

NBO-7.0.7 for LX

Webpage

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

Version

7.0.7

Build Environment

- Intel Parallel Studio XE 2018 update 4

Files Required

- nbo7.0.7-src.tar.gz

Build Procedure

```
#!/bin/sh

VERSION=7.0.7
INSTALL_NAME=nbo707
INSTALL_PREFIX=/local/apl/lx/${INSTALL_NAME}
BASEDIR=/home/users/${USER}/Software/NBO/${VERSION}
TARBALL=${BASEDIR}/nbo${VERSION}-src.tar.gz

#-----
umask 022

module purge
module load intel_parallelstudio/2018update4

if [ -e $INSTALL_PREFIX/bin ]; then
  echo "Remove $INSTALL_PREFIX/bin before installation"
  exit 1
fi
if [ ! -d $INSTALL_PREFIX ]; then
  echo "Create $INSTALL_PREFIX before build."
  exit 1
fi
cd $INSTALL_PREFIX
tar xzf $TARBALL
mv nbo7/* .
rmdir nbo7
sed -i "s/LenBuf=2048/LenBuf=10000/" src/g16nbo/utils.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\${INSTALL_NAME}/' 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\${INSTALL_NAME}\bin/" bin/gaunbo6
sed -i "s/^setenv BINDIR .*/setenv BINDIR \local\apl\lx\${INSTALL_NAME}\bin/" bin/gaunbo7
sed "s/^setenv GAUNBO g16nbo/setenv GAUNBO g09nbo/" bin/gaunbo6 > bin/gaunbo6-g09
sed "s/^setenv GAUNBO g16nbo/setenv GAUNBO g09nbo/" bin/gaunbo7 > bin/gaunbo7-g09
mv bin/gaunbo6 bin/gaunbo6-g16
mv bin/gaunbo7 bin/gaunbo7-g16
chmod 755 bin/gaunbo6-g09
chmod 755 bin/gaunbo7-g09
```

```
chmod 700 src
chmod 600 bin/*.[Fao]
```

```
cd ${INSTALL_PREFIX}/tests/gennbo
make all
```

Notes

- Files are installed under `/local/apl/lx/nbo707` directory.
- 4-bytes integer version is also installed in `/local/apl/lx/nbo707-i4`.