

Molpro 2019.1.2 for LX

ウェブページ

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

バージョン

2019.1.2

ビルド環境

- Intel Parallel Studio 2017 update8
 - ifort 17.0.8
 - icc 17.0.8
 - impi 2017.0.4
- Global Arrays Toolkit 5.7

ビルドに必要なファイル

- Molpro2019.1.2.tar.gz
- ga-5.7.tar.gz
- ~~work.patch~~
 - (2019/12/6) 以下のパッチは適用されていませんでした。申し訳ありません。

```
--- utilities/molpro.template.orig 2018-12-10 16:29:50.000000000 +0900
+++ utilities/molpro.template 2018-12-10 16:39:13.000000000 +0900
@@ -446,6 +446,12 @@
 shift
 done

+MOLPRO_OPTIONS=""
+-d/work/users/$USER/ \
+-l/work/users/$USER/ \
+-W/work/users/$USER/wfu \
+${MOLPRO_OPTIONS}
+
+if test "x${option_d}" = x ; then
+# Now we have to replicate everything inside molpro.exe to try and get the same value of -d that it would
option_d="/tmp"
```

- token

ビルド手順

```
#!/bin/sh

GA_VERSION=5.7
MOLPRO_VERSION=2019.1.2
MOLPRO_DIRNAME=Molpro_release
PARALLEL=12
BASEDIR=/home/users/${USER}/Software/Molpro/2019.1.2
MOLPRO_TARBALL=${BASEDIR}/${MOLPRO_DIRNAME}.tar.gz
PATCH=${BASEDIR}/work.patch
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-3 # gcc 4.9 or later is necessary
      # some fixes required for gcc 6 (qexp etc.)
module load intel_parallelstudio/2017update8

tar xzf /home/users/${USER}/Software/GlobalArrays/${GA_VERSION}/ga-${GA_VERSION}.tar.gz
cd ga-${GA_VERSION}

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"

./configure --with-blas8 \
  --enable-i8 \
  --prefix=${GA_INSTALLDIR}

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

cd ../
tar xzf ${MOLPRO_TARBALL}
cd ${MOLPRO_DIRNAME}
patch -p0 < ${PATCH}

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

CPPFLAGS="-I${GA_INSTALLDIR}/include" \
LDLFLAGS="-L${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

```

```
sed -i -e "s/angs,/ang,/" testjobs/{ch2_singlet.test,ch2_triplet.test}
sed -i -e "s/angs$/ang/" testjobs/{oh_radical.test,ozone_avdz.test}
sed -i -e "s/ANGS$/ANG/" testjobs/o2_cic.test

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

make tuning

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

# failed test: loc_eom3.test

#make install # do it manually
```

テスト

- loc_eom3 のテストで数値エラー。2018.2 の時と同様。

メモ

- 距離の単位の "ANGS" が利用できなくなっています。"ANG" と "ANGSTROM" は今まで通り利用できるようです。
 - ch2_singlet, ch2_triplet, oh_radical, ozone_avdz, o2_cic のテストを動作させるにはこの修正が必要でした。