

Molcas 8.0 for PRIMERGY

Webpage

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

Version

8.0

Tools for Compiling

- Intel Compiler 14.0.2.144
- Intel MPI 4.1.0.030
- Intel MKL 14.0.2.144

Necessary Files for Compiling

- molcas80.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/${USER}/build/molcas80/molcas80.tar.gz
set file_license=/home/users/${USER}/build/molcas80/license.dat
#set work=/work/users/${USER}
set work=/dev/shm/${USER}
set prefix=/local/apl/pg/molcas80
#set prefix=${work}/molcas80
#-----
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 -xHost/" cfg/intel.comp ... NG
#sed -i "s/-O2/-O2 -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_2013_sp1.2.144/bin/compilervars.csh intel64
#sed -i "s/-O2/-O2 -xAVX/" 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/impi/4.1.0.030/intel64/ -par_run /opt/intel/impi/4.1.0.030/intel
  -par_args NONE -blas MKL -blas_lib -WI,--start-group -mkl -static-intel -WI,--end-group
make -j 12 build
make install
```

