

ABINIT 7.8.2 for PRIMERGY

Webpage

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

Version

7.8.2

Tools for Compiling

- Intel Compiler 14.0.2.144
- Intel MPI 4.1.0.030
- Intel MKL 14.0.2.144

Necessary Files for Compiling

- [abinit-7.8.2.tar.gz](#)

Attention

- Compile option "-xSSE4.2" is set because verification would be failed with "-xAVX".
- Environment variable, MKL_CBWR=SSE4_2, is needed in calculation.

Procedure of Compiling

```
#!/bin/csh -f
umask 022
unsetenv LANG
set file_abinit=/home/users/${USER}/build/abinit782/abinit-7.8.2.tar.gz
set work=/work/users/${USER}
set prefix=/local/apl/pg/abinit782
#-----
cd ${work}
if (-d abinit-7.8.2) then
  rm -rf abinit-7.8.2
endif
tar xzf ${file_abinit}
cd abinit-7.8.2
mkdir rccs
cd rccs
# If you use ifort version 13.1.1.163, internal error occur
# in src/66_wfs/prep_fourwf.F90.
source /opt/intel/composer_xe_2013_sp1.2.144/bin/compilervars.csh intel64
cp ../configure .
sed -i 's/xHost/xSSE4.2/g' ./configure
sed -i 's/-lmkl_sequential -lmkl_core -lpthread -lm/-mkl=sequential/' ./configure
sed -i 's/lapack_libs="mkl_intel_lp64"/lapack_libs=""/' ./configure
sed -i 's/-l$ac_lib \${abi_linalg_blas}/\${abi_linalg_blas}/' ./configure
sed -i 's/search_zgemm=\$ac_res/search_zgemm=-mkl=sequential/' ./configure
./configure --prefix=${prefix} --with-linalg-flavor=mkl --with-fft-flavor=fftw3-mkl CC=mpiicc FC=mpiifort CXX=mpicpc
make multi_multi_nprocs=12
make install
```