

Molpro2012.1-pl15 for UV2000

Webpage

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

Version

2012.1.15

Tools for Compiling

- ▶ Intel Compiler 14.0.2.144
- ▶ SGI MPT 2.07
- ▶ Intel MKL 14.0.2.144

Necessary Files for Compiling

- ▶ molpro.2012.1.15.tar.gz
- ▶ [dirs.mk.patch](#)
- ▶ [work.patch](#)
- ▶ token

Patch Files

dirs.mk.patch

```
--- Molpro/src/make/dirs.mk.orig 2014-05-22 22:54:44.000000000 +0900
+++ Molpro/src/make/dirs.mk 2014-06-05 11:13:18.000000000 +0900
@@ -21,6 +21,10 @@
DIRECTORIES+=Molcas/shared_util
DIRECTORIES+=Molcas/slapaf
DIRECTORIES+=Molcas/slapaf_util
+DIRECTORIES+=vscf
+DIRECTORIES+=basis
+DIRECTORIES+=neci
+DIRECTORIES+=tdfft
DIRECTORIES+=util
DIRECTORIES+=argos
DIRECTORIES+=ccsd
@@ -53,9 +57,7 @@
DIRECTORIES+=netlib/slatec/lin
DIRECTORIES+=netlib/dftemplates
DIRECTORIES+=dalton
-DIRECTORIES+=basis
DIRECTORIES+=explicit
-DIRECTORIES+=vscf
DIRECTORIES+=cosmo
DIRECTORIES+=dft
DIRECTORIES+=sapt
@@ -75,7 +77,5 @@
DIRECTORIES+=slater
DIRECTORIES+=instanton
DIRECTORIES+=aims
-DIRECTORIES+=neci
-DIRECTORIES+=tdfft

ALLDIRECTORIES=$(PREDIRECTORIES) $(DIRECTORIES)
```

work.patch

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

Procedure of Compiling

```
#!/bin/csh -f
umask 022
unsetenv LANG
set work=/work/users/${USER}
set molpro=molpro2012.1-pl15
set file_molpro=/home/users/${USER}/build/${molpro}/molpro.2012.1.15.tar.gz
set file_token=/home/users/${USER}/build/${molpro}/token
set patch_dirsmk=/home/users/${USER}/build/${molpro}/dirs.mk.patch
set patch_work=/home/users/${USER}/build/${molpro}/work.patch
# prepare
cd ${work}
if (-d ${molpro}) then
  mv ${molpro} ${molpro}-erase
  rm -rf ${molpro}-erase &
endif
if (-d "ga-5-3") then
  rm -rf ga-5-3 &
endif
tar xzf ${file_molpro}
patch -p0 < ${patch_dirsmk}
patch -p0 < ${patch_work}
mv Molpro ${molpro}
#
cd ${work}/${molpro}/src/ga-5-3
setenv GA_FOPT "-O3 -w -xAVX"
sed -i 's/lmkl/mkl/g' tascel/configure comex/configure configure
#
./configure --with-blas8 --enable-i8 --disable-cxx --prefix=${work}/ga-5-3
make -j 16
make install
cp config.log ${work}/ga-5-3
#
cd ${work}/${molpro}
cp ${file_token} lib/token
sed -i 's/-link_info/-ilp64 -link_info/' configure
./configure -batch -icc -ifort -mpp -mppbase ${work}/ga-5-3 -noboost -prefix /local/apl/uv/${molpro}
sed -i 's/-Wl,/' CONFIG
sed -i 's|^LAUNCHER.*$|LAUNCHER=/opt/sgi/mpt/mpt-2.07/bin/mpiurun -np %n /usr/bin/dplace -s1 %x|' CONFIG
sed -i 's/^VERBOSE.*$|VERBOSE=/' CONFIG
make -j 16
make tuning
make install
```