

Molcas 8.0 sp1 for UV2000

ウェブページ

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

バージョン

8.0 sp1

ビルド環境

- ▶ Intel Compiler 15.0.2.164
- ▶ SGI MPT 2.11
- ▶ Intel MKL 15.0.2.164

ビルドに必要なファイル

- ▶ molcas80sp1.tar.gz
- ▶ ga-5-3.tgz
- ▶ license.dat

ビルド手順

```
#!/bin/csh -f
umask 022
set file_molcas=/home/users/${USER}/build/molcas80sp1/molcas80sp1.tar.gz
set file_ga=/home/users/${USER}/build/molcas80sp1/ga-5-3.tgz
set file_license=/home/users/${USER}/build/molcas80sp1/license.dat
set prefix=/local/apl/uv/molcas80sp1
set work=/work/users/${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 molcas80sp1) then
  rm -rf molcas80sp1
endif
tar xzf ${file_molcas}
cd molcas80sp1
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 ompi -par_root /opt/sgi/mpt/mpt-2.11/ -par_run /opt/sgi/mpt/mpt-2.11/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-2.11/bin/mpirun -np $CPUS /usr/bin/dplace -s1 $program""|" molcas.rte
make -j 12 build
make install
```