

ABINIT 8.8.3 for LX

Webpage

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

Version

8.8.3

Build Environment

- Intel Compiler 17.0.4.196
- Intel MKL 2017 update 3
- Intel MPI 2017.0.3

Files Required

- abinit-8.8.3.tar.gz

Build Procedure

```
#!/bin/sh

VERSION=8.8.3
INSTALLDIR=/local/apl/lx/abinit883

WORKDIR=/work/users/${USER}
TARBALL=/home/users/${USER}/abinit-${VERSION}.tar.gz

#-----
umask 0022

cd ${WORKDIR}
if [ -d abinit-${VERSION} ]; then
  mv abinit-${VERSION} abinit_erase
  rm -rf abinit_erase &
fi

module purge
module load intel_parallelstudio/2017update4

tar xzf ${TARBALL}
cd abinit-${VERSION}

export LANG=C
export CC=mpiicc
export FC=mpiifort
export CXX=mpiicpc
export CFLAGS="-fPIC"

./configure --prefix=${INSTALLDIR} \
  --with-linalg-flavor=mkl \
  --with-fft-flavor=fftw3-mkl \
  --enable-mpi-inplace \
  --with-mpi-level=2 \
  --with-dft-flavor=bigdft+libxc+atompaw+wannier90

make multi multi_nprocs=12
## test
# ulimit -s unlimited
# cd tests
# ./runtests.py -w Test_suite_serial >& tests_serial.log
# ./runtests.py -n4 -w Test_suite_n4 >& tests_n4.log
```

```
# cd ../
make install
```

Notices

- GPU and OpenMP are NOT enabled.
- BigDFT(1.7.2.25), AtomPAW(4.0.1.0), Wannier90(2.0.1.1), libxc(3.0.0) are enabled (via fallbacks).
- Serial and parallel (n=4) tests were performed. The result files of these tests are available in the following locations.
 - serial: /local/apl/lx/abinit883/share/abinit-test/tests_serial.log (individual log files in Test_suite_serial/)
 - Some of tests yielded error messages. But they were caused by file format difference or minor numerical errors, can be negligible.
 - libxc:t45, v7:t68, v3:t88,t89,t90, v67mbpt:t38,t39, v7:t87, v8:t43,t63
 - parallel(n=4): /local/apl/lx/abinit883/share/abinit-test/tests_n4.log (individual log files in Test_suite_n4/)
 - (error for np=1 tests are excluded here) Some of tests failed to run. Please be careful if you want to use those functions.
 - v67mbpt:t19(np=3) - minor numerical error
 - wannier90:t12,t13(np=3) - numerical error(?)
 - **v5:t23(np=2) - crash**
 - v7:t27-t31(np=2) - numerical error(?)
 - libxc:t44-t45(np=4) - minor numerical error(?)
 - **tutorial:tpositron_3,tpositron_4(np=4) - crash**
 - **v5:t07(np=4) - crash**
 - v7:t29(np=4) - numerical error(?)
 - **v7:t71(np=4) - crash**