

Molpro 2018.2 for LX

Webpage

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

Version

2018.2

Build Environment

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

Files Required

- Molpro2018.2.0.tar.gz
- ga-5.7.tar.gz
- work.patch

```
--- 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

Build Procedure

```
#!/bin/sh

GA_VERSION=5.7
MOLPRO_VERSION=2018.2
MOLPRO_DIRNAME=Molpro_release
PARALLEL=12
BASEDIR=/home/users/qq7/Software/Molpro/2018.2.0
MOLPRO_TARBALL=${BASEDIR}/Molpro2018.2.0.tar.gz
PATCH=${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

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 zxf /home/users/qf7/Software/GlobalArrays/5.7/ga-5.7.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 zxf ${MOLPRO_TARBALL}
cd ${MOLPRO_DIRNAME}
patch -p0 < ${PATCH}

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
```

```
MOLPRO_OPTIONS=-n2 make quicktest
```

```
MOLPRO_OPTIONS=-n2 make test
```

```
# failed tests
```

```
# hamiltonian.test loc_eom3.test
```

```
#make install # do it manually
```

Test

- The following two tests yield errors. The official binary package also has the same problem. Results from our build and official binary are consistent.
 - hamiltonian.test: returns error upon finishing the job. Output values seem to be OK.
 - loc_eom3.test: numerical error happens.

Note

- Intel MPI version is more stable than Open MPI version in terms of number of failed tests.
 - Open MPI version failed on some more tests, and some errors happen upon finishing the job. In most cases, the outputted values (energies) are correct, though.