

Quantum Espresso 5.0.1 fot PG

ウェブページ

Quantum ESPRESSO ([Download Page](#))

バージョン

5.0.1

ビルド環境

Intel Composer XE 2011 sp1.8.273

Intel MPI 4.0.2.003

ビルドに必要なファイル

- espresso-5.0.1.tar.gz
- diff.patch
- FFTW to Intel MKL Wrappers (fftw3xf)

diff.patchの内容

```

*** ./make.sys 2012-09-19 16:27:31.403356218 +0900

--- ../espresso-5.0.1-ori/make.sys 2012-09-19 12:36:11.386356201 +0900
*****
*** 87,93 ****
# Typically LD coincides with F90 or MPIF90, LD_LIBS is empty

LD = mpiifort
! LDFLAGS = -static-intel
LD_LIBS =

# External Libraries (if any) : blas, lapack, fft, MPI
--- 87,93 ----
# Typically LD coincides with F90 or MPIF90, LD_LIBS is empty

LD = mpiifort
! LDFLAGS = -static-intel $(MKLRROOT)/lib/intel64/libmkl_blas95_lp64.a $(MKLRROOT)/lib/intel64/libmkl_lapack95_lp64.a $(I
LD_LIBS =

# External Libraries (if any) : blas, lapack, fft, MPI
*****
*** 96,102 ****
# BLAS_LIBS = /your/path/to/espresso/BLAS/blas.a
# BLAS_LIBS_SWITCH = internal

! BLAS_LIBS = -lmkl_intel_lp64 -lmkl_sequential -lmkl_core
BLAS_LIBS_SWITCH = external

# If you have nothing better, use the local copy :
--- 96,102 ----
# BLAS_LIBS = /your/path/to/espresso/BLAS/blas.a
# BLAS_LIBS_SWITCH = internal

! BLAS_LIBS = -lmkl_intel_lp64 -lmkl_intel_thread -lmkl_core
BLAS_LIBS_SWITCH = external

# If you have nothing better, use the local copy :
*****
*** 108,114 ****
LAPACK_LIBS =
LAPACK_LIBS_SWITCH = external

! SCALAPACK_LIBS = -lmkl_scalapack_lp64 -lmkl_blacs_openmpi_lp64

# nothing needed here if the the internal copy of FFTW is compiled
# (needs -D_FFTW in DFLAGS)
--- 108,114 ----
LAPACK_LIBS =
LAPACK_LIBS_SWITCH = external

! SCALAPACK_LIBS = -lmkl_scalapack_lp64 -lmkl_blacs_intelmpi_lp64

# nothing needed here if the the internal copy of FFTW is compiled
# (needs -D_FFTW in DFLAGS)

```



```
#!/bin/csh -f
umask 022
set file_espresso=/home/users/${USER}/build/espresso-5.0.1.tar.gz
set work=/local/apl/pg/
set espresso=espresso501
set patch=/home/users/${USER}/build/espresso-5.0.1/diff.patch
#-----
cd ${work}
if (-d ${espresso}) then
mv ${espresso} ${espresso}-erase
rm -rf ${espresso}-erase &
endif
#-----

tar zxf ${file_espresso}
mv espresso-5.0.1 ${espresso}
cd ${work}/${espresso}

./configure CC=icc FC=ifort MPIF=mpiifort F77=ifort MPIF90=mpiifort LIBDIRS="${MKLROOT}/include/fftw /home/users/$

#-----
patch -p0

#-----

make all |& tee make.log
```

