $LD_LIBRARY_PATH | sed -e 's/\//\\\\/g'`
sed -i -e "s/^VERBOSE.*$/VERBOSE=/" \
    -e "s/^LD_ENV.*$/LD_ENV=$LD_LIBRARY_PATH_ESC/" CONFIG
unset LD_LIBRARY_PATH_ESC

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

make tuning

```

```
## manually modify tuning parameters!
#sed -i -e "s/tuning-mindgm.*/tuning-mindgm 0001/" \
# -e "s/tuning-mindgc.*/tuning-mindgc 0001/" \
# -e "s/tuning-mindgr.*/tuning-mindgr 0001/" \
# -e "s/tuning-mindgl.*/tuning-mindgl 0001/" \
# -e "s/tuning-mindgv.*/tuning-mindgv 0001/" lib/tuning.rc

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

# failed tests
# loc_eom3.test and PNO-[RU]CCSD tests

#make install
#install -m 644 lib/.token ${INSTALLDIR}/molpro*/lib
```

最後の install は手動で実行しています。

## テスト

- GA のテストは全てパス
- PNO-LCCSD 関連は動作しないため全てエラー
  - (h2odim\_pnolmp2.test, h2o\_rhfpr.test, h2odim\_pnolccsdtf12.test, h2o\_pnormp2f12.test, auh\_cabs.test, c2h4\_pnoccd.test, ch3oh\_srmp2.test, embed\_pno-lccsd-in-dft.test, form\_pnoccd.test, gly1\_pnolmp2f12\_xyz.test, gly1\_pnolmp2f12\_zmat.test, gly2\_pnof12.test, gly2\_pnolccd.test, gly2\_pnolccsd.test, gly2\_pnolmp2.test, gly2\_pnolmp2\_2.test, gly2\_pnolmp2f12.test, gly2\_pnorccsd.test, gly2\_pnotriples.test, gly2\_pnotriples\_disk.test, h2o\_pno\_litf.test, h2o\_pnolccsdf12.test, h2o\_pnormp2f12.test, h2o\_pnotriples.test, h2o\_rhfpr.test, h2odim\_mltp.test, h2odim\_pno\_singdom.test, h2odim\_pnolccsd.test, h2odim\_pnolccsd\_f12.test, h2odim\_pnolccsd\_proj.test, h2odim\_pnolccsdf12.test, h2odim\_pnolccsdtf12.test, h2odim\_pnolmp2.test, h2odim\_pnolmp2\_2.test, h2odim\_pnolmp2\_3.test, h2odim\_pnolmp2f12.test, h2odim\_pnorccsd.test, h2odim\_pnormp2.test, ldfhf.test, ldfhf2.test)

## メモ

- PNO-LCCSD 関連はソースコードレベルで動かないようになっています。
- パフォーマンスについても基本的には GCC 版の方が上である可能性が高いです。まずは GCC 版をお試し下さい。
- Intel Parallel Studio 2020 update 2 の MPI を使うと GA が一部正常に動作せずフリーズするため回避。