Molpro2015.1-pl0 for UV2000

ウェブページ

http://www.molpro.net/

バージョン

2015.1.0

ビルド環境

- Intel Compiler 15.0.2
- SGI MPT 2.11
- Intel MKL 2015.2.164

ビルドに必要なファイル

- Molpro2015.tar.gz
- work.patch
- token

パッチファイル

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

ビルド手順

```
#!/bin/csh -f
umask 022
unsetenv LANG
set work=/work/users/${USER}
set molpro=molpro2015.1-pl0
set file_molpro=/home/users/${USER}/build/${molpro}/Molpro2015.tar.gz
set file_token=/home/users/${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-5-4") then
  rm -rf ga-5-4 &
endif
tar zxf ${file_molpro}
patch -p0 < ${patch_work}
mv Molpro2015 ${molpro}
#
cd ${work}/${molpro}/src/ga-5-4
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-5-4
make -j 16
make install
cp config.log ${work}/ga-5-4
#
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-5-4/lib --disable-boost --enable-slater --prefix=/local/apl/uv/${mo
sed -i 's|^LAUNCHER.*$|LAUNCHER=/opt/sgi/mpt/mpt-2.11/bin/mpirun -np %n /usr/bin/dplace -s1 %x|' CONFIG
sed -i 's/^VERBOSE.*$/VERBOSE=/' CONFIG
make -j 16
make tuning
```