NWChem-6.8 for LX

Webpage

http://www.nwchem-sw.org/index.php/Main_Page

Version

6.8

Tools for Compiling

- Intel Compiler 17.0.4.196
- Intel MPI 2017.4.196
- Intel MKL 2017.4.196

Necessary Files for Compiling

- nwchem-6.8-release.revision-v6.8-47-gdf6c956-src.2017-12-14.tar.bz2

Procedure of Compiling

```
#!/bin/csh -f
umask 022
unsetenv LANG
set work=/work/users/${USER}
set nwchem=nwchem68
set file_nwchem=/home/users/${USER}/build/${nwchem}/nwchem-6.8-release.revision-v6.8-47-gdf6c956-src.2017-12-14.tar.bz2
# prepare
cd ${work}
if (-d ${nwchem}) then
  mv ${nwchem} ${nwchem}-erase
  rm -rf ${nwchem}-erase &
endif
bunzip2 -c ${file_nwchem} | tar xf -
mv nwchem-6.8 ${nwchem}
#
setenv NWCHEM_TOP ${work}/${nwchem}
setenv NWCHEM_TARGET LINUX64
setenv ARMCI_NETWORK MPI-PR
setenv NWCHEM_MODULES "all python"
setenv USE_NOFSCHECK TRUE
setenv USE_NOIO TRUE
setenv PYTHONHOME /usr
setenv PYTHONVERSION 2.7
setenv PYTHONLIBTYPE so
setenv USE_PYTHON64 y
setenv USE_CPPRESERVE y
setenv USE_MPI y
setenv USE_MPIF y
setenv USE_MPIF4 y
setenv MPI_HOME /local/apl/lx/intel2017update4/compilers_and_libraries_2017.4.196/linux/mpi/intel64
setenv MPI_LOC $MPI_HOME
setenv MPI_LIB $MPI_LOC/lib
setenv MPI_INCLUDE $MPI_LOC/include
setenv LIBMPI "-lmpigf -lmpigi -lmpi_ilp64 -lmpi"
setenv BLASOPT "-mkl -qopenmp"
setenv USE_OPENMP y
setenv FC ifort
setenv CC icc
cd $NWCHEM_TOP/src
sed -i 's/^RELEASE :=.*$/RELEASE :=/' config/makefile.h
make nwchem_config
make
```