

## Molpro2015.1-pl19 for UV2000

### Webpage

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

### Version

2015.1.19

### Tools for Compiling

- ▶ Intel Compiler 15.0.2
- ▶ SGI MPT 2.13
- ▶ Intel MKL 2015.2.164

### Remarks

- ▶ Tests (embed\_test2\_high.test, h2odim\_enepart.test, h2odim\_enepart\_direct.test, h2odimer1\_imp2.test, h2odimer2\_imp2.test) did not pass in Intel Compiler 17.0.2.
- ▶ Test (h2o\_slater.test) did not pass in Intel Compiler 16.0.2.

### Necessary Files for Compiling

- ▶ Molpro2015.1.19.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 mrcx executables
export PATH="`echo ${exe} | sed -e 's/[^\v]*/g':${PATH}"
```

```
+MOLPRO_OPTIONS="\
+-d/work/users/${USER}/\
+I/work/users/${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/${USER}
set molpro=molpro2015.1-pl19
set file_molpro=/home/users/${USER}/build/${molpro}/Molpro2015.1.19.tar.gz
set file_token=/home/users/${USER}/build/${molpro}/token
set patch_work=/home/users/${USER}/build/${molpro}/work_patch
#
eval `usr/bin/modulecmd tcsh load intel-15.0/15.0.2`
# 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 xzf ${file_molpro}
patch -p0 < ${patch_work}
mv Molpro2015 ${molpro}
#
cd ${work}/${molpro}/src/ga-5-5
setenv GA_FOPT "-O3 -w -xAVX"
sed -i 's/mkl/mkl/g' tascel/configure comex/configure configure
#
./configure --with-blas8 --enable-i8 --disable-cxx --prefix=${work}/ga-5-5
```

```
make -j 16
make install
cp config.log ${work}/ga-5-5
#
setenv CXX mpicxx
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=/local/apl/uv/${molpro}
sed -i 's|^LAUNCHER.*$|LAUNCHER=/opt/sgi/mpt/mpt-2.13/bin/mpirun -np %n /usr/bin/dplace -s1 %x|' CONFIG
sed -i 's/^VERBOSE.*$|VERBOSE=/' CONFIG
make -j 16
make tuning
make MOLPRO_OPTIONS=-n2 quickestest
#make MOLPRO_OPTIONS=-n2 test
```

---