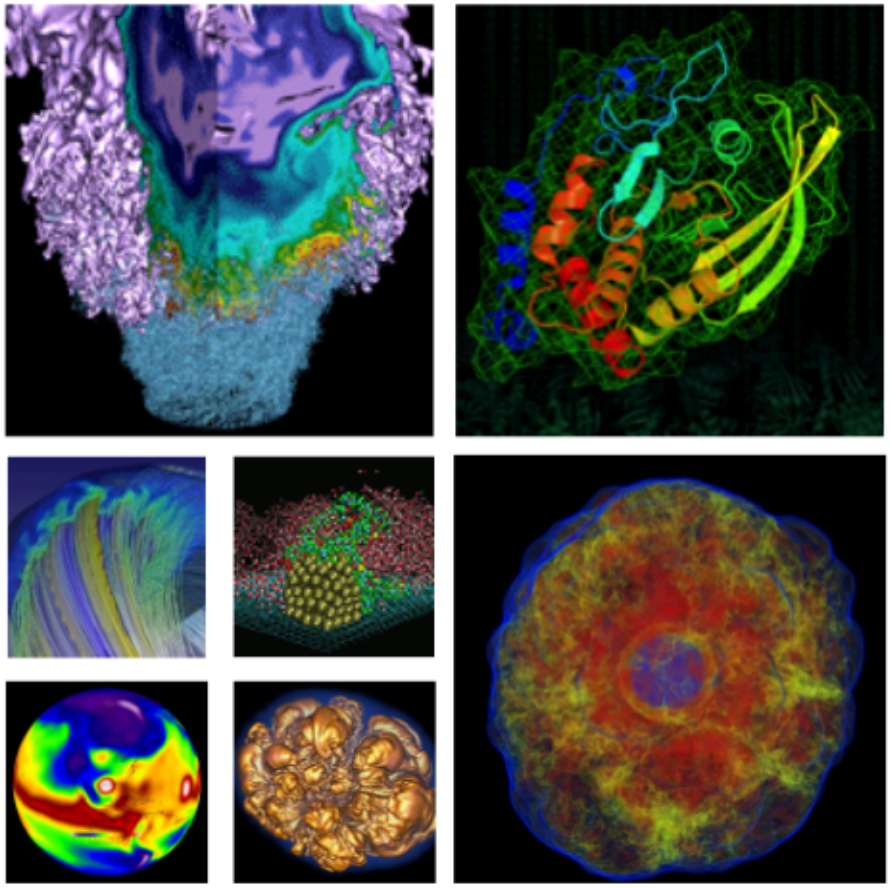
Building Applications on Edison



Jack Deslippe

NERSC User Services

10/10/2013

U.S. DEPARTMENT OF ENERGY | Office of Science

BERKELEY LAB

Outline

- Applications Already Available at NERSC
- Available Compilers
- Available Libraries

Applications Already Available

Did you know that NERSC offers precompiled executables for more than 100 applications?

Applications Already Available

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Example, Materials Science:

Quantum ESPRESSO, NAMD, LAMMPS, NWCHEM, VASP, BerkeleyGW, SIESTA, Abinit, Gamess, GROMACS, GPAW MEEP, cpmd, libxc, etsf_io, atompaw, Wiek2K, Gaussian, PARATEC, cp2k, Wannier90, Amber, Yambo, XCrysden, Q-Chem

Applications Already Available

http://www.nersc.gov/users/software/all-software-list/

Show 25 entries Search:

#	Package	Platform	Category	Version	Module	Install Date	Date Made Default
0	ABINIT	carver	applications/ material sciences	6.0.3	abinit/6.0.3	2010-05-06	
1	ABINIT	carver	applications/ material sciences	6.10.3	abinit/6.10.3	2012-01-10	
2	ABINIT	carver	applications/ material sciences	6.2.2	abinit/6.2.2	2010-08-16	
3	ABINIT	carver	applications/ material sciences	6.4.1	abinit/6.4.1	2010-11-24	2012-01-12
4	ABINIT	franklin	applications/ material sciences	5.6	abinit/5.6	2008-12-03	2008-12-03
5	ABINIT	franklin	applications/ material sciences	5.8.4	abinit/5.8.4	2009-12-06	2009-12-15
6	ABINIT	franklin	applications/ material sciences	6.10.3	abinit/6.10.3	2012-01-10	
7	ABINIT	franklin	applications/ material sciences	6.4.3	abinit/6.4.3	2011-02-22	2011-03-24
8	ABINIT	hopper	applications/ material sciences	6.10.3	abinit/6.10.3	2012-01-09	

The NERSC Software Database on the web shows all of our available pre-compiled applications for Hopper, Edison, Carver

Applications Already Available

Many application pages contain compilation instructions

e.g. Abinit

Compilation Instructions

Some advanced users may be interested in tweaking the Abinit build parameters and building Abinit themselves in their own directory. In order to aid in this process, and to provide a greater degree of transparency, the build instructions for the Abinit module are listed below. The following procedure was used to build Abinit 6.8.2 on Hopper.

```
% module swap PrgEnv-pgi PrgEnv-gnu
```

```
% module swap gcc gcc/4.5.2
```

```
% module load netcdf atompaw etsf_io wannier90 libxc
```

```
% ./configure -prefix="`pwd`/.." FC=ftn CC=CC CXX=CC FCFLAGS="-O3" CFLAGS="-O3" CXXFLAGS="-O3" --with-fc-vendor=gr
```

```
% make
```

```
% make install
```

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Compilers vs. Compiler Wrappers

ifort, icc vs ftn, cc, CC

The compiler wrappers are the same as the underlying compilers with the addition of flags included by default and libraries linked by default (like MPI libraries for example)

The same compiler wrapper command (.e.g. ftn) can refer to any underlying compiler available on the system (e.g. pgi, gnu, intel etc...)

Available Compilers

Available Compilers Across Machines:

	Edison	Hopper	Carver
PGI		✗	✗
GNU	✗	✗	✗
Intel	✗	✗	✗
Pathscale		✗	
Cray	✗	✗	

Default

Available Compilers

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PGI		✖	✖
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Intel	✖	✖	✖
Pathscale		✖	
Cray	✖	✖	

Default

Edison Swap between Compilers With Modules:

% module swap PrgEnv-intel PrgEnv-gnu

Available Compilers

Useful Compiler Options on Edison:

	Intel	GNU	Cray
Optimization	-fast -no-ipo	-O3 -fast-math	
OpenMP	-openmp	-fopenmp	
Version	-V	--version	-V
Verbose	-v	-v	-v
Debugging	-g -warn all -CB	-g -fbounds-check	-g -R bs
Math Libs	-mkl=cluster		

➔ The "-v" option displays the complete link and compile line unwrapped from ftn

➔ The "-Wl,-y<symbol_name>" reports which library the linker is currently using for the symbol <symbol_name>"

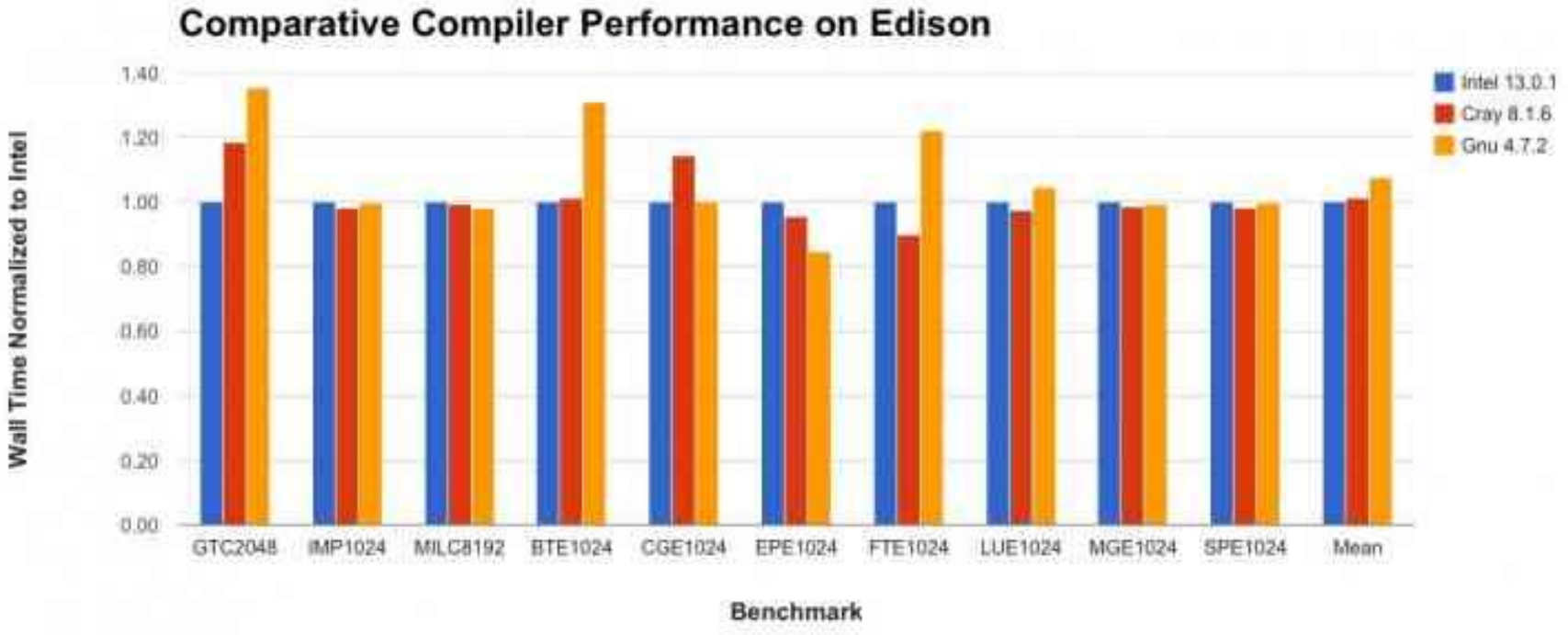
Intel -fast option

- The Intel and PGI compiler -fast options have different effects:

- PGI
  - "A generally optimal set of options is chosen for targets that support SSE capability."
  - Same as -fastsse.

- Intel
  - Includes interprocedural optimization which can increase compile time by an order of magnitude or cause it to fail.
  - Always turn it off with -no-ipo when using -fast.
  - -fast -no-ipo generally improves performance over the default (no optimization arguments) on Edison.
  - Includes vectorization. AVX (4 Double-Precision operations).

Comiler Comparison



Intel and Cray compilers general provide best performance.

http://www.nersc.gov/users/computational-systems/edison/performance-and-optimization/compiler-comparisons/

Using MKL on Edison:

Add to the end of your link-line

-mkl=cluster : Single-Threaded MKL with BLAS/LAPACK/scaLAPACK/FFTW

-mkl (same as -mkl=parallel) : Multi-Threaded MKL (No ScaLAPACK)

-mkl=sequential : Single-Threaded MKL (No ScaLAPACK)

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Add to the end of your link-line

-mkl=cluster : Single-Threaded MKL with BLAS/LAPACK/scaLAPACK/FFTW

-mkl (same as -mkl=parallel) : Multi-Threaded MKL (No ScaLAPACK)

-mkl=sequential : Single-Threaded MKL (No ScaLAPACK)

In order to link to multi-threaded MKL libraries including ScaLAPACK must add:

$(MKLROOT)/lib/intel64/libmkl_scalapack_lp64.a -Wl,--start-group $(MKLROOT)/lib/intel64/libmkl_intel_lp64.a $(MKLROOT)/lib/intel64/libmkl_intel_thread.a $(MKLROOT)/lib/intel64/libmkl_core.a $(MKLROOT)/lib/intel64/libmkl_blacs_intelmpi_lp64.a -Wl,--end-group -lpthread -lm

For linking with other compilers than intel. Use the following online tool: http://software.intel.com/sites/products/mkl/MKL_Link_Line_Advisor.html

MKL on Edison

Usin

Add to th

-mkl=clus

-mkl (sar

-mkl=seq

In order t

$(MKLR(
/lib/intel6
/lib/intel6
lpthread

For linkin
com/sites/p

Intel® Math Kernel Library (MKL) Link Line Advisor v2.2 Reset

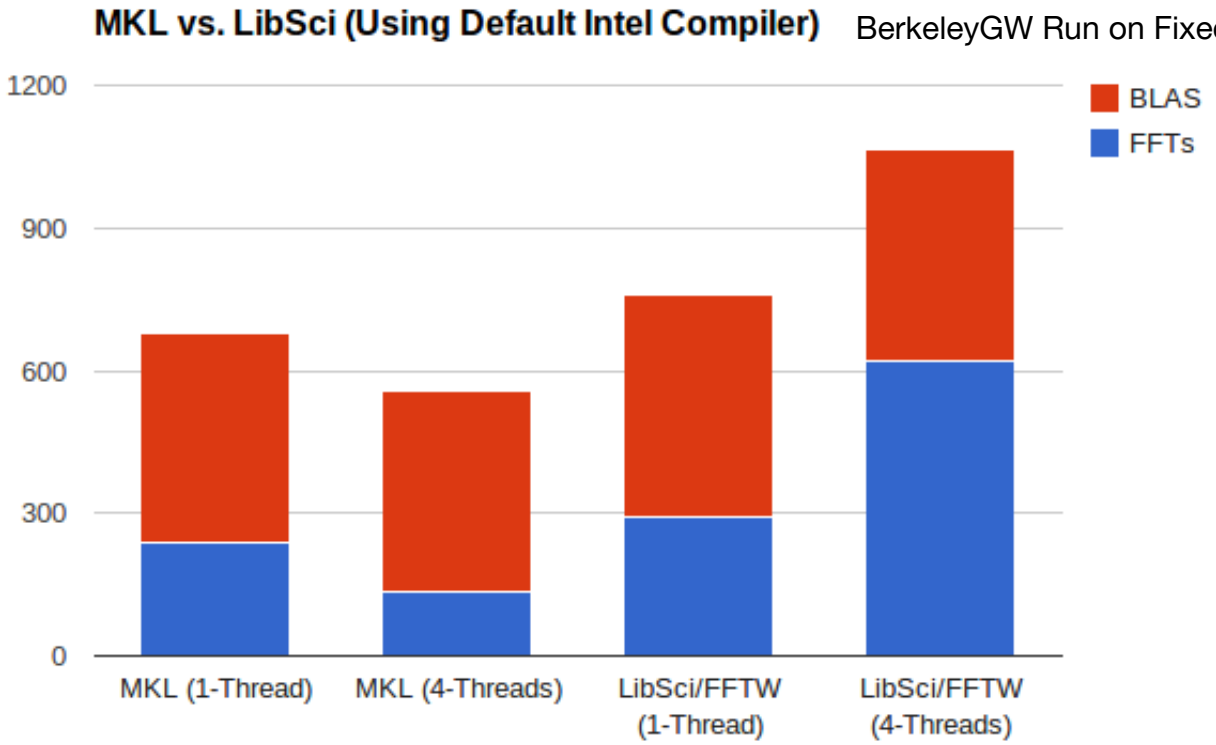
Select Intel® product:	Intel(R) MKL 11.0
Select OS:	Linux*
Select compiler:	GNU Fortran
Select architecture:	<Select architecture>
Select dynamic or static linking:	<Select linking>
Select interface layer:	<Select interface>
Select sequential or multi-threaded layer:	<Select threading>
Select OpenMP library:	<Select OpenMP>
Select cluster library:	CDFT (BLACS required) ScaLAPACK (BLACS required) BLACS
Select MPI library:	<Select MPI>
Select the Fortran 95 interfaces:	BLAS95 LAPACK95
Link with Intel® MKL libraries explicitly:	

Use this link line:

OOT)
-end-group -

ntel.

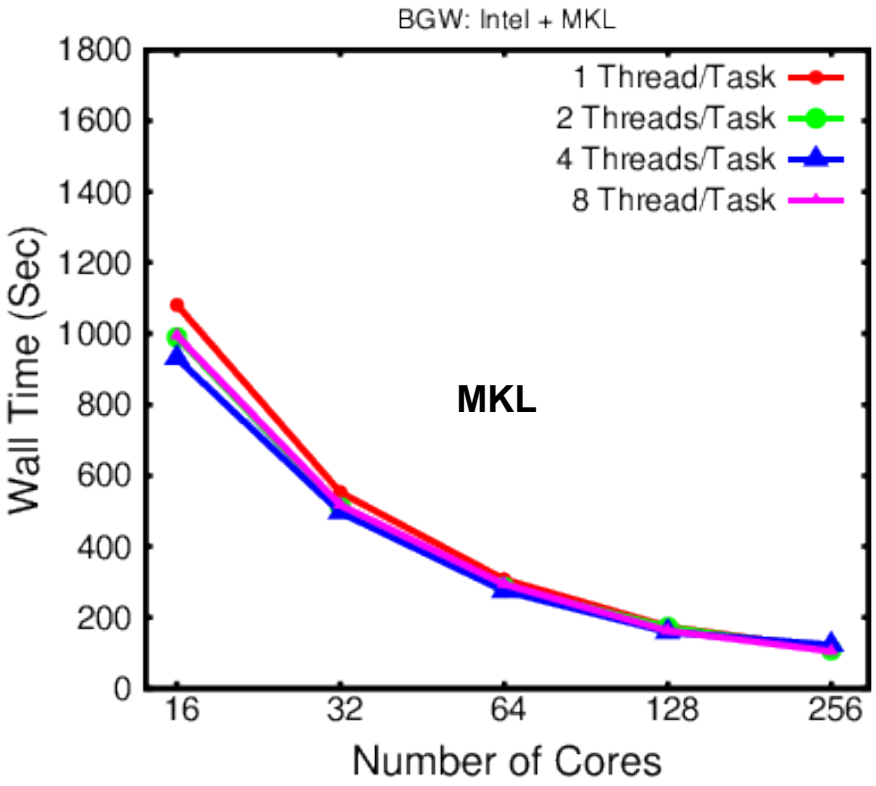
Math Library Performance

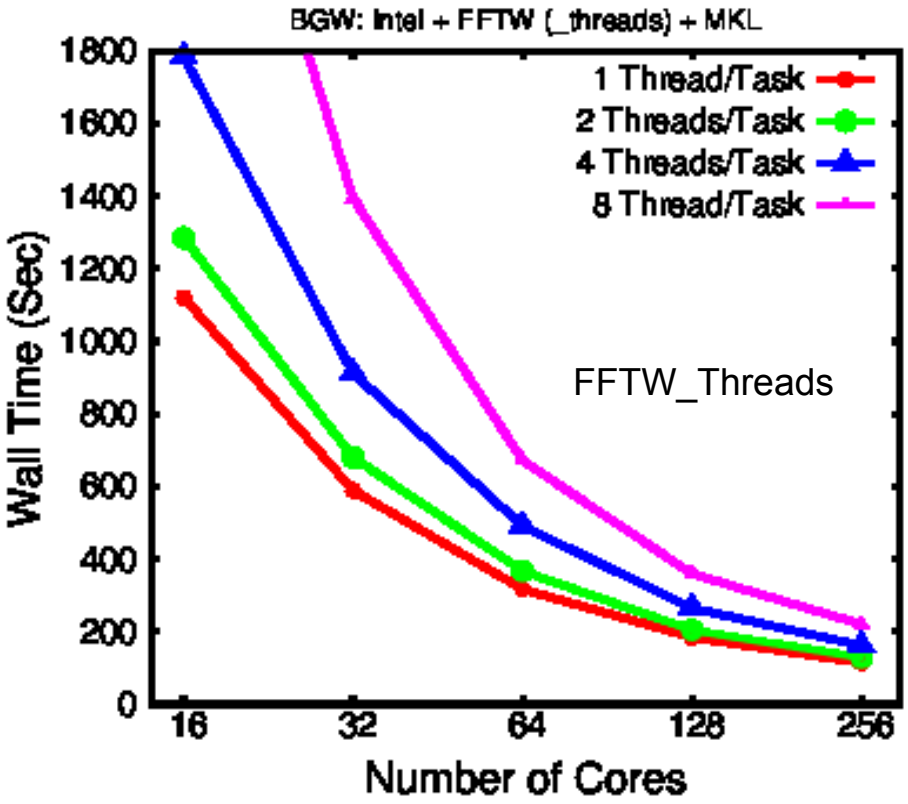


➔ MKL and LibSci give comparable dense linear algebra performance.
- ◆ Both Provide good support with threads.

➔ MKL FFTs consistently outperform FFTW.
- ◆ MKL FFTs scale well with threads. FFTW does not

FFT Library Performance





MKL gives better threaded FFTW performance than Cray provided FFTW pthread in codes that use OpenMP

Available Compilers

Tips for using compilers:

- Use the compiler wrappers for parallel programs:
  edison: **ftn, cc, CC** not **ifort, icc, gcc, gfortran ...**

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- Edison statically links by default (carver dynamically links)

> You can dynamically link on Edison by adding -dynamic flag to compilation and "setenv CRAY_ROOTFS DSL" in batch script and/or use CCM.

Available Compilers

Tips for using compilers:

To show libraries linked automatically with ftn

```
% ftn -v test.f90 -o test.x
...
--start-group -lscicpp_gnu -lsci_gnu_mp -lstdc++ -l gfortran -l m -lmpichf90_gnu -lmpich_gnu -
lmpichf90_gnu -lmpl -lsma -lxpmem -ldmapp -lugni -lpmi -Wl,--as-needed -lalpslli -lalpsutil -Wl,--no-as-
needed -ludreg -u pthread_mutex_destroy -u pthread_create -lpthread -Wl,--end-group -lgomp -lpthread -l
gfortran -l m
Using built-in specs.
...
```

To show which library "dgemm" is used from:

```
% ftn -Wl,-ydgemm_  test.f90 -o test.x
/scratch/scratchdirs/jdeslip/cc8ImteH.o: reference to dgemm_
/opt/xt-libsci/11.0.03/gnu/46/mc12/lib/libsci_gnu_mp.a(dgemm.o): definition of dgemm_
```

Modules

Software libraries at NERSC are managed in modules.

Modules add and remove executables and libraries from your $PATH and $LD_LIBRARY_PATH as well as define environment variables.

They are used by doing "module load" command

e.g. "% module load fftw"

Available Libraries

Most math and science libraries are available

e.g.:

```
% module avail fftw

------------------------ /opt/cray/modulefiles
------------------------
fftw/2.1.5.5           fftw/2.1.5.6           fftw/3.3.0.1
fftw/3.3.0.3           fftw/3.3.0.4(default)
```

```
% module show fftw/2.1.5.5

setenv          FFTW_DIR /opt/fftw/2.1.5.5/lib
setenv          FFTW_INC /opt/fftw/2.1.5.5/include
setenv          FFTW_POST_LINK_OPTS -L/opt/fftw/2.1.5.5/lib
setenv          FFTW_INCLUDE_OPTS -I/opt/fftw/2.1.5.5/include
prepend-path    CRAY_LD_LIBRARY_PATH /opt/fftw/2.1.5.5/lib
prepend-path    INFOPATH /opt/fftw/2.1.5.5/info
append-path     PE_PRODUCT_LIST FFTW
setenv          CRAY_FFTW_DIR /opt/fftw/2.1.5.5
```

Summary of Good Practices

- Use developer recommended compiler and compiler options
- Use compiler wrappers
- Test your application against lower optimization levels and included tests
- Use system provided libraries

More Information

NERSC Website:

- http://www.nersc.gov/users/computational-systems/edison/programming/

Man Pages:

% man ifort

eMail Us:

consult@nersc.gov

EXTRA SLIDES

Fix the Problem Game

Jack is having trouble building and running some of his favorite applications at NERSC.

Can you help fix the problem?

Rules: No looking ahead.

Prizes: Eternal glory in the minds of those around you.

Round 1

Quantum ESPRESSO on Edison:

```
% cat README
...
Quick installation instructions for the impatient:
   ./configure [options]
   make all
...
```

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Quick installation instructions for the impatient:
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That seems easy enough...

```
% ./configure ... (Success!)
% make all ... come back in 20 minutes ... (Success!)

% aprun -n 5 ~/PresentationDir/espresso-4.3.2/bin/pw.x -in ./in

    Program PWSCF v.4.3.2      starts on 25Jan2012 at 15:19:44
    Program PWSCF v.4.3.2      starts on 25Jan2012 at 15:19:44
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    This program is part of the open-source Quantum ESPRESSO suite
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     .....
```

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% cat README
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Quick installation instructions for the impatient:
   ./configure [options]
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     .....
```

The output looks weird and repeated....

Round 1

Solution

Use the compiler wrappers, ftn, cc, CC. They can often be specified in configure:

./configure FC=ftn CC=CC CXX=CC or in make.sys file

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./configure FC=ftn CC=CC CXX=CC or in make.sys file

```
% cat make.sys
.....
DFLAGS        =  -D__PGI -D__ACML
FDFLAGS       = $(DFLAGS)
MPIF90        = ifort
#F90          = ifrot
CC            = icc
F77           = ifort


.....
```

```
% cat make.sys_fixed
.....
DFLAGS        =  -D__PGI -D__ACML -D__MPI
FDFLAGS       = $(DFLAGS)
MPIF90        = ftn
#F90          = ftn
CC            = cc
F77           = ftn


.....
```

Round 2

BerkeleyGW on Edison

```
% cat arch.mk
...
FCPP    = /usr/bin/cpp -ansi
F90free = ftn -Mfree
LINK    = ftn

LAPACKLIB =
FFTWLIB      =

FOPTS   = -fast
FNOOPTS = $(FOPTS)
...
```

Round 2

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FCPP    = /usr/bin/cpp -ansi
F90free = ftn -Mfree
LINK    = ftn

FOPTS   = -fast
FNOOPTS = $(FOPTS)

...
```

```
% make

/global/u2/j/jdeslip/PresentationDir/BGW_2.4.x/Xi0/../Common/fftw.f90:270: undefined reference to
`fftwnd_f77_create_plan_'
/global/u2/j/jdeslip/PresentationDir/BGW_2.4.x/Xi0/../Common/fftw.f90:270: undefined reference to
`fftwnd_f77_create_plan_'
/global/u2/j/jdeslip/PresentationDir/BGW_2.4.x/Xi0/../Common/fftw.f90:285: undefined reference to `fftwnd_f77_one_'
/global/u2/j/jdeslip/PresentationDir/BGW_2.4.x/Xi0/../Common/fftw.f90:287: undefined reference to `fftwnd_f77_one_'
```

Round 2

Solution

"undefined reference" errors usually mean you are missing a library at link time. In this case, we are missing the fftw library.

Note that ftn links lapack/blas equivalents automatically.

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F90free = ftn -Mfree
LINK    = ftn

LAPACKLIB =
FFTWLIB      =

FOPTS   = -fast
FNOOPTS = $(FOPTS)
...
```

```
% module load fftw
% cat arch.mk -fixed
...
FCPP    = /usr/bin/cpp -ansi
F90free = ftn -Mfree
LINK    = ftn

LAPACKLIB =
FFTWLIB      = -L$(FFTW_DIR) -ldfftw

FOPTS   = -fast
FNOOPTS = $(FOPTS)
...
```

Round 3

BerkeleyGW on Carver

```
% module load fftw mkl
% cat arch.mk
...
F90free = mpif90 -Mfree
LINK    = mpif90
FOPTS   = -fast

FFTWPATH     = $(FFTW_ROOT)
FFTWLIB      = -L$(FFTW_LIBDIR) -ldfftw
FFTWINCLUDE  = $(FFTW_INC)

LAPACKLIB    = $(MKL)
SCALAPACKLIB = -L$(MKL_LIBDIR) -lmkl_scalapack_lp64 -lmkl_blacs_openmpi_lp64
...

% make (SUCCESS!)
```

Round 3

BerkeleyGW on Carver

```
% module load fftw mkl
% cat arch.mk
...
F90free = mpif90 -Mfree
LINK    = mpif90
FOPTS   = -fast

FFTWPATH     = $(FFTW_ROOT)
FFTWLIB      = -L$(FFTW_LIBDIR) -ldfftw
FFTWINCLUDE  = $(FFTW_INC)

LAPACKLIB    = $(MKL)
SCALAPACKLIB = -L$(MKL_LIBDIR) -lmkl_scalapack_lp64 -lmkl_blacs_openmpi_lp64
...

% make (SUCCESS!)
```

(later that day...)

```
% mpirun -np 2 xi0.cplx.x
xi0.cplx.x: error while loading shared libraries: libmkl_scalapack_lp64.so: cannot open shared object file: No such file
xi0.cplx.x: error while loading shared libraries: libmkl_scalapack_lp64.so: cannot open shared object file: No such file
```

Round 3

Solution

On carver, we link against shared object files. These need to be present at runtime.

These need to be in your $LD_LIBRARY_PATH

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```
% module load mkl fftw
```

(or)

```
% export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:/usr/common/usg/mkl/10.2.2.025/lib/em64t:/usr/common/usg/fftw/2.1.5/lib
```

Round 4

etsf_io on Hopper

```
% module swap PrgEnv-pgi PrgEnv-gnu
% module load netcdf
% ./configure --prefix="`pwd`/../" CC=cc CXX=cc FC=ftn F77=ftn FCFLAGS="-O3" F77FLAGS="-O3" CFLAGS="-O3" CXXFLAGS="-O3" --with-netcdf-module-path="$CRAY_NETCDF_DIR/gnu/45/include" --enable-fortran

checking for module extension for compiler 'gcc'... mod
checking for ranlib... ranlib
checking for ar... ar
checking for /opt/cray/netcdf/4.1.3/gnu/45/include/netcdf.mod... yes
checking for netcdf library... no
Action: install NetCDF and set the library link path with --with-netcdf-ldflags.
configure: error: "No 'NetCDF' library found."
```

But... This worked for me one month ago just fine!?!?!?

Round 4

Solution

To debug ./configure errors. Look at generated config.log.

```
% cat config.log
....
configure:3866: ftn -o conftest -O3 -I/opt/cray/netcdf/4.1.3/gnu/45/include   conftest.f90  -lnetcdf >&5
conftest.f90:3.12:

  use netcdf
           1
Fatal Error: Wrong module version '4' (expected '6') for file 'netcdf.mod' opened at (1)
configure:3872: $? = 1
configure: failed program was:
|
| program main
|   use netcdf
|   integer :: s, ncid
|   s = nf90_open(path = "", mode = NF90_NOWRITE, ncid = ncid)
| end program main
....
```

ftn --version shows gcc 4.6, but netcdf module was compiled with gcc 4.5.

Round 2

User MPI Code

```
 % cat jobscript.e3250732

Initial temperature 500.0000000000002 500.0000000000001
Application 5341714 exit signals: Floating point exception
```

do ia=rank+1,nsites,nprocs

```
 % cat Makefile
...
FC = ftn #mpif90 -fpp          # Modified
DEFINES = -DMPI

FILESF77= mdheff.F readinput.f readepqr3ndonsite.f  ran1.f timer.f
OBJS77= $(FILESF77:.f=.o)
.f.o:
        $(FC) -c $(FFLAGS) $(DEFINES) $<
....
```

Round 2

User MPI Code

```
 % cat jobscript.e3250732

Initial temperature 500.0000000000002 500.0000000000001
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```

nprocs=0

```
do ia=rank+1,nsites,nprocs
```

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...
FC = ftn #mpif90 -fpp          # Modified
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OBJS77= $(FILESF77:.f=.o)
.f.o:
        $(FC) -c $(FFLAGS) $(DEFINES) $<
....
```

Round 2

Solution

The $(DEFINES) was not included in the compilation of the .F files.

```
 % cat Makefile
...
FC = ftn #mpif90 -fpp          # Modified
FLAGSOPM =  #-O2 -march=pentium3 -mtune=core2 -assume byterecl -funroll-loops -fp-model precise -pc64 # Modified
DEFINES = -DMPI

FILESF77= mdheff.F readinput.f readepqr3ndonsite.f  ran1.f timer.f
OBJS77= $(FILESF77:.f=.o)
.f.o:
        $(FC) -c $(FFLAGS) $(DEFINES) $<
.F.o:
        $(FC) -c $(FFLAGS) $(DEFINES) $<
....
```