

ウェブページ

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

バージョン

2012.1.37

ビルド環境

- Intel Compiler 16.0.2
- SGI MPT 2.11
- Intel MKL 2016.2.181

ビルドに必要なファイル

- molpro.2012.1.37.tar.gz
- [dirs.mk.patch](#)
- [work.patch](#)
- token

パッチファイル

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+=tddft
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+=dfit
DIRECTORIES+=sapt
@@ -75,7 +77,5 @@
DIRECTORIES+=slater
DIRECTORIES+=instanton
DIRECTORIES+=aims
-DIRECTORIES+=neci
-DIRECTORIES+=tddft

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 mrcc executables
export PATH=`echo ${exe} | sed -e 's/[^V]*$//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/${USER}
set work=/dev/shm/${USER}
set molpro=molpro2012.1-pl37
set file_molpro=/home/users/${USER}/build/${molpro}/molpro.2012.1.37.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-5-4") then
rm -rf ga-5-4 &
endif
tar xzf ${file_molpro}
patch -p0 < ${patch_dirsmk}
patch -p0 < ${patch_work}
mv Molpro ${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
#
cd ${work}/${molpro}
cp ${file_token} lib/token
sed -i 's/-link_info/-ilp64-link_info/' configure
./configure -batch -icc -ifort -mpp -mppbase ${work}/ga-5-4 -noboost -slater -prefix /local/apl/uv/${molpro}
sed -i 's/-WI,///g' CONFIG
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

```