

Molcas 8.2 for UV2000

Webpage

<http://www.molcas.org/>

Version

8.2

Tools for Compiling

- ▶ Intel Compiler 17.0.4.196
- ▶ SGI MPT 2.13
- ▶ Intel MKL 17.0.4.196

Necessary Files for Compiling

- ▶ molcas82.tar.gz
- ▶ license.dat

Attention

- ▶ Compile option "-xSSE4.2" is set because verification would be failed with "-xAVX".
- ▶ Unless ./configure is executed twice, the built-in blas routine is used.

Procedure of Compiling

```
#!/bin/csh -f
umask 022
set file_molcas=/home/users/${USER}/build/molcas82/molcas82.tar.gz
set file_license=/home/users/${USER}/build/molcas82/license.dat
set work=/work/users/${USER}
set prefix=/local/apl/uv/molcas82
#-----
eval `usr/bin/modulecmd tosh load intel-17.0/17.0.4`
setenv MPICC mpicc
setenv MPICXX mpicxx
setenv MPIF77 mpif90
setenv CC mpicc
setenv CXX mpicxx
setenv F77 mpif90
cd ${work}
if (-d molcas82) then
  rm -rf molcas82
endif
tar xzf ${file_molcas}
cd molcas82
cp ${file_license} .
chmod 644 license.dat
chmod 700 src
mkdir bin
cp sbin/molcas.driver bin/molcas
chmod +x bin/molcas
#
sed -i "s/-O2/-O2 -xSSE4.2" cfg/intel.comp
#
setenv PATH $prefix/bin:$PATH
setenv MOLCAS_NPROCS 1
# (Workaround) Need to execute './configure' twice.
./configure -compiler intel -parallel -mpiroot /opt/sgi/mpt/mpt-2.13/ -mpirun /opt/sgi/mpt/mpt-2.13/bin/mpirun -blas MKL -blas_lib '-Wl,--start-group -mkl -static-intel -Wl,--end-group'
./configure -compiler intel -parallel -mpiroot /opt/sgi/mpt/mpt-2.13/ -mpirun /opt/sgi/mpt/mpt-2.13/bin/mpirun -blas MKL -blas_lib '-Wl,--start-group -mkl -static-intel -Wl,--end-group'
# (Workaround for parallel compilation)
sed -i 's/all: build/all: build\nutils: ${UTILS}' Makefile
sed -i 's/^${UTILS}: .*${UTILS}: ${DIRS} ${EXTERNALS} ${MODULES}' Makefile
sed -i 's/^${UTILS} \\\$utils $' Makefile
# (Workaround for intel compiler)
sed -i 's/(SUBROUTINE CHO_SETMAXSHL.*)\\1\n!DIR$ NOOPTIMIZE" src/cholesky_util/cho_setmaxshl.f'
#
make Driver
# Alternative command "make -j 16 utils"
grep -E '^UTILS' Makefile | sed 's/UTILS = //' | xargs -P 16 -n 1 make
# Alternative command "make -j 16 build"
grep -E '^PROGRAMS' Makefile | sed 's/PROGRAMS = //' | xargs -P 16 -n 1 make
make build
sed -i 's/remove_tree/rmtree/g' sbin/verify
setenv MOLCAS_NPROCS 4
```

