

Molpro2015.1-pl33 for LX

ウェブページ

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

バージョン

2015.1.33

ビルド環境

- Intel Compiler 15.0.1
- Intel MKL 11.2.1
- Open MPI 2.1.3 (intel)
- Global Arrays Toolkit 5.5

ビルドに必要なファイル

- Molpro2015.1.33.tar.gz
- work.patch (下参照)
- ga-5-5 (スクリプト中で取得)
- token

work.patch

```
--- Molpro2015/utilities/molpro.template.orig 2014-07-01 09:18:27.834620536 +0900
+++ Molpro2015/utilities/molpro.template 2014-07-01 09:19:40.493339561 +0900
@@ -100,6 +100,13 @@
# add executable directory to PATH for finding mrcc executables
export PATH="`echo ${exe} | sed -e 's/V[^V]*$/g`:${PATH}"

+MOLPRO_OPTIONS="\
+-d/work/users/${USER}/\
+-l/work/users/${USER}/\
+-W/work/users/${USER}/wfu\
+${MOLPRO_OPTIONS}"
+export MOLPRO_OPTIONS
+
if [ "x${LAUNCHER}" = x ]; then
mode="serial"
if [ "x${verbose}" = x1 ]; then echo " # SERIAL mode"; fi
```

ビルド手順

```
#!/bin/sh

GA_VERSION=5-5
MOLPRO_VERSION=2015.1-pl33
MOLPRO_DIRNAME=Molpro2015.1.33
PARALLEL=12
BASEDIR=/home/users/${USER}
MOLPRO_TARBALL=${BASEDIR}/Molpro2015.1.33.tar.gz
PATCH=${BASEDIR}/work.patch
TOKEN=${BASEDIR}/token

GA=https://svn.pnl.gov/svn/hpctools/branches/ga-${GA_VERSION}
WORKDIR=/work/users/${USER}
GA_INSTALLDIR=${WORKDIR}/ga-temporary
INSTALLDIR=/local/apl/lx/molpro${MOLPRO_VERSION}
GA_INC=${GA_INSTALLDIR}

#-----
umask 0022
```

```

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

svn checkout ${GA} --username anonymous --password anonymous --non-interactive

# using environment modules
module purge
module load intel/15.0.1
module load mkl/11.2.1
module load mpi/openmpi/2.1.3/intel

cd ga-${GA_VERSION}

export F77=mpif90
export CC=mpicc
export CXX=mpicxx
export MPIF77=mpif90
export MPICC=mpicc
export MPICXX=mpicxx
export GA_FOPT="-O3 -w -xHost"
export GA_COPT="-O3 -w -xHost"
export GA_CXXOPT="-O3 -w -xHost"

sed -i 's/Imkl/mkl/g' armci/configure tascel/configure comex/configure configure

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

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

unset F77
unset CC
unset CXX
unset MPIF77
unset MPICC
unset MPICXX

cd ../
tar zxvf ${MOLPRO_TARBALL}
cd ${MOLPRO_DIRNAME}
patch -p1 < ${PATCH}
sed -i -e "s/2012\,1/2015.1/" configure # why...?

./configure -batch \
  -i8 \
  -icc \
  -ifort \
  -j ${PARALLEL} \
  -openmpi \
  -slater \
  -noboost \

```

```
-mpp \  
-mppbase ${GA_INC} \  
-x86_64 \  
-prefix ${INSTALLDIR}  
  
LD_LIBRARY_PATH_ESC=`echo $LD_LIBRARY_PATH | sed -e 's/V/\\\\\\\\/g`  
sed -i -e "s/^VERBOSE.*$/VERBOSE=/" \  
-e "s/^LD_ENV=.*$/LD_ENV=$LD_LIBRARY_PATH_ESC/" CONFIG  
  
make -j ${PARALLEL}  
cp $TOKEN lib/.token  
  
make tuning  
MOLPRO_OPTIONS=-n2 make quicktest  
MOLPRO_OPTIONS=-n2 make test  
#make install # do it manually
```

最後のmake installは手動で実行します。

注意点

インプット条件により、正常に動作しないケースがあります。テストジョブで確認。
その場合、実行時に --tuning-mindgm 0001 や --tuning-mindgv 0001 等のチューニングオプションを渡すと
(多少数値精度に変化があるようですが)動作する場合があります。
これらチューニング用パラメータの名前とデフォルト値はlib/tuning.rcに記述があります。