

Molcas 8.0 sp1 for PRIMERGY

Webpage

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

Version

8.0 sp1

Tools for Compiling

- ▶ Intel Compiler 15.0.2.164
- ▶ Intel MPI 5.0.3.048
- ▶ Intel MKL 15.0.2.164

Necessary Files for Compiling

- ▶ molcas80sp1.tar.gz
- ▶ license.dat

Attention

Compile option "-xSSE4.2" is set because verification would be failed with "-xAVX".

Procedure of Compiling

```
#!/bin/csh -f
umask 022
set file_molcas=/home/users/${USER}/build/molcas80sp1/molcas80sp1.tar.gz
set file_license=/home/users/${USER}/build/molcas80sp1/license.dat
set work=/work/users/${USER}
set prefix=/local/apl/pg/molcas80sp1
#-----
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 -xHost/" cfg/intel.comp ... NG
#sed -i "s/-O2/-O2 -xSSE4.1/" cfg/intel.comp ... OK
# Verification failed with AVX code in MPI.
source /opt/intel/composer_xe_2015.2.164/bin/compilervars.csh intel64
#sed -i "s/-O2/-O2 -xAVX/" cfg/intel.comp ... NG
#sed -i "s/-O2/-O2 -xHost/" cfg/intel.comp ... NG
#sed -i "s/-O2/-O3 -no-prec-div -xSSE4.2/" cfg/intel.comp ... NG (087)
sed -i "s/-O2/-O2 -xSSE4.2/" cfg/intel.comp # ... OK
setenv PATH $prefix/bin:$PATH
setenv MOLCAS_CPUS 1
./configure -compiler intel -parallel impi -par_root /opt/intel/mpi/5.0.3.048/intel64/ -par_run /opt/intel/mpi/5.0.3.048/intel64/bin/mpirun -par_args NONE -blas MKL -blas_lib -WI,-start-group -mkl -static-intel -WI,-end-group
make -j 12 build
make install
#
setenv MOLCAS_CPUS 4
molcas verify
```