

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 tcsh 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 -
./configure -compiler intel -parallel -mpiroot /opt/sgi/mpt/mpt-2.13/ -mpirun /opt/sgi/mpt/mpt-2.13/bin/mpirun -blas MKL -
# (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 $/' Makefile
# (Workaround for intel compiler)
sed -i 's/(SUBROUTINE CHO_SETMAXSHL.*)\n\n!DIR\n$ 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
molcas verify

```