

Quantum ESPRESSO-5.1.1 for PRIMERGY

ウェブページ

<http://www.quantum-espresso.org/>

バージョン

5.1.1

ビルド環境

- ▶ Intel Compiler 13.1.1.163
- ▶ Intel MPI 4.1.0.030
- ▶ Intel MKL 2013.3.163
- ▶ fftw-3.2

ビルドに必要なファイル

- ▶ espresso-5.1.1.tar.gz

ビルド手順

```
#!/bin/csh -f
umask 022
unsetenv LANG
set file_espresso=/home/users/${USER}/build/espresso511/espresso-5.1.1.tar.gz
set work=/work/users/${USER}
set espresso=espresso511
#-----
cd ${work}
if (-d ${espresso}) then
mv ${espresso} ${espresso}-erase
rm -rf ${espresso}-erase &
endif
#-----
tar xzf ${file_espresso}
mv espresso-5.1.1 ${espresso}
cd ${work}/${espresso}
./configure CC=icc FC=ifort F77=ifort MPIF90=mpiifort --prefix=/local/apl/pg/${espresso} --with-scalapack=no
sed -i 's/traceback/traceback -xHost/' make.sys
make all |& tee make.log
```