

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**
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