

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
PARALLELEL=12
BASEDIR=/home/users/qf7/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 xzf /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 xzf ${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.