Quantum Espresso 5.0.1 for UV

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
MPT 2.0.5

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-ori 2012-09-20 10:56:53.388355740 +0900
+++ make.sys 2012-09-20 18:52:19.027355347 +0900
@@ -37,7 +37,8 @@
# IFLAGS = how to locate directories where files to be included are
# In most cases, IFLAGS = -I../include

-IFLAGS = -I../include
+# IFLAGS = -I../include -I${MPI_ROOT}/include
+IFLAGS = -I../include -I$(MKLROOT)/include/intel64/lp64 -I$(MKLROOT)/include -I$(MPI_ROOT)/include

# MOD_FLAGS = flag used by f90 compiler to locate modules
# Each Makefile defines the list of needed modules in MODFLAGS
@@ -69,9 +70,9 @@
# C flags must include DFLAGS and IFLAGS
# F90 flags must include MODFLAGS, IFLAGS, and FDFLAGS with appropriate syntax

-CFLAGS = -O3 $(DFLAGS) $(IFLAGS)
-F90FLAGS = $(FFLAGS) -nomodule -fpp $(FDFLAGS) $(IFLAGS) $(MODFLAGS)
-FFLAGS = -O2 -assume byterecl -g -traceback -par-report0 -vec-report0
+CFLAGS = -O3 $(DFLAGS) $(IFLAGS) -I$(MKLROOT)/include/intel64/lp64 -I$(MKLROOT)/include
+F90FLAGS = $(FFLAGS) -nomodule -fpp $(FDFLAGS) $(IFLAGS) $(MODFLAGS) -I$(MKLROOT)/include/intel64/lp64 -I$(MK
+FFLAGS = -O2 -assume byterecl -g -traceback -par-report0 -vec-report0 -I$(MKLROOT)/include/intel64/lp64 -I$(MKLROO

# compiler flags without optimization for fortran-77
# the latter is NEEDED to properly compile dlamch.f, used by lapack
@@ -87,7 +88,7 @@
# Typically LD coincides with F90 or MPIF90, LD_LIBS is empty

LD = mpif90
-LDFLAGS = -static-intel
+LDFLAGS = -static-intel $(MKLROOT)/lib/intel64/libmkl_blas95_lp64.a $(MKLROOT)/lib/intel64/libmkl_lapack95_lp64.a $(
LD_LIBS =

# External Libraries (if any) : blas, lapack, fft, MPI
@@ -96,7 +97,7 @@
# BLAS_LIBS = /your/path/to/espresso/BLAS/blas.a
# BLAS_LIBS_SWITCH = internal

-BLAS_LIBS = -lmkl_intel_lp64 -lmkl_sequential -lmkl_core
+BLAS_LIBS = -lmkl_intel_lp64 -lmkl_intel_thread -lmkl_core
BLAS_LIBS_SWITCH = external

# If you have nothing better, use the local copy :
@@ -108,7 +109,7 @@
```

```
@@ -108,7 +109,7 @@
LAPACK_LIBS =
LAPACK_LIBS_SWITCH = external

-SCALAPACK_LIBS = -lmkl_scalapack_lp64 -lmkl_blacs_openmpi_lp64
+SCALAPACK_LIBS = -lmkl_scalapack_lp64 -lmkl_blacs_sgimpt_lp64

# nothing needed here if the the internal copy of FFTW is compiled
# (needs -D__FFTW in DFLAGS)
@@ -118,6 +119,7 @@
# For parallel execution, the correct path to MPI libraries must
# be specified in MPI_LIBS (except for IBM if you use mpxlf)

+# MPI_LIBS = -L${MPI_ROOT}/lib
MPI_LIBS =

# IBM-specific: MASS libraries, if available and if -D__MASS is defined in FDFLAGS
@@ -126,7 +128,8 @@

# ar command and flags - for most architectures: AR = ar, ARFLAGS = ruv

-AR = ar
+#AR = ar
+AR = xiar
ARFLAGS = ruv

# ranlib command. If ranlib is not needed (it isn't in most cases) use
```

ビルド手順 (make.csh)

```
#!/bin/csh -f
umask 022
set file_espresso=/home/users/${USER}/build/espresso-5.0.1.tar.gz
set work=/local/apl/uv
set espresso=espresso501
set patch=/home/users/${USER}/build/espresso-5.0.1/ccuv/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=mpif90 MPIF90=mpif90 LIBDIRS="${MLROOT}/include/fftw /home/users/${USER}/mkl/

#-------------------------------------------------------------
patch make.sys < ${patch}

#-------------------------------------------------------------
make all |& tee make.log

exit 0
```