

Molpro2015.1-pl27 for LX

Webpage

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

Version

2015.1.27

Tools for Compiling

- ▶ Intel Compiler 17.0.4.196
- ▶ Intel MPI 2017.4.196
- ▶ Intel MKL 2017.4.196

Necessary Files for Compiling

- ▶ Molpro2015.1.27.tar.gz
- ▶ [work.patch](#)
- ▶ token

Patch Files

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 mrcr executables
export PATH="echo ${exe} | sed -e 's/^[^/]*/g':${PATH}"

+MOLPRO_OPTIONS="\
+-d/work/users/$USER/ \
+!work/users/$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
```

Procedure of Compiling

```
#!/bin/csh -f
umask 022
unsetenv LANG
set work=/work/users/${USER}
set molpro=molpro2015.1-pl27
set prefix=/local/apl/lx/${molpro}
set file_molpro=/home/users/${USER}/build/${molpro}/Molpro2015.1.27.tar.gz
set file_token=/home/users/${USER}/build/${molpro}/token
set patch_work=/home/users/${USER}/build/${molpro}/work.patch
# prepare
cd ${work}
if (-d ${molpro}) then
mv ${molpro} ${molpro}-erase
rm -rf ${molpro}-erase &
endif
if (-d "ga-5-5") then
rm -rf ga-5-5 &
endif
tar zxf ${file_molpro}
patch -p0 < ${patch_work}
mv Molpro2015 ${molpro}
#
cd ${work}/${molpro}/src/ga-5-5
setenv F77 mpiifort
setenv CC mpiicc
setenv MPICC mpiicc
setenv MPICXX mpiicc
setenv MPIF77 mpiifort
setenv GA_FOFT "-O3 -w -xAVX"
sed -i 's/lmkl/mkl/g' tascel/configure comex/configure configure
## To use /usr/lib64/liblapack.so for test
setenv LD_LIBRARY_PATH /usr/lib64:${LD_LIBRARY_PATH}
./configure --with-blas8 --enable-i8 --disable-cxx --prefix=${work}/ga-5-5
```

```
make -j 12
make install
cp config.log ${work}/ga-5-5
unsetenv F77
unsetenv CC
unsetenv MPICC
unsetenv MPICXX
unsetenv MPIF77
#
setenv CXX mpiicc
setenv FC ifort
cd ${work}/${molpro}
cp ${file_token} lib/.token
sed -i 's/-link_info/-ilp64 -link_info/' configure
./configure --enable-integer8 --enable-mpp=${work}/ga-5-5/lib --disable-boost --enable-slater --prefix=${prefix}
sed -i 's/^LAUNCHER:*/LAUNCHER=mpirun -np %n %x/' CONFIG
sed -i 's/^VERBOSE:*/VERBOSE=/' CONFIG
make -j 12
make tuning
make MOLPRO_OPTIONS=-n2 quicktest
make MOLPRO_OPTIONS=-n2 test
```
