

## Molcas 8.0 for UV2000

### Webpage

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

### Version

8.0

### Tools for Compiling

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

### Necessary Files for Compiling

- ▶ molcas80.tar.gz
- ▶ ga-5-3.tgz
- ▶ license.dat

### Procedure of Compiling

```
#!/bin/csh -f
umask 022
set file_molcas=/home/users/${USER}/build/molcas80/molcas80.tar.gz
set file_ga=/home/users/${USER}/build/molcas80/ga-5-3.tgz
set file_license=/home/users/${USER}/build/molcas80/license.dat
set prefix=/local/apl/uv/molcas80
set work=/work/users/${USER}
#-----
cd ${work}
if (-d ga-5-3) then
  rm -rf ga-5-3
endif
tar xzf ${file_ga}
cd ga-5-3
./configure --with-blas8 --enable-i8 --disable-cxx --prefix=${work}/ga-5-3
make -j 16
make install
#-----
cd ${work}
if (-d molcas80) then
  rm -rf molcas80
endif
tar xzf ${file_molcas}
cd molcas80
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/-O3 -no-prec-div -xAVX/" cfg/intel.comp
sed -i "s/-lmpi -lmpi_f77 -lmpi/" cfg/mpi.comp
setenv PATH $prefix/bin:$PATH
./configure --compiler intel --parallel omp --par_root /opt/sgi/mpt/mpt-2.07/ --par_run /opt/sgi/mpt/mpt-2.07/bin/mpirun --par_args NONE \
-blas MKL --blas_lib -Wl,--start-group -mkl -static-intel -Wl,--end-group -ga ${work}/ga-5-3
sed -i 's|mpirun -np $CPUS|mpirun -np $CPUS /usr/bin/dplace -s1|' molcas.rte
sed -i 's|[RUNBINARYSER=.*]|RUNBINARYSER=""|opt/sgi/mpt/mpt-2.07/bin/mpirun -np $CPUS /usr/bin/dplace -s1 $program|' molcas.rte
make -j 12 build
make install
```