

NBO-7.0.2 for LX

Webpage

<http://nbo7.chem.wisc.edu/>

Version

7.0.2

Build Environment

- Intel Compiler 18.0.2.199
- Intel MKL 2018 Update 2

Files Required

- nbo7.0-src.tar.gz

Build Procedure

```
#!/bin/csh -f
umask 022
set file_nbo=/home/users/${USER}/build/nbo702/nbo7.0-src.tar.gz
set prefix=/local/apl/lx/nbo702
#-----
if (-e $prefix/bin) then
echo "Remove $prefix to be clean."
exit 1
endif
if (! -d $prefix) then
echo "Create $prefix before build."
exit 1
endif
cd $prefix
tar xf $file_nbo
mv nbo7/* .
rmdir nbo7
sed -i "s/LenBuf=2048/LenBuf=10000/" src/g16nbo/utlis.F
sed -i 's/^FC = .*/FC = ifort/' Make.config
sed -i 's/^CC = .*/CC = icc/' Make.config
sed -i "s/^NBODIR = .*/NBODIR = \local\apl\lx\nbo702/" Make.config
sed -i 's/^LAPACK = .*/LAPACK = true/' Make.config
sed -i 's/^LAPACKLIB = .*/LAPACKLIB = -mkl/' Make.config
sed -i 's/^BLAS = .*/BLAS = true/' Make.config
sed -i 's/^BLASLIB = .*/BLASLIB = -mkl/' Make.config
make
sed -i "s/^setenv BINDIR .*/setenv BINDIR \local\apl\lx\nbo702\bin/" bin/gaunbo6
sed -i "s/^setenv BINDIR .*/setenv BINDIR \local\apl\lx\nbo702\bin/" bin/gaunbo7
sed "s/^setenv GAUNBO g09nbo/setenv GAUNBO g16nbo/" bin/gaunbo6 > bin/gaunbo6-g16
sed "s/^setenv GAUNBO g09nbo/setenv GAUNBO g16nbo/" bin/gaunbo7 > bin/gaunbo7-g16
mv bin/gaunbo6 bin/gaunbo6-g09
mv bin/gaunbo7 bin/gaunbo7-g09
chmod 755 bin/gaunbo6-g16
chmod 755 bin/gaunbo7-g16
chmod 700 src
chmod 600 bin/*.[Fao]
```

Notices

- Files are installed under /local/apl/lx/nbo702 directory.